Molecular Sieve Bench Testing and Computer Modeling

Contract NAS8-38250-17

Final Report

McDonnell Douglas Aerospace - Huntsville
MCDONNELL DOUGLAS

Molecular Sieve Bench Testing and Computer Modeling

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PREFACE

This document has been prepared by the Product Development Group of McDonnell Douglas Aerospace - Huntsville (MDA-HSV) to document the mathematical model and numerical simulation of adsorption of H₂O and CO₂ on 5A zeolite. The work was performed under the Molecular Sieve Bench Testing and Computer Modeling contract (NAS8-38250-17) to ION Electronics.
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>PREFACE</td>
<td>ii</td>
</tr>
<tr>
<td>CONTENTS</td>
<td>iv</td>
</tr>
<tr>
<td>APPENDICIES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>viii</td>
</tr>
<tr>
<td>Section 1 INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>Section 2 DEVELOPMENT AND ANALYSIS OF A MATHEMATICAL MODEL</td>
<td>3</td>
</tr>
<tr>
<td>2.1 Gas/Solid Equilibrium</td>
<td>3</td>
</tr>
<tr>
<td>2.1.1 Single Component Isotherm</td>
<td>3</td>
</tr>
<tr>
<td>2.1.2 Multicomponent Isotherm</td>
<td>4</td>
</tr>
<tr>
<td>2.2 Mathematical Model For Nonisothermal Multicomponent Adsorption In a</td>
<td>5</td>
</tr>
<tr>
<td>Packed Bed</td>
<td></td>
</tr>
<tr>
<td>2.2.1 One Dimension Adsorption Mathematical Model</td>
<td>6</td>
</tr>
<tr>
<td>2.2.1.1 Mass Balance Equation</td>
<td>6</td>
</tr>
<tr>
<td>2.2.1.2 Total Material Balance</td>
<td>6</td>
</tr>
<tr>
<td>2.2.1.3 Gas Phase Energy Equation</td>
<td>6</td>
</tr>
<tr>
<td>2.2.1.4 Solid Phase Energy Equation</td>
<td>7</td>
</tr>
<tr>
<td>2.2.1.5 Column Wall Energy Equation</td>
<td>7</td>
</tr>
<tr>
<td>2.2.1.6 Momentum Equation</td>
<td>8</td>
</tr>
<tr>
<td>2.2.2 Solid Phase Transport Equation</td>
<td>8</td>
</tr>
<tr>
<td>2.2.3 Monodisperse Pore Diffusion Model</td>
<td>11</td>
</tr>
<tr>
<td>2.2.4 Bidisperse Pore Diffusion Model for Zeolite</td>
<td>13</td>
</tr>
<tr>
<td>2.2.5 Two Dimension Adsorption Mathematical Model</td>
<td>14</td>
</tr>
<tr>
<td>2.2.5.1 Mass Equation</td>
<td>14</td>
</tr>
<tr>
<td>2.2.5.2 Gas Phase Energy Equation</td>
<td>15</td>
</tr>
<tr>
<td>2.2.5.3 Solid Phase Energy Equation</td>
<td>15</td>
</tr>
<tr>
<td>2.2.5.4 Column Wall Energy Equation</td>
<td>15</td>
</tr>
<tr>
<td>2.2.5.5 Bed Energy Equation Based On Effective Conductivity</td>
<td>16</td>
</tr>
<tr>
<td>2.2.5.6 Momentum Equation</td>
<td>16</td>
</tr>
<tr>
<td>2.2.6 Porosity Variation</td>
<td>16</td>
</tr>
<tr>
<td>2.2.7 Calculation Of Thermal Conductivity For 2-D Flow</td>
<td>17</td>
</tr>
<tr>
<td>2.2.7.1 Stagnant Conductivity ko</td>
<td>17</td>
</tr>
<tr>
<td>2.2.7.2 Effective Radial Conductivity kfr</td>
<td>16</td>
</tr>
<tr>
<td>2.2.7.3 Effective Axial Conductivity keff,x</td>
<td>18</td>
</tr>
<tr>
<td>2.2.8 Calculation Of Mass Diffusivity For 2-D Flow</td>
<td>19</td>
</tr>
<tr>
<td>2.2.8.1 Effective Diffusivity</td>
<td>19</td>
</tr>
<tr>
<td>2.2.8.2 Effective Radial Diffusivity Dfr,x</td>
<td>19</td>
</tr>
<tr>
<td>2.2.8.3 Effective Axial diffusivity Deff,x</td>
<td>19</td>
</tr>
<tr>
<td>2.2.9 Effective Radial Thermal Conductivity Based on Fahien Equations</td>
<td>20</td>
</tr>
<tr>
<td>2.2.10 Effective Radial Diffusivity Based on Fahien Equations</td>
<td>21</td>
</tr>
<tr>
<td>2.2.11 Heat Transfer Coefficient Between Wall Surface and Packed Bed, hw</td>
<td>21</td>
</tr>
</tbody>
</table>
# CONTENTS (continued)

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 3  NUMERICAL ANALYSIS</td>
<td>23</td>
</tr>
<tr>
<td>3.1 The Discrete Numerical Equations</td>
<td>23</td>
</tr>
<tr>
<td>3.1.1 Discretized Spatial Finite Difference With Unequal Grid Size</td>
<td>24</td>
</tr>
<tr>
<td>3.2 Discretized Partial Differential Equations (PDE's)</td>
<td>25</td>
</tr>
<tr>
<td>3.2.1 Discretized Component Mass Balance</td>
<td>25</td>
</tr>
<tr>
<td>3.2.2 Discretized Gas Phase Energy</td>
<td>25</td>
</tr>
<tr>
<td>3.2.3 Discretized Solid Phase Energy Equation</td>
<td>26</td>
</tr>
<tr>
<td>3.2.4 Discretized Column Wall Equation</td>
<td>26</td>
</tr>
<tr>
<td>3.2.5 Discretized Total Material Equation</td>
<td>26</td>
</tr>
<tr>
<td>3.2.6 Discretized Momentum Equation</td>
<td>27</td>
</tr>
<tr>
<td>3.2.7 Discretized Boundary Condition</td>
<td>27</td>
</tr>
<tr>
<td>3.3 Numerical Approach</td>
<td>28</td>
</tr>
<tr>
<td>3.4 Convergence And Stability Of Numerical Techniques</td>
<td>29</td>
</tr>
<tr>
<td>Section 4  COMPUTER MODEL VERIFICATION</td>
<td>31</td>
</tr>
<tr>
<td>4.1 Test Apparatus</td>
<td>31</td>
</tr>
<tr>
<td>4.2 Thermal Characterization with Inert Gas Heating</td>
<td>31</td>
</tr>
<tr>
<td>4.2.1 Molecular Sieve 5A</td>
<td>32</td>
</tr>
<tr>
<td>4.2.1.1 FLOW1MOL Model Thermal Verification</td>
<td>32</td>
</tr>
<tr>
<td>4.2.1.2 2DMOL Model Thermal Verification</td>
<td>35</td>
</tr>
<tr>
<td>4.3 Carbon Dioxide Adsorption</td>
<td>37</td>
</tr>
<tr>
<td>4.3.1 Molecular Sieve 5A</td>
<td>37</td>
</tr>
<tr>
<td>4.3.1.1 FLOW1MOL Model Verification</td>
<td>37</td>
</tr>
<tr>
<td>4.3.1.2 2DMOL Model Verification</td>
<td>43</td>
</tr>
<tr>
<td>4.4 Water Adsorption</td>
<td>46</td>
</tr>
<tr>
<td>4.4.1 Molecular Sieve 5A</td>
<td>46</td>
</tr>
<tr>
<td>4.4.1.1 FLOW1MOL Model Verification</td>
<td>47</td>
</tr>
<tr>
<td>4.4.1.2 2DMOL Model Verification</td>
<td>51</td>
</tr>
<tr>
<td>4.5 Water and Carbon Dioxide Adsorption</td>
<td>55</td>
</tr>
<tr>
<td>4.5.1 Molecular Sieve 5A</td>
<td>55</td>
</tr>
<tr>
<td>4.5.1.1 FLOW1MOL Model Verification</td>
<td>57</td>
</tr>
<tr>
<td>4.5.1.2 2DMOL Model Verification</td>
<td>61</td>
</tr>
<tr>
<td>4.6 Carbon Dioxide Desorption</td>
<td>66</td>
</tr>
<tr>
<td>4.6.1 Molecular Sieve 5A</td>
<td>66</td>
</tr>
<tr>
<td>4.6.1.1 FLOW1MOL Model Verification</td>
<td>66</td>
</tr>
<tr>
<td>4.6.1.2 2DMOL Model Verification</td>
<td>70</td>
</tr>
<tr>
<td>4.7 Water Desorption</td>
<td>73</td>
</tr>
<tr>
<td>4.7.1 Molecular Sieve 5A</td>
<td>73</td>
</tr>
<tr>
<td>4.7.1.1 FLOW1MOL Model Verification</td>
<td>74</td>
</tr>
<tr>
<td>4.7.1.2 2DMOL Model Verification</td>
<td>78</td>
</tr>
<tr>
<td>4.8 FLOW3MOL MODEL RESULTS</td>
<td>81</td>
</tr>
<tr>
<td>4.9 VACMOL Model Results</td>
<td>83</td>
</tr>
<tr>
<td>Section 5  CONCLUSIONS AND RECOMMENDATIONS</td>
<td>86</td>
</tr>
<tr>
<td>5.1 Conclusion</td>
<td>86</td>
</tr>
<tr>
<td>5.2 Recommendations</td>
<td>86</td>
</tr>
<tr>
<td>Section 6  REFERENCES</td>
<td>88</td>
</tr>
</tbody>
</table>
## Appendices

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>DERIVATION OF IAST EQUATION (EQ 2.8)</td>
<td>A-1</td>
</tr>
<tr>
<td>B</td>
<td>DERIVATION OF MOMENTUM, ENERGY, AND MOLAR CONCENTRATION BALANCES FOR TWO DIMENSIONS</td>
<td>B-1</td>
</tr>
<tr>
<td>C</td>
<td>DESCRIPTION OF COMPUTER PROGRAMS</td>
<td>C-1</td>
</tr>
<tr>
<td>D</td>
<td>FLOW1MOL FORTRAN CODE</td>
<td>D-1</td>
</tr>
<tr>
<td>E</td>
<td>2DMOL FORTRAN CODE</td>
<td>E-1</td>
</tr>
<tr>
<td>F</td>
<td>VACMOL FORTRAN CODE</td>
<td>F-1</td>
</tr>
<tr>
<td>G</td>
<td>FLOW3MOL FORTRAN CODE</td>
<td>G-1</td>
</tr>
<tr>
<td>Section</td>
<td>Figure Description</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>1-1</td>
<td>Space Station 4-Bed Molesieve</td>
<td>1</td>
</tr>
<tr>
<td>2-1</td>
<td>Intraparticle Mechanism of Diffusion for Monodisperse Sorbent</td>
<td>9</td>
</tr>
<tr>
<td>2-2</td>
<td>Intraparticle Mechanisms of Bidisperse-pore Sorbent</td>
<td>9</td>
</tr>
<tr>
<td>3-1</td>
<td>Shows the grids with different sizes</td>
<td>24</td>
</tr>
<tr>
<td>4-1</td>
<td>5A Thermal Characterization Test Specifications</td>
<td>32</td>
</tr>
<tr>
<td>4-2</td>
<td>Variations of H_FW for FLOW1MOL</td>
<td>33</td>
</tr>
<tr>
<td>4-3</td>
<td>Variations of H_OW for FLOW1MOL</td>
<td>34</td>
</tr>
<tr>
<td>4-4</td>
<td>Final Thermal Verification of FLOW1MOL for 5A</td>
<td>34</td>
</tr>
<tr>
<td>4-5</td>
<td>Variations of H_FW for 2DMOL</td>
<td>35</td>
</tr>
<tr>
<td>4-6</td>
<td>Variations of H_OW for 2DMOL</td>
<td>36</td>
</tr>
<tr>
<td>4-7</td>
<td>Final Thermal Verification of 2DMOL for 5A</td>
<td>36</td>
</tr>
<tr>
<td>4-8</td>
<td>Specifications for 01-26-94 CO2 Adsorption Testing</td>
<td>38</td>
</tr>
<tr>
<td>4-9</td>
<td>CO2 Partial Pressures for 01-26-94 Test</td>
<td>39</td>
</tr>
<tr>
<td>4-10</td>
<td>CO2 Model Temperature Comparisons With and Without Nitrogen Coadsorption</td>
<td>39</td>
</tr>
<tr>
<td>4-11</td>
<td>CO2 Model Breakthrough Comparisons With and Without Nitrogen Coadsorption</td>
<td>40</td>
</tr>
<tr>
<td>4-12A</td>
<td>Input Data Set &quot;A&quot; for FLOW1MOL Comparison with 01-26-94 Test</td>
<td>41</td>
</tr>
<tr>
<td>4-12B</td>
<td>Input Data Set &quot;B&quot; for FLOW1MOL Comparison with 01-26-94 Test</td>
<td>42</td>
</tr>
<tr>
<td>4-13</td>
<td>Input Data Set &quot;A&quot; for 2DMOL Comparison with 01-26-94 Test</td>
<td>43</td>
</tr>
<tr>
<td>4-14</td>
<td>Input Data Set &quot;B&quot; for 2DMOL Comparison with 01-26-94 Test</td>
<td>44</td>
</tr>
<tr>
<td>4-15</td>
<td>CO2 Model Breakthrough Comparisons for 01-26-94 Test with 2DMOL Results</td>
<td>45</td>
</tr>
<tr>
<td>4-16</td>
<td>CO2 Temperature Comparisons for 01-26-94 Test with 2DMOL Results</td>
<td>45</td>
</tr>
<tr>
<td>4-17</td>
<td>Specifications for 01-26-94 H2O Adsorption Testing</td>
<td>46</td>
</tr>
<tr>
<td>4-18</td>
<td>H2O Breakthrough for 04-07-94 Test</td>
<td>47</td>
</tr>
<tr>
<td>4-19</td>
<td>Input Data Set &quot;A&quot; for FLOW1MOL Comparison with 04-07-94 Test</td>
<td>48</td>
</tr>
<tr>
<td>4-20</td>
<td>Input Data Set &quot;B&quot; for FLOW1MOL Comparison with 04-07-94 Test</td>
<td>49</td>
</tr>
<tr>
<td>4-21</td>
<td>H2O Breakthrough Comparisons for 04-07-94 Test with FLOW1MOL Results</td>
<td>50</td>
</tr>
<tr>
<td>4-22</td>
<td>H2O Temperature Comparisons for 04-07-94 Test with FLOW1MOL Results</td>
<td>50</td>
</tr>
<tr>
<td>4-23</td>
<td>Input Data Set &quot;A&quot; for 2DMOL Comparison with 04-07-94 Test</td>
<td>52</td>
</tr>
<tr>
<td>4-24</td>
<td>Input Data Set &quot;B&quot; for 2DMOL Comparison with 04-07-94 Test</td>
<td>53</td>
</tr>
<tr>
<td>4-25</td>
<td>H2O Breakthrough Comparisons for 04-07-94 Test with 2DMOL Results</td>
<td>54</td>
</tr>
<tr>
<td>4-26</td>
<td>H2O Temperature Comparisons for 04-07-94 Test with 2DMOL Results</td>
<td>54</td>
</tr>
<tr>
<td>4-27</td>
<td>Specifications for 05-06-94 H2O/CO2 Adsorption Testing</td>
<td>55</td>
</tr>
<tr>
<td>4-27</td>
<td>H2O Breakthrough for 05-06-94 Test</td>
<td>56</td>
</tr>
<tr>
<td>4-28</td>
<td>H2O/CO2 Temperatures for 05-06-94 Test</td>
<td>56</td>
</tr>
<tr>
<td>4-29</td>
<td>CO2 Breakthrough for 05-06-94 Test</td>
<td>57</td>
</tr>
<tr>
<td>4-30</td>
<td>Input Data Set &quot;A&quot; for FLOW1MOL Comparison with 05-06-94 Test</td>
<td>58</td>
</tr>
<tr>
<td>4-31</td>
<td>Input Data Set &quot;B&quot; for FLOW1MOL Comparison with 05-06-94 Test</td>
<td>59</td>
</tr>
<tr>
<td>4-32</td>
<td>H2O Breakthrough Comparisons for 05-06-94 Test with FLOW1MOL Results</td>
<td>60</td>
</tr>
<tr>
<td>4-33</td>
<td>H2O/CO2 Temperature Comparisons for 05-06-94 Test with FLOW1MOL Results</td>
<td>60</td>
</tr>
<tr>
<td>4-34</td>
<td>CO2 Breakthrough Comparisons for 05-06-94 Test with FLOW1MOL Results</td>
<td>61</td>
</tr>
<tr>
<td>4-35</td>
<td>Input Data Set &quot;A&quot; for 2DMOL Comparison with 05-06-94 Test</td>
<td>62</td>
</tr>
<tr>
<td>4-36</td>
<td>Input Data Set &quot;B&quot; for 2DMOL Comparison with 05-06-94 Test</td>
<td>63</td>
</tr>
<tr>
<td>4-37</td>
<td>CO2 Breakthrough Comparisons for 05-06-94 Test with 2DMOL Results</td>
<td>64</td>
</tr>
<tr>
<td>4-38</td>
<td>H2O/CO2 Temperature Comparisons for 05-06-94 Test with 2DMOL Results</td>
<td>64</td>
</tr>
<tr>
<td>4-39</td>
<td>H2O/CO2 Breakthrough Comparisons for 05-06-94 Test with 2DMOL Results</td>
<td>65</td>
</tr>
<tr>
<td>4-40</td>
<td>Specifications for 01-27-94 CO2 Desorption Testing</td>
<td>66</td>
</tr>
<tr>
<td>4-41</td>
<td>Input Data Set &quot;A&quot; for FLOW1MOL Comparison with 01-27-94 Test</td>
<td>67</td>
</tr>
<tr>
<td>4-42</td>
<td>Input Data Set &quot;B&quot; for FLOW1MOL Comparison with 01-27-94 Test</td>
<td>68</td>
</tr>
<tr>
<td>4-43</td>
<td>CO2 Breakthrough Comparisons for 01-27-94 Test with FLOW1MOL Results</td>
<td>69</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES (CONTINUED)

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-44</td>
<td>CO2 Temperature Comparisons for 01-27-94 Test with FLOW1MOL Results</td>
<td>69</td>
</tr>
<tr>
<td>4-45</td>
<td>Input Data Set &quot;A&quot; for 2DMOL Comparison with 01-27-94 Test</td>
<td>70</td>
</tr>
<tr>
<td>4-46</td>
<td>Input Data Set &quot;B&quot; for 2DMOL Comparison with 01-27-94 Test</td>
<td>71</td>
</tr>
<tr>
<td>4-47</td>
<td>CO2 Breakthrough Comparisons for 01-27-94 Test with 2DMOL Results</td>
<td>72</td>
</tr>
<tr>
<td>4-48</td>
<td>CO2 Temperature Comparisons for 01-27-94 Test with 2DMOL Results</td>
<td>72</td>
</tr>
<tr>
<td>4-49</td>
<td>Specifications for 04-19-94 H2O Desorption Testing</td>
<td>73</td>
</tr>
<tr>
<td>4-50</td>
<td>Input Data Set &quot;A&quot; for FLOW1MOL Comparison with 04-19-94 Test</td>
<td>75</td>
</tr>
<tr>
<td>4-51</td>
<td>Input Data Set &quot;B&quot; for FLOW1MOL Comparison with 04-19-94 Test</td>
<td>76</td>
</tr>
<tr>
<td>4-52</td>
<td>H2O Breakthrough Comparisons for 04-19-94 Test with FLOW1MOL Results</td>
<td>77</td>
</tr>
<tr>
<td>4-53</td>
<td>Temperature Comparisons for 04-19-94 Test with FLOW1MOL Results</td>
<td>77</td>
</tr>
<tr>
<td>4-54</td>
<td>Input Data Set &quot;A&quot; for 2DMOL Comparison with 04-19-94 Test</td>
<td>78</td>
</tr>
<tr>
<td>4-55</td>
<td>Input Data Set &quot;B&quot; for 2DMOL Comparison with 04-19-94 Test</td>
<td>79</td>
</tr>
<tr>
<td>4-56</td>
<td>Breakthrough Comparisons for 04-19-94 Test with 2DMOL Results</td>
<td>80</td>
</tr>
<tr>
<td>4-57</td>
<td>Temperature Comparisons for 04-19-94 Test with 2DMOL Results</td>
<td>80</td>
</tr>
<tr>
<td>4-58</td>
<td>Temperature Comparisons for 04-19-94 Test with 2DMOL Results</td>
<td>81</td>
</tr>
<tr>
<td>4-59</td>
<td>Carbon Dioxide Breakthrough Results for FLOW3MOL</td>
<td>82</td>
</tr>
<tr>
<td>4-60</td>
<td>Water Breakthrough Results for FLOW3MOL</td>
<td>82</td>
</tr>
<tr>
<td>4-61</td>
<td>Temperature Results for FLOW3MOL</td>
<td>83</td>
</tr>
<tr>
<td>4-62</td>
<td>Temperature Results for VACMOL</td>
<td>84</td>
</tr>
<tr>
<td>4-63</td>
<td>Partial Pressure Results for VACMOL</td>
<td>84</td>
</tr>
<tr>
<td>4-64</td>
<td>Total Pressure Results for VACMOL</td>
<td>85</td>
</tr>
<tr>
<td>4-65</td>
<td>Velocity Results for VACMOL</td>
<td>85</td>
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<td>Velocity Results for VACMOL (first 0.25 hours)</td>
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**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>a</td>
<td>Surface area of pellets per unit volume of pellet ft²/ft³</td>
</tr>
<tr>
<td>A</td>
<td>Surface area ft²</td>
</tr>
<tr>
<td>B</td>
<td>Langmuir constant</td>
</tr>
<tr>
<td>C</td>
<td>Constant in Darcy equation</td>
</tr>
<tr>
<td>C</td>
<td>Gas stream concentration, lb mole/ft³</td>
</tr>
<tr>
<td>Cip</td>
<td>Gas phase concentration of iᵗʰ component in the pores of particles, lb mole/ft³</td>
</tr>
<tr>
<td>C*</td>
<td>Volume average pore Gas phase concentration of iᵗʰ component, lb mole/ft³</td>
</tr>
<tr>
<td>C'i</td>
<td>Gas phase concentration of iᵗʰ component at the surface of the solid phase lb mole/ft³</td>
</tr>
<tr>
<td>C₁₀</td>
<td>Gas phase concentration of iᵗʰ component at boundary or initial lb mole/ft³</td>
</tr>
<tr>
<td>cₚg</td>
<td>Heat capacity of gas phase, Btu/lbm-R</td>
</tr>
<tr>
<td>cₚs</td>
<td>Heat capacity of solid particle, Btu/lbm-R</td>
</tr>
<tr>
<td>cₚw</td>
<td>Heat capacity of column particle, Btu/lbm-R</td>
</tr>
<tr>
<td>d, dᵢ</td>
<td>Column diameter, ft</td>
</tr>
<tr>
<td>D</td>
<td>Diffusivity, ft²/hr</td>
</tr>
<tr>
<td>Dˡ</td>
<td>Axial diffusivity, ft²/hr</td>
</tr>
<tr>
<td>Dₘᵢ</td>
<td>Knudsen diffusivity, ft²/hr</td>
</tr>
<tr>
<td>Dₛᵢ</td>
<td>Surface diffusivity, ft²/hr</td>
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<tr>
<td>Dₑ</td>
<td>Effective diffusivity, ft²/hr</td>
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<tr>
<td>Dₘᵣ</td>
<td>Molecular diffusion in mixture, ft²/hr</td>
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<tr>
<td>D₀</td>
<td>Stagnant diffusivity, ft²/sec</td>
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<tr>
<td>Dᵢf</td>
<td>Fluid flow diffusivity, ft²/sec</td>
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<td>Effective axial diffusivity, ft²/sec</td>
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<td>Dₑᵣ</td>
<td>Effective radial diffusivity, ft²/sec</td>
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<tr>
<td>Dᵢfₓ</td>
<td>Axial diffusivity of fluid flow, ft²/sec</td>
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<td>Dᵢfᵣ</td>
<td>Radial diffusivity of fluid flow, ft²/sec</td>
</tr>
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<td>dₑᵣ</td>
<td>Bed diameter, ft</td>
</tr>
<tr>
<td>Eₛᵢ</td>
<td>Surface diffusivity energy of activation of species i</td>
</tr>
<tr>
<td>G</td>
<td>Superficial mass velocity, lbₘ/ft² hr</td>
</tr>
<tr>
<td>hₑ</td>
<td>Effective Heat transfer coefficient for column insulation, Btu/ft²-hr</td>
</tr>
<tr>
<td>hₘᵣ</td>
<td>Heat transfer coefficient between the gas stream and the column wall, Btu/ft²-hr</td>
</tr>
<tr>
<td>hₛ</td>
<td>Heat transfer coefficient between the gas stream and the sorbent, Btu/ft²-hr</td>
</tr>
<tr>
<td>ΔH</td>
<td>Heat of Adsorption, Btu/lb mole</td>
</tr>
<tr>
<td>K</td>
<td>Constant in Darcy equation</td>
</tr>
<tr>
<td>k</td>
<td>Fluid flow axial conductivity, dispersion, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kₒ</td>
<td>Stagnant thermal conductivity, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kₑₓ</td>
<td>Effective axial conductivity, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kₑᵣ</td>
<td>Effective radial conductivity, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kᵢfₓ</td>
<td>Axial conductivity of fluid flow, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kᵢfᵣ</td>
<td>Radial conductivity of fluid flow, Btu/ft-hr-R</td>
</tr>
<tr>
<td>kₛ</td>
<td>Solid thermal conductivity, Btu/ft-hr-R</td>
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<tr>
<td>kᵦᵣ</td>
<td>Fluid film mass transfer coefficient of iᵗʰ component, ft/hr</td>
</tr>
<tr>
<td>kₑᵢ</td>
<td>Effective mass transfer coefficient of iᵗʰ component, ft/hr</td>
</tr>
<tr>
<td>Mᵢ</td>
<td>Molecular weight of adsorbate i, lb/lb mole</td>
</tr>
<tr>
<td>n</td>
<td>Number of component</td>
</tr>
<tr>
<td>Nₚₑ</td>
<td>Peclet number, cᵢₚgρₖμ/k</td>
</tr>
</tbody>
</table>
NOMENCLATURE

\( \text{Re} \)  
Reynolds number, \( d_p \rho_g u/\mu \)

\( N_S \)  
Schmidt number, \( \mu/D \rho_g \)

\( N_i \)  
Molar flux of component i, lb mole/ft²-hr

\( P \)  
Total pressure, mmHg or lbf/ft²

\( P_i \)  
Partial pressure of component i, mmHg or lbf/ft²

\( P_{CA} \)  
critical pressure of component A, Atm

\( P_{CB} \)  
critical pressure of component B, Atm

\( q \)  
Amount adsorbed in the solid, lb moles/ft³ of solid

\( q_i \)  
Solid phase concentration of i\textsuperscript{th} component in equilibrium with gas phase, lbs moles/ft³ of solid

\( \bar{q}_i \)  
Volume average solid phase concentration of component i, lb moles/ft³ of solid

\( q_{mi} \)  
Langmuir constant

\( r \)  
Radial position, ft

\( r_e \)  
Mean pore radius, Å

\( r_p \)  
Radial spatial particle dimension, ft

\( R \)  
Ideal gas constant 555 mm Hg ft³/lb mol

\( R_i \)  
Inside wall diameter of column, ft

\( R_o \)  
Outside wall diameter of column, ft

\( R_p \)  
Particle radius, ft

\( t \)  
Time, hr

\( T \)  
Temperature, K

\( T_a \)  
Ambient temperature, R

\( T_g \)  
gas temperature, R

\( T_w \)  
Wall temperature, R

\( T_s \)  
Solid temperature, R

\( T_{CA} \)  
Critical temperature of component A, K

\( T_{CB} \)  
Critical temperature of component B, K

\( u \)  
Interstitial velocity, ft/hr

\( V \)  
Velocity at the center of packed column, ft/hr

\( x \)  
Axial position

\( x_i \)  
Mole fraction of i\textsuperscript{th} component in the solid phase

\( y_i \)  
Mole fraction of i\textsuperscript{th} component in the gas phase
### GREEK

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<td>( \alpha )</td>
<td>Intraparticle void fraction</td>
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<td>( \alpha \beta )</td>
<td>Constant in effective conductivity equation</td>
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<td>( \varepsilon )</td>
<td>External bed void volume</td>
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<td>( \lambda )</td>
<td>Constant in effective conductivity equation</td>
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<td>( \phi )</td>
<td>Constant in stagnant conductivity equation</td>
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<td>( \rho_{pg} )</td>
<td>Density of gas phase, lb mole/ft(^3)</td>
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<td>( \rho_s )</td>
<td>Density of solid phase, lbs/ft(^3)</td>
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<td>( \rho_w )</td>
<td>Density of column wall, lb mole/ft(^3)</td>
</tr>
<tr>
<td>( \tau_p )</td>
<td>Pore tortuosity factor</td>
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<td>( \tau_s )</td>
<td>Surface tortuosity factor</td>
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<td>( \pi )</td>
<td>Constant or spreading pressure</td>
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<td>( \sigma )</td>
<td>Emissivity</td>
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<tr>
<td>( \Delta H )</td>
<td>Heat of adsorption, BTU/lb of solid</td>
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<td>( \omega )</td>
<td>Over-Relaxation coefficient</td>
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### SUBSCRIPTS

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<td>( i^{th} ) component</td>
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<td>( e )</td>
<td>Effective</td>
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<tr>
<td>( eff )</td>
<td>Effective</td>
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<tr>
<td>( ip )</td>
<td>( i^{th} ) component in the pores</td>
</tr>
<tr>
<td>( o )</td>
<td>Outside, initial</td>
</tr>
<tr>
<td>( p )</td>
<td>Pore</td>
</tr>
<tr>
<td>( pg )</td>
<td>Gas phase</td>
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<td>( ps )</td>
<td>Solid phase</td>
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<td>( * )</td>
<td>Equilibrium value</td>
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SECTION 1
INTRODUCTION

Adsorption is a process involving the selective transfer of one or more solutes from fluid solutions onto and into solids. Physical adsorption is a surface phenomenon. When fluid is in contact with a solid surface, molecules in the fluid phase spontaneously concentrate on the surface without any chemical change. At low temperature, adsorption is usually caused by intermolecular forces, such as Van der waal forces (Ruthven, 1984). Adsorption phenomenon, like any other thermodynamic system which involves the interaction of two phases, is driven by chemical potential differences between the phases. This chemical potential determines the strength with which any given molecule is adsorbed. The differences in the surface energy of adsorbent and the properties of each kind of molecule cause differences in the amount adsorbed in certain kinds of surface, i.e., the selectivity. Separation can be accomplished through selective collection and concentration of fluid molecules onto a solid surface.

Separation of gas mixtures by adsorption can be obtained by using either single column or multi-column configuration. However, for both processes the adsorbent column is alternately saturated and regenerated in a cyclic manner.

One example of a cyclic selective process is the Four-Bed Molecule Sieve (4BMS) used in International Space Station Alpha for the removal of CO₂ as shown in Figure 1-1.

FIGURE 1-1 SPACE STATION 4-BED MOLE-SIEVE

As shown in Figure 1, the actual CO₂ removal system consists of four beds. Two beds operate in the adsorption mode (a desiccant and CO₂ sorbent bed) while the other set of identical beds desorb. The desiccant beds desorb through gas stripping while the sorbent beds are heated and subjected to a vacuum (e.g., the pressure and thermal swing process). Following the air flow path in Figure 1-1, cabin air laden with CO₂ and water enters at the system inlet, then enters desiccant bed (1), which consists of Silica Gel and 13X sorbent materials. The desiccant bed is required to remove virtually all water from the air stream. The dry air is next pulled through the air blower,
which overcomes the system pressure drop. A heat exchanger, the precooler, removes the heat of compression and heat of adsorption from the desiccant bed before the air enters the 5A sorbent which is responsible for removing the CO₂ from air. Following the precooler, the 5A bed (2), CO₂ removal bed, performs the primary system function of removing CO₂. The other 5A bed (4) is concurrently desorbed with heat from embedded electrical heaters and allowed to vent to space vacuum. At the beginning of a new half cycle, the selector valves cycle to alternate the desorbing and adsorbing beds. Heated air from the hot, previously desorbing CO₂ sorbent bed, trips the downstream desiccant bed (3) of water, which is returned to the cabin in the return air stream.

Because of the complexity of the process, the design of an efficient 4BMS CO₂ removal system mission depends on many mission parameters, such as, duration, crew size, cost of power, volume, fluid interface properties, etc. A need for space vehicle CO₂ removal system models capable of accurately performing extrapolated hardware predictions is inevitable due to the change of the parameters which influences the CO₂ removal system capacity.

The purpose of this study is to (a) investigate the mathematical techniques required for a model capable of accurate extrapolated performance predictions and (b) obtain test data required to estimate mass transfer coefficients and verify the computer model. Models have been developed to demonstrate that the finite difference technique can be successfully applied to sorbents and conditions used in spacecraft CO₂ removal systems. The non isothermal, axially dispersed, plug flow model with linear driving force for 5X and pore diffusion for Silica gel are then applied to test data. A more complex model, a non-darcian model (2-dimensional), has also been developed for simulation of the test data. This model takes into account the channeling effect on column breakthrough.
SECTION 2
DEVELOPMENT AND ANALYSIS OF A MATHEMATICAL MODEL

2.1 Gas/Solid Equilibrium

Gas/solid equilibria is the thermodynamic limiting capacity for mass transfer in gas adsorption. It is one of the most important parameters for predicting solute separation from the bulk gas phase. Since the composition, temperature, and pressure change in a wide range with time and location within the adsorption column, a comprehensive gas/solid equilibrium model is needed.

2.1.1 Single Component Isotherm

The most popular single solute isotherms were correlated by Langmuir in 1918. The Langmuir approach assumed the rate of adsorption is equal to that of condensation. The final form of this equation is:

\[ q_i^* = \frac{q_m B_i P_i}{1 + B_i P_i} \]

where \( B_i \) and \( q_m \) are functions of temperature and heat of adsorption. Some of the single solute isotherms were correlated by the Langmuir-Freundlich equation (Sips, 1948):

\[ q_i^* = \frac{q_m B_i P_i^{n_i}}{1 + B_i P_i^{n_i}} \]

where \( n_i \) is a constant close to one.

The pure isotherm constants of CO\(_2\), H\(_2\)O, and N\(_2\) on 13X zeolite are as follows:

for CO\(_2\),

\[
\begin{align*}
q_{m,CO_2} &= (399.3942 - 1.93842889T + 3.25405\times10^{-3}T^2 - 1.82262\times10^{-4}T^3) / 44 / 100 \\
B_{CO_2} &= 35.35358072159 - 1.7016733T + 2.74587\times10^{-4}T^2 - 1.48412\times10^{-7}T^3 \\
n &= -29.3861079 + 1.53889849T - 2.61225877\times10^{-4}T^2 + 1.478185 \times 10^{-7}T^3 
\end{align*}
\]

for H\(_2\)O,

\[
\begin{align*}
q_{m,H_2O} &= (39.914452 - 8.87103\times10^{-2}T + 6.839503\times10^{-4}T^2) / 100 / 18.0 \\
n &= 1.0 
\end{align*}
\]

if partial pressure of H\(_2\)O less or equal than .4 mm Hg

\[
\begin{align*}
q_{m,H_2O} &= (873.44464 - 3.867835T + 5.80375\times10^{-3}T^2 - 2.9346685\times10^{-4}T^3) / 100 / 18 \\
n &= 1.0 
\end{align*}
\]
for partial pressure of greater than .4 mm Hg

\[ q_{m,H_2O} = (95.0938247 - 2.17257754T + 1.4628603 \times 10^{-4}T^2) / 100 / 18 \]

\[ B_{H_2O} = 48.56664 - 2.262024 \times 10^{-4}T + 3.91017 \times 10^{-4}T^2 - 2.3790985 \times 10^{-7}T^3 \]

\( n = 1.0 \)

and for \( N_2 \)

\[ q_{m,N_2} = .00961197026 - 1.637879912 \times 10^{-5}T \quad \text{for } n = 1.0 \]

\[ B_{N_2} = 4.5597278759 \times 10^{-7} \exp(9628.9655743 / T) \quad \text{else} \]

\[ B_{N_2} = 5.808906668 \times 10^{-7} \exp(9911.5734593 / T) \]

where \( q \) is in lb mole of solute per lb of solid, \( T \) in Rankin, and \( P \) in mm Hg.

### 2.1.2 Multicomponent Isotherm

Two types of multicomponent correlation were used in this study. One is based on the Langmuir-Freundlich equation for multicomponent system

\[ q_i = \frac{q_{m_i}B_iP_i^{n_i}}{1 + \sum_j B_jP_j^{n_j}} \quad \text{eq 2.3} \]

and the more reliable method is based on Ideal Adsorption Solution Theory (IAST) of Myers and Prausnitz (1965). For pure-gas adsorption and assuming ideal gas behavior:

\[ \frac{\pi(p_i^*)A}{RT} = \int_0^{p_i^*} \frac{\pi_i}{p_i} dP_i \quad \text{eq 2.4} \]

where \( A \) is the surface area, \( \pi \) is the spreading pressure. The ideal solution assumption is applied to the adsorbed phase and the total amount adsorbed is then related to the mole fraction of each component:

\[ \frac{1}{q_t} = \sum_i \frac{x_i}{q_i} \quad \text{eq 2.5} \]

The Raoult law is also applied to the relation between mole fraction in the gas phase and adsorbed phase:

\[ P_i = P y_i = p_i^*(\pi) x_i \quad \text{eq 2.6} \]

where \( y_i \) and \( x_i \) are mole fraction of the i-th component in the gas phase and in adsorbed phase, respectively, and
\[
\sum x_i = \sum y_i = 1
\]

The IST theory assumes that the spreading pressure is the same for all the components in the mixture.

The solution for the amount adsorbed in the solid phase in equilibrium with the gas phase concentration is obtained by an iterative procedure with the IST theory. For the case of the Langmuir-Freundlich single isotherm, from equations 2.2, 2.4, 2.6, and 2.7 one gets:

\[
\sum_{i=1}^{n} \frac{P_y}{\exp \left( \frac{\pi A n_i}{RT q_m^*} \right) - 1} = 0
\]

The derivation is shown in Appendix A. Knowing the total pressure and the solid temperature, a value of \( \pi \) is guessed and solution will be obtained by iteration until equation 2.8 is satisfied.

### 2.2 Mathematical Model For Nonisothermal Multicomponent Adsorption In a Packed Bed

Separation of solutes from the bulk gas can be accomplished in a packed column which is filled with a specific adsorbent that preferentially adsorbs certain constituents from the bulk gas. In the simplest case of packed column adsorbent particles, the following mass transport processes are considered: axial dispersion in the interparticle fluid phase, fluid to particle mass transfer, and a reversible adsorption in the interior of the particle. Also, adsorption is accompanied by the evolution of heat, and temperature changes affect the adsorption equilibrium relation and, in some cases, adsorption rate. Thus, especially in the gas phase adsorption, not only the effects of mass transfer on adsorption rate but also effects of heat generation and heat transfer in the adsorbent bed must be taken into account.

The dynamic bed behavior can be modeled by heat and mass balance equations. The mathematical model will be used to estimate the breakthrough curve for a certain constituent in the bulk gas. In return, this enables one to obtain the necessary parameters for predicting the transient behavior of the temperature profile and concentration of the gas for different initial parameters such as inlet concentration, temperature, and the fluid velocity.

The heat and mass balances could not be solved analytically; therefore, these equations were solved numerically by finite differences methods, namely the Under-Relaxation and Newman methods. A FORTRAN code was written to find the numerical solutions to the transient equations.

In this study two types of mathematical models were used to predict the dynamic behavior of the bed. A one dimensional model was developed which takes into account only the mass and heat transfer rate of change in the axial direction of the bed. On the other hand, a two dimensional model would also estimate these rates in the radial direction of the bed, and therefore this model...
was also developed. The mathematical derivation of a two dimensional model is shown in Appendix B.

2.2.1 One Dimensional Adsorption Mathematical Model

In a one dimensional adsorption model in a packed column any rates of change of variables in the radial direction are assumed to be negligible compared to the axial direction. Also, the porosity of the bed is considered to be constant from the center to the column wall.

2.2.1.1 Mass Balance Equation

In the bulk stream of the gas within the bed, the material balance for the adsorbate concentration is

\[
\frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x^2} - u \frac{\partial C_i}{\partial x} - \varepsilon \frac{\partial \tilde{q}_i}{\partial t}
\]

Boundary/Initial Condition

at \( t < 0 \), \( C_i = C_{i,0} \) for \( 0 < x < L \)

at \( t < 0 \), \( \tilde{q}_i = \tilde{q}_{i,0} \) for \( 0 < x < L \)

at \( t \geq 0 \), \( C_i = C_{i,0} \) for \( x = 0 \)

at \( t \geq 0 \), \( \frac{\partial C_i}{\partial x} = 0 \) for \( x = L \)

where \( C_i \) is the concentration of each component in the gas bulk, \( D_i \) is the axial dispersion, \( u \) is the interstitial velocity, \( \varepsilon \) is the void fraction, and \( \tilde{q}_i \) is the adsorbate concentration in the solid phase. The last boundary condition indicates a free stream boundary type. This boundary condition is prescribed for situation where the normal derivative of flux, the gradient of concentration or temperature, at the end of the packed column vanishes. In a numerical sense, the value of the last grid outside the packed bed is set equal to that of last grid of the packed bed.

2.2.1.2 Total Material Balance

Assuming the ideal gas law \( C_i = \frac{P y_i}{R T} \) and knowing \( \sum y_i = 1 \), the above equation can be recast into an overall mass balance equation,

\[
\frac{\partial P}{\partial t} = D_i \frac{\partial^2 P}{\partial x^2} - u \frac{\partial P}{\partial x} - P \frac{\partial u}{\partial x} \left( \frac{\partial T}{\partial t} - D_i \frac{\partial^2 T}{\partial x^2} + u \frac{\partial T}{\partial x} \right) - RT \frac{1 - \varepsilon}{\varepsilon} \sum_{i=1}^{n} \tilde{q}_i
\]

This equation was used to compute the pressure drop along the axial direction in the bed.

2.2.1.3 Gas Phase Energy Equation

The change of gas temperature with respect to time is the result of heat flux from the solid to the gas plus convection of heat due to the fluid flow, as shown by the following equation:
where \( T_g \) is the bulk gas temperature, \( T_w \) is the wall temperature, \( T_s \) is the solid temperature, \( \rho_g \) is the bulk density, \( c_p \) is the specific heat of the bulk gas, \( k_f \) is the effective conductivity of the bulk gas, \( h_s \) is the heat transfer coefficient between the solid and the gas phase (Petrovic and Thodos, 1968), and \( h_w \) is the heat transfer coefficient between the wall and the gas phase.

### 2.2.1.4 Solid Phase Energy Equation

The following energy equation for the solid phase includes the term for heat flux from the solid phase to the gas phase plus heat generation due to adsorption.

\[
\rho_s c_p \frac{\partial T_s}{\partial t} = k_f \frac{\partial^2 T_s}{\partial x^2} + h_s a_s (T_s - T_g) - \sum_{i=1}^{n} \Delta H_i \frac{\partial q_i}{\partial t}
\]

**Boundary / Initial Conditions**

at \( t < 0 \), \( T_s = T_{s,i} \) for \( 0 \leq x \leq L \)

at \( t \geq 0 \), \( T_s = T_i \) for \( x = 0 \)

at \( t \geq 0 \), \( \frac{\partial T_s}{\partial x} = 0 \) for \( x = L \)

**eq 2.12**

### 2.2.1.5 Column Wall Energy Equation

The wall temperature \( T_w \) is given by

\[
\rho_w c_w \frac{\partial T_w}{\partial t} = 2\pi R h_w (T_s - T_w) - 2\pi R h_o (T_w - T_o)
\]

**Initial Condition**

at \( t < 0 \), \( T_w = T_{w,o} \)

**eq 2.13**

where \( T_{o} \) is the surrounding temperature, \( h_w \) and \( h_o \) are the heat transfer coefficients between the wall and fluid and between the wall and the surrounding, respectively. Axial conductivity in the canister wall is neglected since the area of heat transfer from the fluid to wall and from the wall to fluid is an order of magnitude larger than the area in the axial direction. This is analogous to heat conduction in a slab.
2.2.1.6 Momentum Equation

Bulk resistance to the fluid flow through a solid matrix, as compared to the resistance at and near the surfaces confining the solid matrix, was measured by Darcy (1956). The following equation characterizes the pressure drop in a packed column:

$$\frac{-dP}{dx} = \frac{\mu}{K} u,$$

where $K$ is the permeability of the solid and $\mu$ is the fluid viscosity. This empirical slug-flow equation, which is suitable for slip flow and creeping flow, is valid when the Reynolds number, based on particle diameter, is close to one.

For higher Reynolds number, cross flow within the porous media creates additional pressure drop. For this regime the Ergun equation could be used to estimate the pressure drop, see Ergun (1952) and Beavers (1969):

$$\frac{dP}{dx} = -\frac{\mu}{K} u - \rho Cu^2,$$

where $C$ is the inertial coefficient.

The Darcian terms contain the empirical coefficients $K$ and $C$, which are given by relations developed by Ergun (1952) for flow in a packed bed:

$$K = \frac{d_p^2 \epsilon^3}{150(1 - \epsilon)^2},$$

and

$$C = \frac{1.75(1 - \epsilon)}{d_p \epsilon^3},$$

where $d_p$ is particle diameter.

Equations 2.10 and 2.15 are used to compute the total pressure and the velocity respectively in the axial direction. This was found to give better convergence than using them in the reverse order.

2.2.2 Solid Phase Transport Equation

Mass transfer of solute from bulk gas to sorbed state is driven by equilibrium isotherms. The mass balance equation inside the sorbent material depends on the structure of the pellet. Monodisperse pore-diffusion and bidisperse pore-diffusion are the two models used to predict the mass transport within the pellet. The schematics for the two types of sorbents are illustrated in Figures 2-1 and 2-2. In general, the mass transfer mechanism of an adsorption process includes four steps: fluid-film transfer, pore diffusion, surface adhesion, and surface diffusion. Since the surface adhesion rate approximates the order of the collision frequency of the gas on the solid surface, which is much greater than for the transport processes, equilibrium is assumed to be reached instantaneously at the interfaces (Yang, 1987). Adsorbates initially transfer from
the bulk gas stream through an external film around the particles and reach the external surface of the particles. Molecules of adsorbate then diffuse into the pores of the particles, are adsorbed on the active sites, and then diffuse along the surface. The film transfer and pore diffusion are treated as sequential steps, since no accumulation of adsorbates are allowed; in other words, conservation of mass applies. However, pore and surface diffusion generally take place in parallel. Any combination of the resulting three steps can constitute the rate-controlling mechanism. The external mass transfer rate is defined in terms of an effective transfer coefficient (\( k_f \)) as a linear driving force equation.

FIGURE 2-1 INTRAPARTICLE MECHANISM OF DIFFUSION FOR MONODISPERSE SORBENT

FIGURE 2-2 INTRAPARTICLE MECHANISMS OF BIDISPERSE-PORE SORBENT
\[ N_n = -k_n(C_m - C_{\text{surf},i}) \]  

\text{eq 2.18}

For the low Reynolds number region covered in the present study, the correlation of Petrovic and Thodos (1968) is used:

\[ k_n = \frac{0.357}{\varepsilon} (N_{Re})^{0.64} (N_{Sc,i})^{0.33} \frac{D_{mi}}{2R_p}, \]

\text{eq 2.19}

for \( 3 < N_{Re} < 2000 \). \( N_{Re} \) is the Reynolds number and \( N_{Sc} \) is Schmidt number.

Molecular diffusion of a component in a mixture is described by the Stefan-Maxwell equation. For single component diffusion in a mixture, however, the diffusion coefficient \( D_{mi} \) is approximately related to the binary coefficients by the following relationship (Bird et al., 1960):

\[ D_{mi} = \frac{1 - y_j}{\sum_{j} y_j D_{ij}} \]

\text{eq 2.20}

For binary mixtures at low pressure, \( D_{ij} \) can be estimated by the following equation, (Slattery and Bird, 1958):

\[ D_{AB} = \frac{1}{p} (P_{ei}P_{eb})^{\frac{3}{2}} (T_{eA}T_{eb})^{\frac{3}{2}} \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{\frac{3}{2}} \left( \frac{T}{\sqrt{T_{eA}T_{eb}}} \right)^b \]

For nonpolar gaspairs:
- \( a = 2.745 \times 10^{-4} \)
- \( b = 1.823 \)

For \( H_2O \) with a nonpolar gas:
- \( a = 3.640 \times 10^{-4} \)
- \( b = 2.334 \)

\text{eq 2.21}

The Knudsen diffusion coefficient can be estimated by the following equation (Satterfield, 1980):

\[ D_{ki} = 4.67 \times 10^{-4} \frac{r_e}{\tau_p} \left( \frac{T}{M_i} \right)^{0.5} \]

\text{eq 2.22}

where \( r_e \) is the mean diameter of the pore size and \( \tau_p \) the pore tortuosity factor and is approximately between 1-4 (Satterfield, 1980).

The surface diffusion is an activated process which can be expressed by an Arrhenius-type expression (Smith, 1981):
\[ D_{si} = D_{so,i} \exp\left(\frac{-E_{si}}{RT}\right) \]

where \( E_{si} \) is the activation energy for the surface diffusion and \( D_{so,i} \) is the pre-exponential factor.

### 2.2.3 Monodisperse Pore Diffusion Model

The pore structure of pellets are simulated by this model are monodisperse. Sorbents in this category include activated carbon, alumina, and silica gel. The mass balance for component \( i \) inside the pores of a spherical particle at the axial location \( x \) in the bed yield:

\[
\alpha \frac{\partial C_{wp}}{\partial t} + \frac{1}{r_p^2} \frac{\partial (r_p^2 N_{ir})}{\partial r_p} + \frac{\partial q_i}{\partial t} = 0
\]

where \( \alpha \) is the intraparticle void fraction, \( N_{ir} \) is the flux of component \( i \), \( r_p \) is particle radius, and \( q_i \) is the amount adsorbed on the solid phase.

Equation 2.24 can be simplified by employing the following particle volume-averaged quantities:

\[
\bar{C}_i = \frac{3}{R_p^3} \int C_{ir} r_p^2 dr
\]

and

\[
\bar{q}_i = \frac{3}{R_p^3} \int q_{ir} r_p^2 dr
\]

By integrating equation 2.24 with respect to \( r_p \), using the volume averaged quantities and noting that \( N_{ir} = 0 \) at \( r = 0 \), the result is

\[
\alpha \frac{\partial \bar{C}_{wp}}{\partial t} + \frac{3}{R_p} N_{ir} + \frac{\partial \bar{q}_i}{\partial t} = 0
\]

To further simplify the model, parabolic concentration profile within the particle is assumed (Tsai, 1983), thus

\[
C_{wp} = E_i + F_i r_p^2
\]

where the constant \( E \) and \( F \) can be evaluated by using the surface conditions:

\[
C_{wp} = C_{ws} \text{ at } r = R_p
\]

and

\[
E_i = C_{wp} - F_i R_p^2
\]

where \( C_{wp} \) is the concentration of \( i \) at the surface. By integrating equation 2.28 and using volume averaged quantity:
\[
F_i = (C_i^p - \bar{C}_i^p) \frac{5}{2R_p^2}.
\]

Therefore, by inserting eq 2.31 and 2.30 into eq 2.28 and taking the derivative with respect to \( r \) at the surface of particle:

\[
\left( \frac{\partial C_i^p}{\partial r} \right)_{r=R_p} = (C_i^p - \bar{C}_i^p) \frac{5}{R_p}
\]

The flux \( N_i^p \) is the combined pore and solid diffusions. Pore diffusion is dominated by Knudsen diffusion with a constant diffusivity, \( D_k \). Surface diffusion \( D_s \) obeys Fick's law. Thus,

\[
N_i = -D_k \frac{\partial C_i^p}{\partial r} - D_s \frac{\partial q_i}{\partial r}
\]

A local equilibrium can be assumed between the gas phase in the pore and the solid phase. Since the adsorbate concentrations are dilute, the solid phase concentration of each adsorbate may be assumed to be independent of the gas phase concentration of the other adsorbate. Therefore, the total flux of the \( i^{th} \) component at the pore mouth of the particle is

\[
N_i = -D_k \frac{\partial C_i^p}{\partial r} \bigg|_{r=R_p} - D_s \sum_{j=1}^{n} \frac{q_j}{C_{nj}} \frac{\partial C_j}{\partial r} \bigg|_{r=R_p} \quad i = 1, 2, 3, \ldots n
\]

Assuming gas-solid equilibrium within the pellet,

\[
\frac{\partial q_i}{\partial C_p} = \frac{\partial q_i^*}{\partial C_p}
\]

The time derivative of \( q_i \), is a function of \( T \), and gas concentration in pore side of the pellet, \( C_{pj} \),

\[
\frac{\partial q_i}{\partial t} = \frac{\partial q_i}{\partial T} \frac{\partial T}{\partial t} + \sum_{j=1}^{n} \frac{\partial q_i}{\partial C_j} \frac{\partial C_j}{\partial t} \quad j = 1, 2, \ldots n
\]

Equations 2.32-2.36 are substituted into equation 2.27, to obtain the final rate equation for monodisperse pellet is

\[
(\varepsilon + \frac{\partial q_i}{\partial C_i^p}) \frac{\partial C_i^p}{\partial t} = \frac{15D_k}{R_p^3} \sum_{j=1}^{n} \frac{\partial q_j}{\partial C_j} (C_i^p - \bar{C}_i^p) + \frac{15D_s}{R_p^3} (C_i^p - \bar{C}_i^p)
\]

\[
- \frac{\partial q_i}{\partial T} + \sum_{j=1}^{n} \frac{\partial q_j}{\partial C_j} \frac{\partial C_j}{\partial t}
\]
2.2.4 Bidisperse Pore Diffusion Model for Zeolite

Zeolite sorbents consist of crystals, in the size range of 1-9 μm, which are pelletized with a small amount of binder. Diffusion rate is controlled by the crystals in the zeolite sorbents. The mass balance within a spherical crystal is described as

\[
\frac{\partial q_i}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial q_i}{\partial r})
\]

eq 2.38

The rate of change of \( \bar{q}_i \), the volume average \( q_i \), is

\[
\frac{\partial \bar{q}_i}{\partial t} = \frac{3}{R_p^3} \int \frac{\partial q_i}{\partial t} r_p^2 dr
\]

eq 2.39

which results in

\[
\frac{\partial \bar{q}_i}{\partial t} = \frac{3D_s}{R_p} \left( \frac{\partial q_i}{\partial r} \right)_{r=r_p}
\]

eq 2.40

As before, assuming a parabolic distribution

\[ q_i = E_i + F_i r_p^2 \]

eq 2.41

and

\[ q_i = q_i' \text{ at } r_p = R_p \]

eq 2.42

using surface condition

\[ E_i = q_i' - F_i R_p^2 \]

eq 2.43

by integrating equation 2.41 and using the volume average

\[ F_i = (q_i' - \bar{q}_i) \frac{5}{2R_p^2} \]

eq 2.44

obtain

\[ \left( \frac{\partial q_i}{\partial r} \right)_{r=R_p} = (q_i' - \bar{q}_i) \frac{5}{R_p} \]

eq 2.45

and from equation 4.45 and 2.40,

\[ \left( \frac{\partial \bar{q}_i}{\partial t} \right) = 15D_s / R_p^2 (q_i' - \bar{q}_i) \]

eq 2.46

Assuming the mass transfer resistance between the bulk flow of the bed and the solid is not the limiting resistance of gas diffusion into the solid, \( q_i' \) can be replaced by \( \dot{q}_i \) which is in equilibrium with the bulk flow concentration. Thus,

\[ \frac{\partial \bar{q}_i}{\partial t} = 15D_s / R_p^2 (q_i - \bar{q}_i) \]

eq 2.47
This equation is what Glueckauf (1955) suggested. Eq 4.47 is the basis for the Linear Driving Force approximation model,

\[
\frac{\partial \tilde{q}_i}{\partial t} = k_{\text{ef}} a_s (q_i - \tilde{q}_i)
\]

where \(k_{\text{ef}}\) may be obtained by experimental procedure and \(a_s\) is the interfacial surface area.

### 2.2.5 Two Dimensional Adsorption Mathematical Model

For a packed bed the porosity varies with distance from the wall. Near the wall the porosity is higher than the bulk of the bed. This increases the permeability. A few particles away from the wall, the porosity equals the free stream value (Benenati, 1962; Roblee, 1958). As a consequence of the porosity increase in the vicinity of the wall, the velocity of the flow parallel to the wall increases as the wall is approached and goes through a maximum before it decreases to zero (to satisfy the no-slip condition). In general this leads to a net increase in flux, i.e., to the phenomenon called channeling (Nield and Bejan, 1992). During the experimental portion of this study (see Sect. 4.3.1), the effect of channeling was found to be significant for the intended final application of this model. As a result, the effect on momentum, energy, and material balances was considered to be important enough to require the development of a two-dimensional packed bed model.

#### 2.2.5.1 Mass Equation

\[
\frac{\partial C_i}{\partial t} = D_{\text{eff},x} \frac{\partial^2 C_i}{\partial x^2} - \frac{\partial (u_i C_i)}{\partial x} + D_{\text{eff},r} \frac{\partial}{\partial r} \left( r \frac{\partial C_i}{\partial r} \right) - \frac{(1 - \epsilon)}{\epsilon} \frac{\partial C_i}{\partial r}
\]

**Boundary / Initial Conditions**

for \(t < 0\) \(C_i = C_{i,0}\) for \(0 \leq x \leq L\) and \(0 \leq r \leq R\)

for \(t \geq 0\) \(C_i = C_{i,x=0}\) at \(x = 0\) and \(0 \leq r \leq R\)

for \(t \geq 0\) \(\frac{\partial C_i}{\partial x} = 0\) at \(x = L\) and \(0 \leq r \leq R\)

for \(t \geq 0\) \(\frac{\partial C_i}{\partial r} = 0\) at \(r = 0\) and \(r = R\)
2.2.5.2 Gas Phase Energy Equation

\[
\rho_s C_p \frac{\partial T_s}{\partial t} = k_{r,s} \frac{\partial^2 T_s}{\partial x^2} - \frac{\partial u T_s}{\partial x} + \frac{k_{r,s}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_s}{\partial r} \right) - \frac{1}{\varepsilon} h_s a_s (T_s - T_\infty)
\]

Boundary / Initial Conditions

at \( t < 0 \), \( T_s = T_{s,0} \) for \( 0 \leq x \leq L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( T_s = T_{s,0} \) for \( x = 0 \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T_s}{\partial x} = 0 \) for \( x = L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T_s}{\partial r} = 0 \) at \( r = 0 \) for \( 0 \leq x \leq L \)

at \( t \geq 0 \), \( k_{r,s} \frac{\partial T_s}{\partial r} = h_w (T_w - T_s) \) at \( r = R \) for \( 0 \leq x \leq L \)

2.2.5.3 Solid Phase Energy Equation

\[
\rho_s C_p \frac{\partial T_s}{\partial t} = k_{r,s} \frac{\partial^2 T_s}{\partial x^2} + \frac{k_{r,s}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_s}{\partial r} \right) + h_s a_s (T_s - T_\infty) + \sum_{i=1}^{n} \Delta H_i \frac{\partial \dot{q}_i}{\partial t}
\]

Boundary / Initial Condition

at \( t < 0 \), \( T_s = T_{s,0} \) for \( 0 \leq x \leq L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( T_s = T_{s,0} \) for \( x = 0 \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T_s}{\partial x} = 0 \) for \( x = L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T_s}{\partial r} = 0 \) at \( r = 0 \) and \( r = R \) for \( 0 \leq x \leq L \)

Rate of adsorption, \( \frac{\partial \dot{q}_i}{\partial t} \), can be substituted in the above equation either by 2.36 or 2.41. It depends on the adsorbent material. If it is monodisperse or bidisperse type of pellet equation 2.36 or 2.41 will be used, respectively.

2.2.5.4 Column Wall Energy Equation

\[
\rho_c C_p\frac{\partial T_w}{\partial t} = 2\pi R_s h_w (T_s - T_w) - 2\pi R_w h_s (T_w - T_s)
\]

Initial Condition

at \( t < 0 \), \( T_w = T_{w,0} \)

eq 2.52
2.2.5.5 Bed Energy Equation Based On Effective Conductivity

\[
(\varepsilon \rho_s c_p + (1-\varepsilon)\rho_a c_p) \frac{\partial T}{\partial t} = \varepsilon k_{\text{eff},r} \frac{\partial^2 T}{\partial x^2} + \varepsilon \frac{k_{\text{eff},r}}{r} \frac{\partial}{\partial r} (r \frac{\partial T}{\partial r}) - \varepsilon u \rho_s c_p \frac{\partial T}{\partial x} + (1-\varepsilon) \sum_{i=1}^{n} \Delta H_i \frac{\partial q_i}{\partial t}
\]

Boundary / Initial Condition

at \( t < 0 \), \( T = T_i \) for \( 0 \leq x \leq L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( T = T_{\text{out}} \) for \( x = 0 \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T}{\partial x} = 0 \) for \( x = L \) and \( 0 \leq r \leq R \)

at \( t \geq 0 \), \( \frac{\partial T}{\partial r} = 0 \) at \( r = 0 \) for \( 0 \leq x \leq L \)

at \( t \geq 0 \), \( k_{\text{eff},r} \frac{\partial T}{\partial r} = h_w (T_w - T_{\text{in},r}) \) for \( r = R \)

2.2.5.6 Momentum Equation

The governing momentum equation for fully developed flow in cylindrical beds is, from Vafai and Tien (1982).

\[
\frac{\partial P}{\partial x} = -\rho_a u^2 \frac{\mu}{K} u + \frac{1}{\mu} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right),
\]

Boundary Conditions

\[
u = -\frac{K}{m} \frac{\partial P}{\partial x} \text{ at } r = 0 \text{ and } u = 0 \text{ at } r = R,
\]

where \( \epsilon \) is the bed porosity, and \( K \) and \( C \) are the permeability and inertial coefficient which depend on the porosity and the type of porous materials. In the above equation, the second term is the inertial effect which accounts for additional pressure drop resulting from interpore mixing found at higher Reynolds numbers (Vafai, 1981; Ergun, 1952). The third term is the Darcian force representing the pressure loss due to the presence of solid particles. The last term is the viscous shear force representing the resistance to the flow caused by shear stress along the solid boundary. This term accounts for the no-slip boundary condition at the solid boundary. In this study the entrance effect is not considered since the flow is fully developed after one to two particle distance from the entrance (Vafai and Tien, 1981).

2.2.6 Porosity Variation

\[
\epsilon = \epsilon_\infty [1 + a \exp(-by/d_p)]
\]

where \( \epsilon_\infty \) is the free-stream porosity, \( y \) is the distance from the wall, \( d \) is the particle diameter, and \( a \) is taken to be 1.4 (Nield and Bejan, 1992). \( b \) is an experimental parameter that depends on packing and particle size and it varies from 2 to 8.
The empirical coefficients $K$ and $C$ are given by the relations developed by Ergun (1952) for flow in a packed bed:

$$K = \frac{d_p^2 \varepsilon^3}{150(1-\varepsilon)^2}$$

$$C = \frac{1.75(1-\varepsilon)}{d_p \varepsilon^3}$$

The variables $C$ and $K$ are both functions of the bed porosity and particle diameter, $d_p$. The porosity in a packed bed increases from the center of bed, free-stream porosity, to a maximum of one at the bed-wall boundary. This increase is confined to a few particle diameters from the wall (Benenati, 1962; Roblee, 1958).

In the above two dimensional equations, the term which represents the radial diffusion is

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right)$$

where $C$ varies with $r$. Carrying out the derivative

$$\frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial r^2}$$

At the center where $r=0$, the first term is not finite. But

$$\lim_{r \to 0} \left( \frac{1}{r} \frac{\partial C}{\partial r} \right) = \frac{\partial^2 C}{\partial r^2}$$

by L'Hopital's rule. Therefore the term, eq 2.58, in 2-dimensional form for the center point is replaced by

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) = 2 \frac{\partial^2 C}{\partial r^2}$$

Therefore, the diffusional term in the discretized forms of two dimensional PDE's at center grid is replaced by eq 2.61.

### 2.2.7 Calculation Of Thermal Conductivity For 2-D Flow

In this study two different equations were used to calculate the effective conductivity in the packed bed. One is based on the works of Kunii and Smith (1960), and the other one is based on the experimental work of Fahien (1954).

The effective thermal conductivity in the axial and radial direction, $k_{eff,x}$ and $k_{eff,r}$, are related as,

$$k_{eff,x} = k_x + k_{s,x}$$

$$k_{eff,r} = k_r + k_{s,r}$$

These conductivity's can be calculated by the theoretical equations presented below.

### 2.2.7.1 Stagnant Conductivity $k_o$

Kunii and Smith (1960) presented theoretical equations for estimating the stagnant conductivity, $k_o$. The stagnant conductivity can be found if $k_s$, solid thermal conductivity, is given.
\[
\frac{k_r}{k_f} = \varepsilon + (1 - \varepsilon) / \left[ \phi + (2/3)(k_r / k_s) \right]
\]
\[
\text{where } k_f \text{ is the thermal conductivity of fluid and } \phi \text{ is the contribution of solid to solid heat transfer through fluid film around a contacting point of neighboring particles. } \phi \text{ is given by}
\]
\[
\phi = \phi_1 + (\phi_1 - \phi_2) \left[ (\varepsilon - .26)/.216 \right]
\]
\[
\text{for } .476 \geq \varepsilon \geq .26
\]
\[
\phi = \phi_1
\]
\[
\text{for } \varepsilon > .476
\]
\[
\phi = \phi_2
\]
\[
\text{for } \varepsilon < .26
\]
where \( \phi_1 \) and \( \phi_2 \) are given in a schematic form, and are being interpolated linearly in tabular form in the computer program.

2.2.7.2 Effective Radial Conductivity \( k_{r,*} \)

Packed bed thermal conductivity in the radial direction is given by Baron (1952) as

\[
\frac{C_p \rho A}{k_{r,*}} = N_{peu} = 8 - 10
\]

where \( N_{peu} \) is Peclet number, therefore the effective thermal conductivity in the radial direction would be (Yagi and Kunii, 1952).

\[
\frac{k_{r,*}}{k_r} = \frac{k_r}{k_r} + (\alpha \beta)N_{r*} N_{pr}
\]
\[
\text{where } (\alpha \beta) = 1 / N_{peu} = .1 \text{ to } .125
\]

2.2.7.3 Effective Axial Conductivity \( k_{e,*} \)

A similar equation can be derived for effective thermal conductivity in the axial direction, (Yagi, Kunii, and Wakao, 1960).

\[
\frac{k_{e,*}}{k_r} = \frac{k_r}{k_r} + \lambda N_{r*} N_{pr}
\]
\[
\text{where } \lambda = .5 \text{ to } 1.0
\]

In the above equations, the radial and axial conductivity are the combination of two terms. The first term is the stagnation conductivity, which varies from a bulk conductivity to fluid conductivity with distance from the center to the column wall. Therefore, it depends on the porosity variation which also is a function of bed parameters. The second term is due to the dynamic or dispersion conductivity which incorporates the mixing caused by flow through the particles. Incorporating the effects of porosity variation into the effective conductivity, the effective conductivity reduces to (Hunt, 1987)
\[
\frac{k_{\text{eff},r}}{k_r} = (1 + a^r \exp(-bR)) \frac{k_r}{k_r} + (\alpha \beta) \frac{l(R)}{d} N_{Re_r} N_{Pr}
\]

where \((\alpha \beta) = 1 / N_{Re_r} = .1 \text{ to } .15\) \hspace{1cm} \text{eq 2.68}

and in the axial direction

\[
\frac{k_{\text{eff},x}}{k_r} = (1 + a^x \exp(-bR)) \frac{k_r}{k_r} + \lambda \frac{l(R)}{d} N_{Re_r} N_{Pr}
\]

where \(\lambda = .5 \text{ to } 1.0\) \hspace{1cm} \text{eq 2.69}

where \(a^r\) is chosen such that \(k_r/k_f\) equals one at the wall as velocity becomes zero. The variation of dispersion, mixing length, is

\[
\frac{l(R)}{d} = R_i / R_i - r / R_i \text{ for } R_i - r \leq 1
\]

where \(R_i\) is tube diameter. An expression similar to porosity variation was used to predict the mixing length variation (Hunt, 1987).

### 2.2.8 Calculation Of Mass Diffusivity For 2-D Flow

A similar theoretical approach can be taken for the calculation of mass diffusivity in the radial and axial direction as that used for thermal diffusivity in the previous section.

#### 2.2.8.1 Effective Diffusivity

Effective diffusivity follows the same expression as in thermal conductivity:

\[
D_{\text{eff},x} = D_r + D_{r,x}
\]

\[
D_{\text{eff},r} = D_r + D_{r,r}
\]

\hspace{1cm} \text{eq 2.71}

#### 2.2.8.2 Effective Radial Diffusivity \(D_{r,r}\)

The effective diffusivity in the radial direction by analogy to heat transfer is:

\[
\frac{D_{\text{eff},r}}{D_r} = \frac{D_r}{D_r} + (\alpha \beta) N_{Re_r} N_{Sc},
\]

where \((\alpha \beta) = 1 / N_{Re_r} = .1 \text{ to } .125.\) \hspace{1cm} \text{eq 2.72}

#### 2.2.8.3 Effective Axial diffusivity \(D_{\text{eff},x}\)

A similar equation can be derived for effective diffusivity in the axial direction:

\[
\frac{D_{\text{eff},x}}{D_r} = \frac{D_r}{D_r} + \lambda N_{Re_r} N_{Sc},
\]

where \(\lambda = .5 \text{ to } 1.0.\) \hspace{1cm} \text{eq 2.73}
Incorporating the effects of porosity variation into the effective diffusivity, the effective diffusivity reduces to (Hunt, 1987),

\[
\frac{D_{e,rr}}{D_r} = (1 + a' \exp(-bR)) \frac{D_r}{D_r} + (\alpha \beta) \frac{I(R)}{d} N_{rs}, N_{sc},
\]

where \((\alpha \beta) = 1/N_{rs} = .1\) to \(.125.\) \(eq\ 2.74\)

and in the axial direction,

\[
\frac{D_{e,zz}}{D_z} = (1 + a' \exp(-bR)) \frac{D_z}{D_z} + \lambda \frac{I(R)}{d} N_{rs}, N_{sc},
\]

where \(\lambda = .5\) to \(1.0.\) \(eq\ 2.75\)

### 2.2.9 Effective Radial Thermal Conductivity Based on Fahien Equations

In contrast to weak effect of mass diffusion on radial mass fraction, the thermal conductivity profile has a strong effect on both temperature and mass adsorption. A thermal conductivity profile for different ratio of \(d_p/d_t\) was approximated by Fahien (1954),

\[
k_{e,rr} = \langle k \rangle (k^*_0 + 3(k^*_0 - k^*_w) \frac{r^2}{r_M^2} + 2(k^*_0 - k^*_w) \frac{r^3}{r_M^3}) \quad 0 \leq r \leq r_M
\]

\[
k_{e,rr} = \langle k \rangle (k^*_0 - (k^*_M - k^*_w) \frac{r - r_M}{1 - r_M}) \quad r > r_M
\]

\[
k^*_M = \frac{3.0 - 9k^*_0 r_M^2 - k^*_w r_M^3 - 3r_M^2 + 2}{1 - r_M}
\]

\[
r_M = 1 - \frac{2}{\alpha}
\]

\[
\alpha = d_t / d_p
\]

\(eq\ 2.76\)

where \(k^*_0\) is the effective radial conductivity at the center of the column wall, \(k^*_M\) is the maximum effective thermal conductivity, \(k^*_w\) is the effective thermal conductivity near the wall, \(\langle k \rangle\) is the average effective thermal conductivity, and \(r_M\) is the location of maximum in conductivity profile. These conductivity's are obtained by Argo and Smith (1953) equation using the void fraction values as a function of radial position. According to Argo and Smith

\[
k_{e} = \varepsilon \left[ k_s + \frac{d_t C_{mG}}{N_{rs}} + 4 \left( \frac{\sigma}{2 - \sigma} \right) d_p (0.173)(T_s^{3/100^4}) \right] + (1 - \varepsilon) \frac{h k_s d_p}{2 k_s + h d_p}
\]

\(eq\ 2.78\)

where \(\sigma\) is the emissivity of the solid particle, \(T_s\) is the average temperature. In the above equation,

\[
h = h_c + h_r + h_p
\]

\(eq\ 2.79\)
\[ h_c = 1.95C_{pg}G N_{Re}^{-0.5}N_{Re} < 350 \]
\[ h_c = 1.06C_{pg}G N_{Re}^{-0.4}N_{Re} > 350 \]  
\[ \text{eq } 2.80 \]

\[ h_r = \frac{k_r(2k_s + h_d)}{d_p k_s} \]
\[ k_r = 4\left(\frac{\sigma}{2 - \sigma}\right)d_p (0.173) \left(\frac{T_s^3}{100^4}\right) \]
\[ \text{eq } 2.81 \]

\[ h_p = \frac{k_p(2k_s + h_d)}{d_p k_s} \]
\[ \log_{10} k_p = 1.76 + 0.0129k_s/\sigma \]  
\[ \text{eq } 2.82 \]

2.2.10 Effective Radial Diffusivity Based on Fahien Equations

\[ D_{eff, r} = \begin{cases} < D > (D_0^* + 3(D_M^* - D_0^*)r^2 + 2(D_M^* - D_0^*)r^3) & 0 \leq r \leq r_M \\ < D > (D_M^* \frac{r - r_M}{1 - r_M}) & r > r_M \end{cases} \]
\[ \text{eq } 2.83 \]

\[ D_M^* = \frac{3.0 - 9D_0^*r_M^2}{1 + r_M + 1.1r_M^2} \]

\[ D_0^* \] is obtained from work of Fahien and Smith (1955) to be

\[ D_0^* = \frac{9}{8V_o(1 + 4.85\alpha^{-2})} \]  
\[ \text{eq } 2.84 \]

where \( V_o \) is velocity at the center of packed bed.

2.2.11 Heat Transfer Coefficient Between Wall Surface and Packed Bed, \( h_w \)

The effective thermal conductivity in the wall layer of thickness \( R_p = d_p/2 \), \( k_{ew} \), is defined and \( h_w \) is considered as a correction factor based on the difference \( k_{eff, r} \) and \( k_{ew} \) (Kunii and Suzuki, 1966).

\[ \frac{k_{ew}}{k_f} = \frac{k_{ew}}{k_f} + \frac{1}{\alpha_w N_{Pr} N_{Re}} + \frac{1}{h_w d_p / k_f} \]  
\[ \text{eq } 2.85 \]

where \( \alpha_w \) denotes the contribution of fluid mixing in the wall layer and is taken as 0.2. \( h_w \) represents the heat transfer coefficient of the thermal boundary layer which develops on the wall.
surface. This becomes dominant at high $N_{Re,p}$ and is given by Blasius type equation as (Suzuki, 1990),

$$
\frac{h'_{f}d_{p}}{k_{r}} = C\left(N_{Pr}^{1/3}N_{Re,p}^{3/4}\right)
$$

where $C$ is an experimental coefficient with value of 0.1 to 0.2 (Kunii, Suzuki and Ono, 1968).

$k_{ew0}$ is obtained by the following equation similarly to eq (2.65).

$$
\frac{k_{ew0}}{k_{f}} = \varepsilon_{w} + (1 - \varepsilon_{w})/\left[\phi_{w} + (2/3)(k_{f}/k_{s})\right]
$$

where $\varepsilon_{w}$ denotes void fraction in the wall layer of about 0.7.
SECTION 3
NUMERICAL ANALYSIS

The solution of nonequilibria adsorption/desorption problems must be solved numerically. For an n component mixture, the numerical model would involve the solution of several coupled differential equations: n-1 mass balances equations, n mass balances of rate equations, n equilibrium isotherms, one total mass balance, one momentum equation, one heat balance of fluid flow, one solid phase heat balance, and one heat balance for the wall.

The finite difference technique, which is mostly used for processes with varying boundary and initial conditions, is a convenient method for solving the coupled partial differential equations (PDE's).

In this work, the PDE's were discretized by first or second order differences in time and spatial dimensions. The set of discretized finite difference equations were solved simultaneously by an implicit method. At first, based on the stiffness and the sharpness of the momentum equation and the mass and heat transfer fronts, two different implicit numerical methods were used to simulate the dynamic behavior of the packed bed. For adsorption and flow-through desorption of one and two dimensions, the implicit-iterative method of under relaxation was used. For vacuum desorption, since the convergence of equations are difficult to achieve because of the steep gradient of pressure drop in the packed bed, a more rigorous method had to be used. The implicit method of Newman (1968, 1967) was used to simulate the vacuum desorption process. Later, during the development of the numerical computation, it appeared that the use of Newman method for all the processes reduced the required CPU time and resulted in more stable discretized PDE's.

3.1 The Discrete Numerical Equations

The spatial dimension was discretized using first or second order backward, forward or central differencing depending on the stability of PDE. For instance, having C as a variable, the spatial finite differences for three cases are:

\[
\frac{\partial C^n}{\partial x} = \frac{C^n_{i+1} - C^n_i}{\Delta x} + O(\Delta x) \quad \text{Backward difference}
\]

\[
\frac{\partial C^n}{\partial x} = \frac{C^n_i - C^n_{i-1}}{\Delta x} + O(\Delta x) \quad \text{Forward difference}
\]

\[
\frac{\partial C^n}{\partial x} = \frac{C^n_{i+1} - 2C^n_i + C^n_{i-1}}{2\Delta x} + O(\Delta x^2) \quad \text{Central difference}
\]

\[
\frac{\partial^2 C^n}{\partial x^2} = \frac{C^n_{i+1} - 2C^n_i + C^n_{i-1}}{\Delta x^2} + O(\Delta x^2) \quad \text{Central difference}
\]

The backward finite difference was used in time:

\[
\frac{\partial C_i^{n+1}}{\partial t} = \frac{C_i^{n+1} - C_i^n}{\Delta t} + O(\Delta t)
\]

eq 3.2
3.1.1 Discretized Spatial Finite Difference With Unequal Grid Size

Figure 3.1 shows a situation in which adjacent grids are not the same size. This type of grid spacing was used out in the radial direction in solving the PDE's. To establish the finite difference for the first and second derivatives, Taylor series expansion in powers of \((f\Delta x)\) and \((-\Delta x)\) were used, giving

\[
C_A = C_{i,j} + (f\Delta x) \left. \frac{\partial C}{\partial x_{i,j}} \right|_{i-1,j} + \frac{(f\Delta x)^2}{2!} \left. \frac{\partial^2 C}{\partial x^2_{i,j}} \right|_{i,j} + O(f\Delta x)^3
\]

\[
C_{i-1,j} = C_{i,j} - (\Delta x) \left. \frac{\partial C}{\partial x_{i,j}} \right|_{i-1,j} + \frac{(\Delta x)^2}{2!} \left. \frac{\partial^2 C}{\partial x^2_{i,j}} \right|_{i,j} + O(\Delta x)^3
\]

Equation 3.3

Eliminating \(\left. \frac{\partial C}{\partial x_{i,j}} \right|\) between these equations,

\[
\frac{\partial^2 C}{\partial x^2} = \frac{2}{(\Delta x)^2} \left[ \frac{C_A}{f(1+f)} + \frac{C_{i-1,j}}{(1+f)} - \frac{C_{i,j}}{f} \right]
\]

Equation 3.4

If \(\left. \frac{\partial T}{\partial x_{i,j}} \right|\) is eliminated between eqs 3.3 and 3.4 then

\[
\frac{\partial C}{\partial x} = \frac{1}{(\Delta x)} \left[ \frac{C_A}{f(1+f)} - \frac{f}{(1+f)} C_{i-1,j} - \frac{(1-f)}{f} C_{i,j} \right]
\]

Equation 3.5

with an error of the order of \((\Delta x)^2\).

\[
\begin{array}{c}
i,j \\
\hline
\Delta x & f\Delta x & A \\
\hline
i-1,j & i,j & i+1,j
\end{array}
\]

FIGURE 3-1 SHOWS THE GRIDS WITH DIFFERENT SIZES
3.2 Discretized Partial Differential Equations (PDE's)

Using the approximated values of first and second order derivatives in PDE's, the discretized forms of PDE's for one-dimensional flow will be generated for numerical solution. Theses approximated equations will be solved by the methods mentioned above.

3.2.1 Discretized Component Mass Balance:

\[ \frac{\partial C_i}{\partial t} = D_i \frac{\partial^2 C_i}{\partial x^2} - u \frac{\partial C_i}{\partial x} - \frac{1 - \varepsilon}{\varepsilon} \frac{\partial q}{\partial t} \]

Inserting the finite difference approximations:

\[ \frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D_i \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{(\Delta x)^2} - u_{j}^{n+1} \frac{C_{i,j}^{n+1} - C_{i,j-1}^{n+1}}{\Delta x} - \frac{1 - \varepsilon}{\varepsilon} f_{i,j}^{n+1} \]

collecting \( C_{i,j}^{n+1} \) terms

\[ A = \frac{1}{\Delta t} + \frac{2D_i}{\Delta x^2} + \frac{u_j^{n+1}}{\Delta x} \]

solving for \( C_{i,j}^{n+1} \) and applying under - relaxation method

\[ C_{i,j}^{n+1} = C_{i,j}^{n} + \omega \left( -C_{i,j}^{n} + \frac{1}{A} \left( \frac{C_{i,j}^{n}}{\Delta t} + D_i \frac{C_{i,j+1}^{n+1} + C_{i,j-1}^{n+1}}{(\Delta x)^2} + u_{j}^{n+1} \frac{C_{i,j}^{n+1} - C_{i,j-1}^{n+1}}{\Delta x} - \frac{1 - \varepsilon}{\varepsilon} f_{i,j}^{n+1} \right) \right) \]

3.2.2 Discretized Gas Phase Energy

\[ \rho_{g} c_{ps} \frac{\partial T_{s}}{\partial t} = k_{s} \frac{\partial^2 T_{s}}{\partial x^2} - u_{j} \rho_{g} c_{ps} \frac{\partial T_{s}}{\partial x} + \frac{1 - \varepsilon}{\varepsilon} h_{s} a_{s} (T_{s} - T_{w}) - \frac{4h_{w}}{\varepsilon d} (T_{s} - T_{w}) \]

Inserting the finite difference approximation

\[ \frac{T_{s,j}^{n+1} - T_{s,j}^{n}}{\Delta t} = k_{s} \frac{T_{s,j+1}^{n+1} - 2T_{s,j}^{n+1} + T_{s,j-1}^{n+1}}{(\Delta x)^2} - u_{j}^{n+1} \rho_{g} c_{ps} \frac{T_{s,j}^{n+1} - T_{s,j-1}^{n+1}}{\Delta x} + \frac{1 - \varepsilon}{\varepsilon} h_{s} a_{s} (T_{s,j}^{n+1} - T_{s,j}^{n}) - \frac{4h_{w}}{\varepsilon d} (T_{s,j}^{n+1} - T_{w,j}^{n+1}) \]

collecting \( T_{s,j}^{n+1} \) terms

\[ A = \frac{\rho_{g} c_{ps}}{\Delta t} + \frac{2k_{s}}{(\Delta x)^2} + \frac{u_{j}^{n+1} \rho_{g} c_{ps}}{\Delta x} + h_{s} a_{s} \frac{1 - \varepsilon}{\varepsilon} T_{s,j}^{n+1} + \frac{4h_{w}}{\varepsilon d} T_{s,j}^{n+1} \]

solving for \( T_{s,j}^{n+1} \) and applying under - relaxation method

\[ T_{s,j}^{n+1} = T_{s,j}^{n} + \omega \left( T_{s,j}^{n} + \frac{1}{A} \left( \frac{\rho_{g} c_{ps}}{\Delta t} + k_{s} \frac{T_{s,j+1}^{n+1} + T_{s,j-1}^{n+1}}{(\Delta x)^2} + u_{j}^{n+1} \rho_{g} c_{ps} \frac{T_{s,j}^{n+1} - T_{s,j-1}^{n+1}}{\Delta x} + h_{s} a_{s} \frac{1 - \varepsilon}{\varepsilon} T_{s,j}^{n+1} + \frac{4h_{w}}{\varepsilon d} T_{w,j}^{n+1} \right) \right) \]
3.2.3 Discretized Solid Phase Energy Equation

\[
\rho_c c_w \frac{\partial T_s}{\partial t} = k_x \frac{\partial^2 T_s}{\partial x^2} + h_s a_s (T_s - T_w) - \sum_{i=1}^{n} \Delta H_i \frac{\partial q_i}{\partial t} \quad \text{eq 2.12}
\]

\[
\rho_c c_w \frac{T_{s+1}^j - T_s^j}{\Delta t} = k_x \frac{T_{s+1}^{j+1} - 2T_{s}^{j+1} + T_{s}^{j+1}}{(\Delta x)^2} + h_s a_s (T_{s+1}^j - T_{s}^j) - \sum_{i=1}^{n} \Delta H_i r_{i+1}^j
\]

collecting \( T_{s+1}^j \) terms

\[
A = \frac{\rho_c c_w}{\Delta t} + \frac{2k_x}{(\Delta x)^2} + h_s a_s T_{s+1}^j
\]

solving for \( C_{i+1}^j \) and applying under-relaxation method

\[
T_{s+1}^j = T_s^j + \omega \left( -T_s^j + \frac{1}{A} \left( \frac{\rho_c c_w}{\Delta t} T_{s+1}^j + k_x \frac{T_{s+1}^{j+1} - T_{s}^{j+1}}{(\Delta x)^2} + h_s a_s T_{s+1}^j - \sum_{i=1}^{n} \Delta H_i r_{i+1}^j \right) \right)
\]

3.2.4 Discretized Column Wall Equation

\[
\rho_w c_p \frac{\partial T_w}{\partial t} = 2\pi R_h w (T_s - T_w) - 2\pi R_h h_s (T_w - T_s) \quad \text{eq 2.13}
\]

\[
\rho_w c_p \frac{T_{w+1}^j - T_w^j}{\Delta t} = 2\pi R_h w (T_{s+1}^j - T_{w+1}^j) - 2\pi R_h h_s (T_{w+1}^j - T_{w+1}^j)
\]

Collecting \( T_{w+1}^j \) terms

\[
A = \frac{\rho_w c_p}{\Delta t} + 2\pi R_h w T_{w+1}^j + 2\pi R_h h_s T_{w+1}^j
\]

\[
T_{w+1}^j = T_w^j + \omega \left( -T_w^j + \frac{1}{A} \left( \frac{\rho_w c_p}{\Delta t} T_{w+1}^j + 2\pi R_h w T_{w+1}^j + 2\pi R_h h_s T_{w+1}^j \right) \right)
\]

3.2.5 Discretized Total Material Equation

The total pressure equation was solved numerically using Newman's method.

\[
\frac{\partial P}{\partial t} = D_l \frac{\partial^2 P}{\partial x^2} - u \frac{\partial P}{\partial x} - P \frac{\partial u}{\partial x} + P \left( \frac{\partial T}{\partial t} - D_l \frac{\partial^2 T}{\partial x^2} + u \frac{\partial T}{\partial x} \right) - RT \frac{1 - \varepsilon}{\varepsilon} \sum_{i=1}^{n} \frac{\partial q_i}{\partial t} \quad \text{eq 2.10}
\]

\[
F = -\frac{P_{s+1}^j - P_s^j}{\Delta t} + D_l \frac{P_{s+1}^{j+1} - 2P_{s+1}^j + P_s^j}{(\Delta x)^2} - u \frac{P_{s+1}^j - P_{s+1}^j}{\Delta x} - P \frac{u_{s+1}^j - u_{s+1}^j}{\Delta x} + \frac{u_{s+1}^j}{\Delta x} \quad \text{eq 3.10}
\]

\[
\frac{p_{s+1}^j}{T_{s+1}^j} \left( \frac{T_{s+1}^j - P_{s+1}^j}{\Delta t} - D_l \frac{T_{s+1}^{j+1} - 2T_{s+1}^j + T_{s+1}^j}{(\Delta x)^2} + u \frac{T_{s+1}^j - T_{s+1}^j}{\Delta x} \right) - RT \frac{1 - \varepsilon}{\varepsilon} \sum_{i=1}^{n} r_{i+1}^j
\]
3.2.6 Discretized Momentum Equation

The momentum equation was solved numerically by Newman's method.

\[
\frac{dP}{dx} = -\frac{\mu}{K} u_p - \rho Cu^2
\]

\[
F_2 = \frac{p_{n+1} - p_n}{\Delta t} + \frac{\mu}{K} u_{n+1} + \rho Cu_{n+1}^2
\]

3.2.7 Discretized Boundary Condition

In this study most of the boundary conditions are the homogeneous boundary type. In this type of boundary condition the normal derivative of variables such as temperature, velocity, and concentration at the boundary surface vanishes,

\[
\frac{\partial C}{\partial x} = 0
\]

where C is any variable.

The boundary conditions for all the PDE's were discretized by extending the region at boundaries a distance \( \Delta x \) so that there is an imaginary y node at \( j-1 \) or at \( j+1 \) at the inlet or outlet of the column, respectively. Equation 3.13 can be discretized as,

\[
\frac{C_{j+1} - C_{j-1}}{2\Delta x} = 0
\]

This equation can be solved for \( C_{j+1} \) or \( C_{j-1} \) and to be substituted in the original PDE equation for the imaginary node.

A second type boundary condition, where there is a linear combination of the variable and its normal derivative at the boundary surface, such as boundary surface at the column wall,

\[
k \frac{\partial T}{\partial x} + hT = hT_w
\]

where \( k \) is conductivity, \( T \) is fluid temperature, \( h \) is connective coefficient, and \( T_w \) is the wall temperature. Eq 3.15 can be discretized as,

\[
\frac{T_{j+1} - T_{j-1}}{2\Delta x} + hT_j = hT_w
\]

This equation can be solved for \( T_{j-1} \) and to be substituted in the original PDE equation for the imaginary node.
3.3 Numerical Approach

For each interior grid point, a set of algebraic equations as given above results when finite differences are used to approximate the PDE’s. These system of simultaneous equations may be written in a general matrix form as

$$[A][\phi] = [F] \tag{3.17}$$

where $[A]$ is a square matrix, $[\phi]$ is a column vector containing unknown nodal values of $\phi$, and $[F]$ is the column vector containing the source and the prescribed boundary conditions. From linear algebra, we know that the unique solutions of the above equation exist when the determinant of $[A]$ is nonzero.

An approach to the solution of eq. 3.17 is by using iterative methods. Iterative methods start from a guessed initial field, and sequentially improve the field by using successive iterations until eq 3.13 is satisfied. When the most recent values of the iterate are used, the Gauss-Seidel method results. Iteration can be enhanced by extrapolating the Gauss-Seidel improvement. This technique is called relaxation method (Gerald and Wheatley, 1984), for the case of a simple steady-state one-dimensional diffusion equation:

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{Q}{k} = 0$$

the finite difference approximation will be

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + \frac{Q_i}{k} = 0$$

using the Guess-Siedel method

$$\phi_i^{n+1} = \frac{1}{2}(\phi_{i+1}^n - \phi_{i-1}^n + \Delta x^2 \frac{Q_i}{k})$$

implementing the relaxation method the above equation becomes

$$\phi_i^{n+1} = \frac{\omega}{2}(\phi_{i+1}^n - \phi_{i-1}^n + \Delta x^2 \frac{Q_i}{k}) + (1 - \omega)\phi_i^n \tag{3.18}$$

where $n$ indicates successive iteration, and $\omega$ is called the relaxation factor. Iterative convergence is achieved with $0 < \omega < 2$; $\omega = 1$ correspond to Gauss-Seidel iteration; $0 < \omega < 1$; to successive under-relaxation (SUR); and $1 < \omega < 2$; to successive over-relaxation (SOR). A best, or optimum, value of $\omega$ can be found from numerical test or from analysis. In this study, since the equations are coupled and non linear, the value of $\omega$ was found by numerical test to be between .2 to .5 depending on the stiffness of the PDE.

In the case of vacuum desorption process, because of steep gradients in the pressure front and the velocity equation, the SOR method was not a suitable choice for solving the PDE’s system. Instead, a different numerical method which is more stable and where the radius of convergence is higher was used. This method is lengthy and explained in detail by Newman (1968, 1967). In short, the set of PDE’s are linearized by Newton method resulting in a system of tridiagonol matrix results which can be solved by any ordinary technique. The time of convergence for
Newman method is longer for a given time step but the grid points are three times larger and the time step is up to an order of magnitude larger than SOR.

3.4 Convergence And Stability Of Numerical Techniques

The examination of convergence or the rate of convergence of the numerical methods used in this study relied on actual testing of the iterative methods. Since the set of equations are coupled and nonlinear, the analytical procedure for determination of convergence can not be used. By extensive trial and error of SOR method, the approximated equations were stable for $\omega$ up to 0.5. The component mass balance equations were stable for a wide range of $\omega$ close to 0.5, except for the PDE for H$_2$O component because of the high affinity of zeolite for water. The heat balance equations were also stable for a wide range of $\omega$ close to 0.5. Keeping $\omega$ constant at these values, the number of grids for a bed 20 inches long bed were 75 for CO$_2$ and 150 for water in single component adsorption. The time step ranged from 7 to 18 seconds. In multi-component adsorption the limiting value is determined by what the H$_2$O component was in the single component adsorption case.

In Newman's method, the number of grids could be reduced to 50 and time step increased to as large as 60 seconds. In both methods the iteration was stopped if $(C^{n+1} - C^n)/C^{n+1}$ was less than 1.0E-4 for each grid point. This error criteria was chosen because the difference in two consecutive iteration was less than 1.0e-5 for a gas phase concentration of 1.0e-10. For the first few steps, the number of iterations is large but it decreases to a minimum of 20 to 50 after that.

The stability and the rate of convergence in these PDE's are mostly affected by the rate of adsorption which is related to the isotherms. The second most important criteria is the diffusion coefficients. The implementation of diffusion coefficients makes the PDE's parabolic and in turn causes the equations to be more stable, preventing any initial error from propagating in time.
SECTION 4
COMPUTER MODEL VERIFICATION

4.1 Test Apparatus

Verification of the numerical models is accomplished with test data from the Molecular Sieve Material Bench Test (MSMBT), a Marshall Space Flight Center apparatus. The MSMBT was designed to capture the dynamic adsorption and desorption characteristics of sorbent materials to be used in the International Space Station 4BMS for a range of CO$_2$ and H$_2$O partial pressures. The test apparatus consists of a small packed column 2 inches in diameter and 10 or 20 inches long, depending on the configuration. Instrumentation of the column includes temperature probes and sampling tubes for measurement at sorbent material endpoints and intermediate points. Continuous measurements of the exit CO$_2$ and H$_2$O partial pressures, and all temperatures, are recorded. A gas chromatograph is used to capture the breakthrough at interior bed locations. The MSMBT is fully described elsewhere (Knox, 1992; Mohamadinejad, 1994). Any significant changes made in the test configuration will be discussed in the following sections as appropriate.

The MSMBT is used to obtain data empirically that is not available otherwise or not reliable in the open literature, such as heat of adsorption and lumped mass transfer coefficients. Testing to obtain empirical data is performed in such a way as to isolate the phenomenon of interest as much as possible. Heat transfer coefficients, (not available otherwise due to the use of unique NASA foam insulation for superior adiabatic conditions) for example, were obtained by flowing dry, heated nitrogen through a sorbent bed desorbed in the presence of nitrogen.

The second use of the MSMBT is to verify, following determination of empirical values, the accuracy of the model under conditions similar to those expected in the ISSA. This consists of comparing a series of MSMBT runs at varying conditions to the results of the computer model ran at the same conditions. Of special interest is the capability of the model to predict transient bed temperature and partial pressure for conditions not used to obtain the empirical values.

4.2 Thermal Characterization with Inert Gas Heating

In order to approach adiabatic conditions during adsorption and strip desorption testing, three layers of high performance insulation are used on the column. The inner layers are commercially available felt insulation. A third layer of spray-on foam specifically designed for the Space Transportation System External Tank was added to improve heat retention. However, thermal characteristics were not available for the foam insulation. In order to obtain coefficients for the transfer of heat from the outside (ambient air) through the three layers of insulation to the canister wall (H_OW) and from the carrier gas, or fluid, to the canister wall (H_FW), a test using heated nitrogen gas was conducted.

To simulate the inert gas heating test, the bed inlet temperature measured during the test was curve fit and applied as an input to the computer model. Bed inlet volumetric flow rate was calculated based on the ideal gas law.
4.2.1 Molecular Sieve 5A

Specifications for the thermal characterization test with molecular sieve 5A are shown in Figure 4-1. Volumetric flow rate is required as a model input. This is calculated based on the flow controller rate in standard liters per minute (conditions at point 1) and bed inlet conditions (point 2):

\[ G_2 = \frac{P_2 T_2 G_1}{P_1 T_1} = \frac{14.696}{15.47} \frac{28.04}{535} T_3 \]

eq 4.1

\( P_2 \) (15.47 psia) is the average inlet pressure calculated from test data. Pressure varied less than 0.5% from \( P_2 \) during the test. \( T_2 \) is the test inlet temperature which has been curve fit for use in the model. \( G_1 \) is the volumetric flowrate.

![Thermal Characterization Data Sheet](image)

**FIGURE 4-1 5A THERMAL CHARACTERIZATION TEST SPECIFICATIONS**

4.2.1.1 FLOW1MOL Model Thermal Verification

The determination of heat transfer coefficients and verification of the single material flow-through adsorption and desorption model, FLOW1MOL, is described in this section.

Variations of the heat transfer coefficients, \( H_{OW} \) and \( H_{FW} \), were studied with the computer model. Sensitivity to changes in \( H_{OW} \) is shown in Figure 4-2. Sensitivity to changes in \( H_{FW} \) is shown in Figure 4-3. The test data for the bed outlet is shown as "T5 [°F]", while the model output for variations in the heat transfer coefficient is labeled "T gas@5".

The final values selected for \( H_{FW} \) and \( H_{OW} \) were 2.5 and 0.25, respectively. The comparison with test data is shown in Figure 4-4. The test temperatures for the bed inlet, center, and outlet are labeled based on the measuring thermocouple as "T3 [°F]", "T4 [°F]", and "T5 [°F]".
[°F]" respectively. The corresponding model data is labeled based on node point as "gas T 5", "gas T 50", and "gas T 101" respectively.

As shown in Figure 4-4, the FLOW1MOL thermal model can simulate test data very closely with the adjustment of the heat transfer coefficients. To test the model's predictive capabilities, another nitrogen heating test with different flow rate and heater set point should be run. Independent simulation with FLOW1MOL and comparison of results would indicate predictive accuracy.

![Variations of thermal coefficient H_FW](image)

**FIGURE 4-2 VARIATIONS OF H_FW FOR FLOW1MOL**
FIGURE 4-3 VARIATIONS OF H\_OW FOR FLOW1MOL

FIGURE 4-4 FINAL THERMAL VERIFICATION OF FLOW1MOL FOR 5A
4.2.1.2 2DMOL Model Thermal Verification

The determination of heat transfer coefficients and verification of the two-dimensional adsorption and desorption model, 2DMOL, is described in this section. Variations of the heat transfer coefficients, H_OW and H_FW, were studied with the computer model. Sensitivity to changes in H_OW is shown in Figure 4-5. Sensitivity to changes in H_FW is shown in Figure 4-6. The test data for the bed outlet is shown as "T5 °F", while the model output for variations in the heat transfer coefficient is labeled "T gas@5". Note that the sensitivity of the 2-dimensional model is greatly increased over that of the 1-dimensional model as shown in the previous section. This can be expected due to the existence of radial nodes in this model, allowing a radial gradient in temperature. Since the H_FW is a function of temperature, it changes along the axial direction of the packed column. Simulation of model with the actual test shows that the prediction of H_FW by theoretical equation as it described in Section 2 fits the temperature profile very well.

The final values selected for H_FW and H_OW were 0.3 and 0.25, respectively. The comparison with test data is shown in Figure 4-7. The test temperatures for the bed inlet, center, and outlet are labeled based on the measuring thermocouple as "T3 °F", "T4 °F", and "T5 °F" respectively. The corresponding model data is labeled based on node point as "gas T 5", "gas T 50", and "gas T 101" respectively.

As shown in Figure 4-7, the 2DMOL thermal model can simulate test data very closely with the adjustment of the heat transfer coefficients. The final value selected for H_FW, 0.3, however, is an order of magnitude less than the theoretical value (4.0), calculated in Equation 2.86. This is expected since in the actual adsorption test the bed temperature is around 100° F. Since the heat transfer coefficient is a function of Reynolds number, it would be best to run several experiments with different Reynolds number and fit the obtained results in a empirical equation.

FIGURE 4-5 VARIATIONS OF H_FW FOR 2DMOL
Variations of thermal coefficient $H_{OW}$
(Heat transfer from outside to canister wall)

FIGURE 4-6  VARIATIONS OF $H_{OW}$ FOR 2DMOL

FIGURE 4-7  FINAL THERMAL VERIFICATION OF 2DMOL FOR 5A
4.3 Carbon Dioxide Adsorption

4.3.1 Molecular Sieve 5A

The test ran on 01-26-94 will be used to verify the FLOW1MOL and 2DMOL bed models for carbon dioxide adsorption. Test specifications are shown in Figure 4-8.

Two phenomenon were observed to occur during this adsorption test which are not generally accounted for in mathematical models of this type.

The first phenomenon is the significance of bed channeling in the 1.875 inch ID cylindrical column with sorbent pellets of 8-12 mesh (approx. 2 mm in diameter). The existence of significant bed channeling is evident in Figure 4-9, which shows the breakthrough of CO_{2} in the column. Note the discrepancy in the breakthrough at the material exit centerline (labeled "Outlet") from a point 5 inches downstream of the material exit ("Outlet Beads"). The downstream point measures all gas exiting the column, mixed via turbulence through 5 inches of 3 mm glass beads. Consistent with the assumption of flow channeling at the column wall, the breakthrough is earlier for the mixed gas than at the column centerline. The two-dimensional model was developed to account for the channeling, and to aid in derivation of a technique to intelligently apply a channeling factor to the more CPU efficient single dimension models.

It is important to note that the presence of channeling will be much more pronounced in the 5A sorbent bed heater core. The heater core is configured such that a number of approximately 1/2 inch square channels contain the sorbent material. Channeling occurs at the walls of the packed bed, and the sorbent bed channels have a very high ratio of pellet diameter to wall diameter, which is the critical parameter for flow channeling. The two-dimensional model can be used to simulate the actual 4BMS as long as a good estimate of 5A sorbent bed reactor core channeling is available.

The second phenomenon observed is the importance of including nitrogen co-adsorption for accurate modeling of the carbon dioxide breakthrough with nitrogen as the carrier gas. Figures 4-10 and 4-11 show the test data compared with modeling results with and without coadsorption of N2. As seen in Figure 4-10, the initial adsorption of N2 on an empty bed creates a fast rise in temperature over the entire bed. The higher bed temperature reduces bed CO_{2} adsorption capacity. N2 coadsorption also marginally reduces the bed capacity for CO_{2}. As a result, the earlier breakthrough curves shown in Figure 4-11 reflect the lower bed capacity for modeling with N2 coadsorption. These results also correspond well to the actual test data in both figures.

4.3.1.1 FLOW1MOL Model Verification

The determination of input values, mass transfer coefficients, and verification of the single material flow-through adsorption and desorption model, FLOW1MOL, is described in this section.

Model inputs are shown in Figure 4-12. Determination of appropriate values for each non-obvious input parameter are discussed below.

Inside Diameter: Based on 2 inch OD and wall thickness of 1/16 inch.

Wall Density: For canister wall, stainless steel

Void Fraction: Based on value given in Wright et. al. for Davison 5A
Interfacial Surface Area: Based on Davison Chemical Co. supply.
Pellet Conductivity: Based on Davison Chemical Co. supply.
Pellet Specific Heat: Based on Davison Chemical Co. supply.

Heat Transfer Fluid to Wall: Determined via thermal characterization test (see Sect. 4-2)

<table>
<thead>
<tr>
<th>Adsorb Data Sheet</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Start Time:</strong></td>
</tr>
<tr>
<td><strong>Data File:</strong></td>
</tr>
<tr>
<td><strong>Sorbent Material:</strong></td>
</tr>
<tr>
<td><strong>Carrier Gas:</strong></td>
</tr>
<tr>
<td><strong>Sorbate Gas(es):</strong></td>
</tr>
<tr>
<td><strong>Test Duration:</strong></td>
</tr>
<tr>
<td><strong>Conductor(s):</strong></td>
</tr>
<tr>
<td><strong>Inlet and Initial Conditions</strong></td>
</tr>
<tr>
<td><strong>Carrier Flow Rate:</strong></td>
</tr>
<tr>
<td><strong>CO2 Flow Rate:</strong></td>
</tr>
<tr>
<td><strong>Init./Final Inlet DP:</strong></td>
</tr>
<tr>
<td><strong>Inlet H2O Moie %:</strong></td>
</tr>
<tr>
<td><strong>Inlet pH2O:</strong></td>
</tr>
<tr>
<td><strong>Initial Bed Temp:</strong></td>
</tr>
<tr>
<td><strong>Initial Ambient Temp:</strong></td>
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<tr>
<td><strong>Bed Pressures:</strong></td>
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<td><strong>Inlet Manifold Pressure:</strong></td>
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<tr>
<td><strong>Material Inlet Pressure:</strong></td>
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<tr>
<td><strong>Material CL Pressure:</strong></td>
</tr>
<tr>
<td><strong>Material Exit Pressure:</strong></td>
</tr>
<tr>
<td><strong>DP Sensor Pressure:</strong></td>
</tr>
<tr>
<td><strong>Ambient Pressure:</strong></td>
</tr>
</tbody>
</table>

| **CO2 Calibration:** | |
| **Cal. Gas CO2 % Vol:** | 0.39992% in N2 |
| **Low Pressure Calibration:** | 14.9 psia |
| **Sample 1:** | 12036 279388 |
| **Sample 2:** | 12048 2739601 |

| **High Pressure Calibration:** | 15.3 psia |
| **Sample 1:** | 12309 2797320 |

**FIGURE 4-8 SPECIFICATIONS FOR 01-26-94 CO2 ADSORPTION TESTING**
FIGURE 4-9 CO₂ PARTIAL PRESSURES FOR 01-26-94 TEST

FIGURE 4-10 CO₂ MODEL TEMPERATURE COMPARISONS WITH AND WITHOUT NITROGEN COADSORPTION
Heat Transfer Outside to Wall: Determined via thermal characterization test (see Section 4-2)

Pellet Density: Based on Davison Chemical Co. supply.

Heat of Adsorption: Based on Davison Chemical Co. supply.

Mass Transfer Coefficients: Determined empirically based on comparison of test data to model results

Results of the model comparison are shown by the solid lines in Figures 4-10 and 4-11. As is evident, the comparison is very favorable. Note in particular the excellent agreement of coadsorption temperature effects in Figure 4-10. The immediate temperature increase caused by N2 adsorption is properly reflected by the model. In addition, although not exact in magnitude, the subsequent dramatic drop at both the midpoint and outlet positions is also properly modeled.

Also note the proper change in slope of the breakthrough curve in Figure 4-12 from the midpoint to outlet positions. This change is due to increasing bed temperatures and the subsequent broadening of the mass transfer zone which is an indication of a nonequilibrium conditions between the gas and solid phase during the adsorption of CO2 on 5A material. The comparison of the experimental data with models predicts the mass transfer coefficient of CO2 to be .017 ft/hr.
<table>
<thead>
<tr>
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<th>Description</th>
<th>Units</th>
<th>Current Value</th>
</tr>
</thead>
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<td>hours</td>
<td>3</td>
</tr>
<tr>
<td>DELT1</td>
<td>time step</td>
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<td>NJ</td>
<td>Number of nodes</td>
<td>n/a</td>
<td>101</td>
</tr>
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<td>DELZ1</td>
<td>distance between nodes</td>
<td>feet</td>
<td>0.00833333</td>
</tr>
<tr>
<td>TO</td>
<td>Ambient temperature</td>
<td>°R</td>
<td>537</td>
</tr>
<tr>
<td>GF</td>
<td>Volumetric flow rate</td>
<td>CFH</td>
<td>55.5</td>
</tr>
<tr>
<td>TO</td>
<td>Inlet temperature</td>
<td>°R</td>
<td>537</td>
</tr>
<tr>
<td>NC</td>
<td>Number of components</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>INERT</td>
<td>Inert gas (1=N2; 2=He)</td>
<td>n/a</td>
<td>1</td>
</tr>
<tr>
<td>P TOT</td>
<td>Total Inlet Pressure</td>
<td>psia</td>
<td>15.89</td>
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<td>BC C(1)</td>
<td>Inlet partial pressure</td>
<td>psia</td>
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<td>Inlet partial pressure</td>
<td>psia</td>
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<td>Inlet partial pressure</td>
<td>psia</td>
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</tr>
<tr>
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<td>Inlet partial pressure</td>
<td>psia</td>
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</tr>
<tr>
<td>Z</td>
<td>Bed length</td>
<td>feet</td>
<td>0.83333333</td>
</tr>
<tr>
<td>DE</td>
<td>External Diameter</td>
<td>feet</td>
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</tr>
<tr>
<td>DI</td>
<td>Inside Diameter</td>
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<td>Wall Density</td>
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<td>void fraction (eta)</td>
<td>dimless</td>
<td>0.35</td>
</tr>
<tr>
<td>AINT</td>
<td>Interfacial Surface Area</td>
<td>ft^2/ft^3</td>
<td>635</td>
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<td>CON S</td>
<td>Pellet (solid) conductivity</td>
<td>BTU/°F·ft</td>
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<tr>
<td>CP S</td>
<td>Pellet (solid) specific heat</td>
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<td>H FW</td>
<td>Heat transfer fluid to wall</td>
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<td>2.5</td>
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<tr>
<td>H OW</td>
<td>Heat transfer outside to wall</td>
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<td>M W(3)</td>
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<td>28</td>
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<td>M W(4)</td>
<td>Molecular Weight</td>
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<td>heat of adsorption</td>
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<td>-30000</td>
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<td>heat of adsorption</td>
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</tr>
<tr>
<td>HEAT(4)</td>
<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
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<td>Mass Transfer Coefficient</td>
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<td>Mass Transfer Coefficient</td>
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<td>Mass Transfer Coefficient</td>
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<td>IND(1)</td>
<td>Indicator for CO2 present</td>
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</tr>
<tr>
<td>IND(2)</td>
<td>Indicator for H2O present</td>
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<tr>
<td>IND(3)</td>
<td>indicator for N2 present</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>IND(4)</td>
<td>Indicator for O2 present</td>
<td></td>
<td>0</td>
</tr>
</tbody>
</table>

**FIGURE 4-12** INPUT DATA SET "A" FOR FLOW1MOL COMPARISON WITH 01-26-94 TEST
### Variable | Description | Units | Current Value
--- | --- | --- | ---
LABEL(1) | Output Labels |  | ppCO2
LABEL(2) |  |  | pp N2
LABEL(3) |  |  | gas T
LABEL(4) |  |  | p tot
AOUT(1) | C array indices to output |  | 1
AOUT(2) |  |  | 2
AOUT(3) |  |  | 5
AOUT(4) |  |  | 9
IOUT(1) | Node locations to be output |  | 5
IOUT(2) |  |  | 25
IOUT(3) |  |  | 50
IOUT(4) |  |  | 75
IOUT(5) |  |  | 101
SB | Cross sectional surface area | ft^3 | 0.019175
CON WA | Wall thermal conductivity | Btu/hr/ft/R | 32.875
CON WI Q |  |  | 0.29
CON WI K |  |  | 0.19
CP WA |  |  | 0.109848
CP WI Q |  |  | 0.21
CP WI K |  |  | 0.21
RO WI Q |  |  | 3.5
RO WI K |  |  | 16
X WA | Canister Wall Thickness | feet | 0.00541667
X WI Q | Q-felt insulation thickness | feet | 0.0416667
X WI K | K-felt insulation thickness | feet | 0.02083333
RA |  |  | 0.0045893
RAV |  |  | 0.0091785
EPSIN |  |  | 0.317
RHOS |  |  | 43
ALPHA1 |  |  | 575
R P |  |  | 0.00472441
D P |  |  | 0.00944882
BC L1 | boundary temperature for fluid |  | 537
BC L2 | boundary temperature for solid |  | 537
BC L3 | boundary temperature for canister wall |  | 537
BC L5 | fluid pressure at each grid(?) |  | 15.886
BC L6 |  |  | 15.886
IN L1 | inlet temperature for fluid |  | 537
IN L2 | inlet temperature for solid |  | 537
IN L3 | inlet temperature for canister wall |  | 537
IN L5 | fluid pressure at each grid(?) |  | 15.886
IN L6 |  |  | 15.886
R | Gas Constant |  | 0.19875
PI |  |  | 3.141593
TEST |  |  | 0

**FIGURE 4-12** INPUT DATA SET "B" FOR FLOW1MOL COMPARISON WITH 01-26-94 TEST
4.3.1.2 2DMOL Model Verification

The determination of input values, mass transfer coefficients, and verification of the two-dimensional single material flow-through adsorption and desorption model, 2DMOL, is described in this section.

Model inputs are shown in Figure 4-13 and 4-14.

<table>
<thead>
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<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Current Value</th>
</tr>
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<tbody>
<tr>
<td>END</td>
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<td>DELT</td>
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<td>55.6</td>
</tr>
<tr>
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<td>Inlet temperature</td>
<td>°R</td>
<td>537</td>
</tr>
<tr>
<td>NG</td>
<td>Number of components</td>
<td>n/a</td>
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<td>Inert gas (1=N2; 2=He)</td>
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<td>Z</td>
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</tr>
<tr>
<td>D E</td>
<td>External Diameter</td>
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</tr>
<tr>
<td>D I</td>
<td>Inside Diameter</td>
<td>feet</td>
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</tr>
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<td>RO WA</td>
<td>Wall Density</td>
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</tr>
<tr>
<td>EPSEX</td>
<td>void fraction (eta)</td>
<td>dimless</td>
<td>0.35</td>
</tr>
<tr>
<td>AINT</td>
<td>Interfacial Surface Area</td>
<td>ft^2/ft^3</td>
<td>635</td>
</tr>
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<td>CP S</td>
<td>Pellet (solid) specific heat</td>
<td>BTU/°F-lb</td>
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<td>M W(2)</td>
<td>Molecular Weight</td>
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</tr>
<tr>
<td>M W(3)</td>
<td>Molecular Weight</td>
<td>lb/lb-mol</td>
<td>28</td>
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<tr>
<td>M W(4)</td>
<td>Molecular Weight</td>
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<td>heat of adsorption</td>
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<td>HEAT(4)</td>
<td>heat of adsorption</td>
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<tr>
<td>K F(4)</td>
<td>Mass Transfer Coefficient</td>
<td>ft/hr</td>
<td>0.1</td>
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**FIGURE 4-13** INPUT DATA SET "A" FOR 2DMOL COMPARISON WITH 01-26-94 TEST
FIGURE 4-14 INPUT DATA SET "B" FOR 2DMOL COMPARISON WITH 01-26-94 TEST

Results of the model comparison are shown in Figures 4-15 and 4-16. As is evident, the comparison is very favorable. Note that two sets of model data are presented; averaged data and centerline data. The centerline data for node 51 is the central node radially and the last bed material node axially. Averaged data for node 51 is also at the last bed node axially, but is an average of all the radial nodes. The averaged data is thus representative of gas after mixing in the glass beads, or the test data labeled "Outlet Beads". Averaging of data was done by two methods, Cubic Spline and Simpson integration (Gerald and Wheatley, 1984). It was found that the Simpson integration method gives better results than the Simpson method.

Based on the above discussion, it is expected that centerline data - the line with filled markers in Figure 4-15 - will compare with the small circular markers. As seen from the figure, this comparison is indeed favorable. Average data should be compared with the small triangular markers, and once again, this is a favorable comparison. As a result, it can be inferred that the two-dimensional model does correctly model the channeling observed in this test.

As seen from Figure 4-16, the temperature comparison is also favorable. The increase in fidelity of the two-dimensional model is evident by comparison of Figure 4-16 with the results from the one-dimensional model in Figure 4-10. The 2DMOL simulation more closely follows the actual temperature peak, both in time and in magnitude.
The short time of breakthrough allows it to use IAST, even though it takes more CPU time than using the Langmuir isotherm. A mass transfer coefficient of .017 ft/hr was used in predicting the CO$_2$ breakthrough curve.

\textbf{FIGURE 4-15} CO$_2$ MODEL BREAKTHROUGH COMPARISONS FOR 01-26-94 TEST WITH 2DMOL RESULTS

\textbf{FIGURE 4-16} CO$_2$ TEMPERATURE COMPARISONS FOR 01-26-94 TEST WITH 2DMOL RESULTS
4.4 Water Adsorption

4.4.1 Molecular Sieve 5A

![Adsorb Data Sheet]

<table>
<thead>
<tr>
<th>Start Time:</th>
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<td>04/07/94 h2o in n2 on 13x adsorb</td>
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</tr>
<tr>
<td>Sorbent Material:</td>
<td>Carrier Gas:</td>
</tr>
<tr>
<td>13x</td>
<td>N2</td>
</tr>
<tr>
<td>Sorbent Gas(es):</td>
<td>Test Duration:</td>
</tr>
<tr>
<td>H2O</td>
<td></td>
</tr>
<tr>
<td>Condutor(s):</td>
<td></td>
</tr>
<tr>
<td>HMJG</td>
<td></td>
</tr>
</tbody>
</table>

**Inlet and Initial Conditions**

- **Carrier Flow Rate:** 26.04 SLPM
- **CO2 Flow Rate:** NA SCCM
- **Init/Final Inlet DP:** 3.8 degrees C
- **Inlet H2O Mole %:** 0.7503
- **Inlet ppH2O:** 6.035196 mmHg
- **Inlet CO2 %:** NA
- **Inlet ppCO2:** 0.0000 mmHg
- **Initial Bed Temp:** degrees F
- **Initial Ambient Temp:** degrees F
- **Final Bed Temp:** degrees F
- **Final Ambient Temp:** degrees F

**Bed Pressures:**

- **Inlet Manifold Pressure:** 15.587 psia
- **Material Inlet Pressure:** 15.554 psia
- **Material CL Pressure:** 15.506 psia
- **Material Exit Pressure:** 15.456 psia
- **DP Sensor Pressure:** 14.872 psia
- **Ambient Pressure:** 14.446 psia

**H2O Calibration:**

- **Low Dewpoint**
  - Sample 1: 9654, 2829155
  - Sample 2: 9667, 2827783
- **Medium Dewpoint**
  - Sample 1: 22579, 2809176
  - Sample 2: 22596, 2810229
- **High Dewpoint**
  - Sample 1: 36444, 2791041
  - Sample 2: 36343, 2789987

**Curve Fit**

- **Partial Pressure**
  - 4.05 mm Hg
  - 9.59 mm Hg
  - 15.67 mm Hg

**Temperatures:**

- **T6 Location:** Wall at Midpoint
- **T11 Location:** Skin
- **T12 Location:** Ambient
- **T14 Location:** Beaker
- **T15 Location:** Chiller
- **D1 Location:** Column exit
- **D2 Location:** Column exit
- **C1 Location:** Column exit
- **C2 Location:** Column exit

**FIGURE 4-17 SPECIFICATIONS FOR 01-26-94 H2O ADSORPTION TESTING**

The test ran on 01-26-94 will be used to verify the FLOW1MOL and 2DMOL bed models for water adsorption. Test specifications are shown in Figure 4-17. Breakthrough for water is shown in Figure 4-18. Note, as in the test of CO2 adsorption, the discrepancy between breakthrough at the material exit measured at the centerline and after gas mixing (marked "Exit" and "Mixed" respectively). The extremely high affinity of zeolite 5A is also evident in the time required for breakthrough.
4.4.1.1 FLOW1MOL Model Verification

The determination of mass transfer coefficients and verification of the single material flow-through adsorption and desorption model, FLOW1MOL, is described in this section.

Model inputs are shown in Figure 4-19 and 4-20. Results of the model comparison are shown by the solid lines in Figures 4-21 and 4-22. For breakthrough, the FLOW1MOL model compares well with test data at the midpoint and fairly well at material exit, except as the breakthrough curve approaches the inlet partial pressure. Deviations from the test data may be explained by the lack of channeling modeled by FLOW1MOL. Channeling appears to have a greater influence in water adsorption than CO₂, perhaps due to the much longer duration of the adsorption run. For temperatures, the comparison is also fairly good, especially during the heating of the column.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Current Value</th>
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<td>hours</td>
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</tr>
<tr>
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<td>time step</td>
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<td>NJ</td>
<td>Number of nodes</td>
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<tr>
<td>DELZ1</td>
<td>distance between nodes</td>
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<tr>
<td>TO</td>
<td>Ambient temperature</td>
<td>°R</td>
<td>532</td>
</tr>
<tr>
<td>G F</td>
<td>Volumetric flow rate</td>
<td>CFH</td>
<td>56.76</td>
</tr>
<tr>
<td>T O</td>
<td>Inlet temperature</td>
<td>°R</td>
<td>532</td>
</tr>
<tr>
<td>NC</td>
<td>Number of components</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>INERT</td>
<td>Inert gas (1=N2; 2=He)</td>
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</tr>
<tr>
<td>P TOT</td>
<td>Total Inlet Pressure</td>
<td>psia</td>
<td>15.68</td>
</tr>
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<td>BC C(1)</td>
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<td>External Diameter</td>
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<tr>
<td>CON S</td>
<td>Pellet (solid) conductivity</td>
<td>BTU/hr ft °R</td>
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<tr>
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<td>M W(4)</td>
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<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-28000</td>
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<tr>
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<td>heat of adsorption</td>
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<tr>
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<td>-8988</td>
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FIGURE 4-19 INPUT DATA SET "A" FOR FLOW1MOL COMPARISON WITH 04-07-94 TEST
### TABLE 4-20 INPUT DATA SET "B" FOR FLOW1MOL COMPARISON WITH 04-07-94 TEST

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<td>LABEL(3)</td>
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<td><em>&quot;gas T&quot;</em></td>
</tr>
<tr>
<td>LABEL(4)</td>
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<td><em>&quot;tot P&quot;</em></td>
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<td>C array indices to output</td>
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<tr>
<td>AOUT(2)</td>
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<td>2</td>
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</tr>
<tr>
<td>AOUT(4)</td>
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<td>10</td>
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</tr>
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<td>IOUT(5)</td>
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<td>61</td>
</tr>
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<td>CON WA</td>
<td>Wall conductivity</td>
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<td>Conductivity for Q-fiber</td>
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<td>CON WI K</td>
<td>Conductivity for Min-K</td>
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<td>Specific Heat for wall</td>
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<td>CP WI K</td>
<td>Specific Heat for Min-K</td>
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</tr>
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<td>Density for Min-K</td>
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</tr>
<tr>
<td>BC L2</td>
<td>boundary temperature for solid</td>
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</tr>
<tr>
<td>BC L3</td>
<td>boundary temperature for canister wall</td>
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</tr>
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</tr>
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<td>BC L6</td>
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</tr>
<tr>
<td>IN L2</td>
<td>initial temperature for solid</td>
<td>532</td>
</tr>
<tr>
<td>IN L3</td>
<td>initial temperature for canister wall</td>
<td>532</td>
</tr>
<tr>
<td>IN L5</td>
<td>initial pressure at each grid</td>
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</tr>
<tr>
<td>IN L6</td>
<td>initial pressure at each grid</td>
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FIGURE 4-21 H₂O BREAKTHROUGH COMPARISONS FOR 04-07-94 TEST WITH FLOW1MOL RESULTS

FIGURE 4-22 H₂O TEMPERATURE COMPARISONS FOR 04-07-94 TEST WITH FLOW1MOL RESULTS
4.4.1.2 2DMOL Model Verification

The determination of mass transfer coefficients and verification of the two-dimensional adsorption and desorption model, 2DMOL, is described in this section.

Input data for the 2DMOL model for the 04-07-94 test are shown in Figures 4-23 and 4-24. The results of the model comparison are shown by the solid lines in Figures 4-25 and 4-26. As expected the center line breakthrough and temperature profile match the one-dimensional flow model. The average breakthrough at the midpoint and the outlet of the bed are shown. The model midpoint average is reasonably good, since the dispersion is moderate compared to the centerline breakthrough. There was no test data point for the average component partial pressure at the midpoint. This can not be done without the distortion of flow regime in the rest of the bed.

The result of the model for the average breakthrough at the outlet shows an early breakthrough compared to test data for breakthrough of H₂O/N₂. This can be attributed to several factors. The equilibrium isotherm, the porosity, and the radial diffusivity of H₂O. This is also apparent from an early breakthrough at the centerline of the bed. Any small deviation in isotherm measurement causes an early/later breakthrough. The porosity variation effect is also a large contributor to the early average breakthrough. In this study, The wall porosity was taken as .85 as it was suggested in theoretical section. Monudin (1976) used a value of .54 in a packed reactor and had good model result with test data. Therefore, it is possible that a smaller porosity value should be taken. The third parameter that affects the average breakthrough is the radial diffusion of H₂O in the bed. Two different equations were used in this work to describe the radial diffusion as it described earlier. The equation by Fahien (1954) predicts the average breakthrough better and was used in this study. Even though this equation gave good result for the adsorption of CO₂/N₂, it is possible that it underestimates the water radial diffusivity.

A mass transfer coefficient of .0035 was used to predict the breakthrough curve. Langmuir isotherm was used to predict H₂O/N₂ isotherm.
<table>
<thead>
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<th>Description</th>
<th>Units</th>
<th>Current Value</th>
</tr>
</thead>
<tbody>
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<td>hours</td>
<td>5</td>
</tr>
<tr>
<td>DELT</td>
<td>time step</td>
<td>hours</td>
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</tr>
<tr>
<td>NJ</td>
<td>Number of axial nodes</td>
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<tr>
<td>NJR</td>
<td>Number of radial nodes</td>
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</tr>
<tr>
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<td>NC</td>
<td>Number of components</td>
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</tr>
<tr>
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<td>Inert gas (1=N2; 2=He)</td>
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<tr>
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<td>External Diameter</td>
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<td>void fraction (eta)</td>
<td>dimless</td>
<td>0.35</td>
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<td>AINT</td>
<td>Interfacial Surface Area</td>
<td>ft^2/ft^3</td>
<td>635</td>
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<td>BTU/lb-mole</td>
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</tr>
<tr>
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<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
</tr>
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</tr>
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FIGURE 4-23 INPUT DATA SET "A" FOR 2DMOL COMPARISON WITH 04-07-94 TEST
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<th>Current Value</th>
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</tr>
<tr>
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<td>Wall specific heat</td>
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FIGURE 4-24 INPUT DATA SET "B" FOR 2DMOL COMPARISON WITH 04-07-94 TEST
FIGURE 4-25 H₂O BREAKTHROUGH COMPARISONS FOR 04-07-94 TEST WITH 2DMOL RESULTS

FIGURE 4-26 H₂O TEMPERATURE COMPARISONS FOR 04-07-94 TEST WITH 2DMOL RESULTS
4.5 Water and Carbon Dioxide Adsorption

4.5.1 Molecular Sieve 5A

The test ran on 05-06-94 will be used to verify the FLOW1MOL and 2DMOL bed models for water and carbon dioxide adsorption. Test specifications are shown in Figure 4-27. Breakthrough for water is shown in Figure 4-28. Note, as in the previous tests, the discrepancy between breakthrough at the material exit measured at the centerline and after gas mixing (marked "matl outlet" and "column outlet" respectively). The extremely high affinity of zeolite 5A is also evident in the time required for breakthrough. It is also evidenced by the fact that the presence of CO₂ is not evident by comparison of this figure with Figure 4-18, which shows water breakthrough for a similar test, except without CO₂.

Figure 4-29 shows the centerline bed temperatures for the test. Note the early peaks resulting from CO₂ adsorption around 0.5 hours.

Figure 4-30 shows the carbon dioxide breakthrough. The roll-up phenomenon is evident in this graph, wherein the weaker adsorbate (CO₂) is driven off the bed by the stronger (H₂O), resulting in an outlet partial pressure greater than at the inlet.
FIGURE 4-27 \(\text{H}_2\text{O}\) BREAKTHROUGH FOR 05-06-94 TEST

FIGURE 4-28 \(\text{H}_2\text{O}/\text{CO}_2\) TEMPERATURES FOR 05-06-94 TEST
4.5.1.1 FLOW1MOL Model Verification

The determination of mass transfer coefficients and verification of the single material flow-through adsorption and desorption model, FLOW1MOL, is described in this section.

Model inputs are shown in Figure 4-30 and 4-31. Determination of appropriate values for each non-obvious input parameter is discussed below (values discussed in previous sections are neglected).

Results of the model comparison are shown by the solid lines in Figures 4-32, 4-33, and 4-34. For breakthrough, the FLOW1MOL model compares well with test data at the midpoint. At the outlet, the model data (representing plug flow) falls, as expected, between the test data for the outlet at the centerline and the outlet following mixing.

For temperatures, the comparison is also fairly good, especially during the heating of the column. As noted for N\textsubscript{2}/CO\textsubscript{2} adsorption, an early temperature peak corresponding to CO\textsubscript{2} adsorption is reflected by the model. In contrast to CO\textsubscript{2} adsorption, the temperature profile remains steady for a large time and suddenly decreases. The period of steady state temperature profile indicates the balance between the heat generated by heat of adsorption of H\textsubscript{2}O and the heat of desorption of CO\textsubscript{2} and N\textsubscript{2} and the heat transferring to the wall of the packed bed. The sudden decrease of temperature or the sharp breakthrough of H\textsubscript{2}O is the reflection of high affinity of water on 5A material. This causes the adsorption of H\textsubscript{2}O to occur in a short length of the bed, with little dispersion taking place. It is possible that in the case of water adsorption the assumption of equilibrium between the gas phase and solid phase is valid to a large extend. Mass transfer coefficients of .0035 ft/hr for H\textsubscript{2}O and .017 ft/hr for CO\textsubscript{2} were used to predict the breakthrough curves.

For carbon dioxide breakthrough, the comparison of model results and test data show that FLOW1MOL properly models the trends exhibited in coadsorption, that is, the roll-up
phenomenon observed earlier. Differences in magnitude are most likely due to the lack of accuracy in the equilibrium isotherms and the approximate nature of the multi-component isotherm equations. The accuracy is expected to improve as more precise isotherm data, particularly on multi-component adsorption, is received. The Langmuir isotherm for mixture of CO₂ and H₂O was used which underestimates the loading of CO₂ and H₂O on 5A. The IAST predicts this loading much closer to the test data. Since the solution to the IAST isotherm is not analytical it is costly in terms of CPU usage.

<table>
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<th>Variable</th>
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<th>Current Value</th>
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<td>-8988</td>
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<td>-8988</td>
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**FIGURE 4-30** INPUT DATA SET "A" FOR FLOW1MOL COMPARISON WITH 05-06-94 TEST

58
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**FIGURE 4-31** INPUT DATA SET "B" FOR FLOW1MOL COMPARISON WITH 05-06-94 TEST
FIGURE 4-32 H₂O BREAKTHROUGH COMPARISONS FOR 05-06-94 TEST WITH FLOW1MOL RESULTS

FIGURE 4-33 H₂O/CO₂ TEMPERATURE COMPARISONS FOR 05-06-94 TEST WITH FLOW1MOL RESULTS
4.5.1.2 2DMOL Model Verification

The determination of mass transfer coefficients and verification of the two-dimensional adsorption and desorption model, 2DMOL, is described in this section.

Input data for the 2DMOL model for the 05-06-94 test are shown in Figures 4-35 and 4-36. Determination of appropriate values for each non-obvious input parameter is discussed below (values discussed in previous sections are neglected).

Results of the model comparison are shown by the solid lines in Figures 4-37 and 4-38. As expected the center line breakthrough and temperature profile match the one dimensional flow model. The average breakthrough at the midpoint and the outlet of the bed are shown. The model midpoint average is reasonably good, since the dispersion is moderate compare to the centerline breakthrough. There was no test data point for the average component partial pressure at the midpoint.

The result of the model for the average breakthrough at the outlet shows an early breakthrough in compared to the test data for breakthrough of H₂O/N₂. This can be attributed to several factors: the equilibrium isotherm, the porosity, and the radial diffusivity of H₂O as were discussed in H₂O/N₂ adsorption.

The Langmuir isotherm was used to predict loading of the H₂O/CO₂ mixture on 5A material. Langmuir isotherm for mixture of CO₂ and H₂O underestimates the loading of CO₂ and H₂O on 5A. The IAST predicts this loading much closer to the test data. Since the solution to the IAST isotherm is not analytical it is costly in terms of CPU usage.
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FIGURE 4-35 INPUT DATA SET "A" FOR 2DMOL COMPARISON WITH 05-06-94 TEST
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FIGURE 4-36 INPUT DATA SET "B" FOR 2DMOL COMPARISON WITH 05-06-94 TEST
FIGURE 4-37 CO₂ BREAKTHROUGH COMPARISONS FOR 05-06-94 TEST WITH 2DMOL RESULTS

FIGURE 4-38 H₂O/CO₂ TEMPERATURE COMPARISONS FOR 05-06-94 TEST WITH 2DMOL RESULTS
FIGURE 4-39 H₂O/CO₂ BREAKTHROUGH COMPARISONS FOR 05-06-94 TEST WITH 2DMOL RESULTS
4.6 Carbon Dioxide Desorption

4.6.1 Molecular Sieve 5A

Strip Desorb Data Sheet

| Start Time: | Data File: | 01/27/94 CO2 13x strip |
| Sorbent Material: | 5A | |
| Carrier Gas: | N2 | Notes: Desorption of 01/26/94 test |
| Sorbate Gas(es): | | |
| Test Duration: | 3 HRS | |
| Conductors: | | JG |

**Inlet and Initial Conditions**

| Carrier Flow Rate: | 28.04 SLPM |
| CO2 Flow Rate: | SCCM |
| Initial/Final Inlet DP: | degrees C |
| Inlet H2O Mole %: | mmHg |
| Inlet ppH2O: | in CO2 %: |
| Initial Bed Temp: | 77 degrees F |
| Initial Ambient Temp: | 77 degrees F |
| Final Bed Temp: | 77 degrees F |
| Final Ambient Temp: | 77 degrees F |

**GC Configuration**

| TCD Vent Flow 1: | 8 R-2-15-AAA |
| TCD Vent Flow 2: | 9.7 R-2-15-AAA |
| Sample Flow @ Port 5: | 11 R-2-15-AAA |
| Detector Current: | 150 mA |
| Column Catalog No.: | C-5000 Attech Cat. |
| TCD/DETT Temp.: | 120/130 degrees C |
| INJ/COL Temp.: | 150/100 degrees C |
| Valve Heat Temp.: | 117 degrees C |

**Temperatures:**

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<td>Exit in Beds</td>
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<td>T12</td>
<td>Ambient</td>
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<td>T14</td>
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</tr>
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<td>T15</td>
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<td>C2</td>
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**FIGURE 4-40** SPECIFICATIONS FOR 01-27-94 CO2 DESORPTION TESTING

The test ran on 01-27-94 will be used to verify the FLOW1MOL and 2DMOL bed models for carbon dioxide desorption. Test specifications are shown in Figure 4-40. Breakthrough for CO2 and temperatures will be shown in the comparative plots in the following sections.

4.6.1.1 FLOW1MOL Model Verification

The determination of mass transfer coefficients and verification of the single material flow-through desorption and desorption model, FLOW1MOL, is described in this section.

Model inputs are shown in Figure 4-41 and 4-42.

Results of the model comparison are shown by the solid lines in Figures 4-43 and 4-44. After the bed was saturated with CO2, the regeneration process was started by using N2 as the purge gas. As it is shown the effluent CO2 concentration has a sharp drop in the first few minutes and the slope of the breakthrough flattens out as time goes by. The initial drop in temperature is due to heat of desorption and finally reaches the inlet condition when there is no depletion of CO2 from the bed. The same mass transfer coefficient of .017 was used. Model predictions of temperature and breakthrough agree well with test data. The IAST was used to predict the mixture isotherm of CO2/N2.
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**FIGURE 4-41 INPUT DATA SET "A" FOR FLOW1MOL COMPARISON WITH 01-27-94 TEST**
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**FIGURE 4-42** INPUT DATA SET "B" FOR FLOW1MOL COMPARISON WITH 01-27-94 TEST
FIGURE 4-43 \( \text{CO}_2 \) BREAKTHROUGH COMPARISONS FOR 01-27-94 TEST WITH FLOW1MOL RESULTS

FIGURE 4-44 \( \text{CO}_2 \) TEMPERATURE COMPARISONS FOR 01-27-94 TEST WITH FLOW1MOL RESULTS
4.6.1.2 2DMOL Model Verification

The determination of mass transfer coefficients and verification of the two-dimensional desorption model, 2DMOL, is described in this section.

Input data for the 2DMOL model for the 01-27-94 test are shown in Figures 45 and 46.

Results of the model comparison are shown by the solid lines in Figures 4-47 and 4-48. The model prediction of centerline and average breakthrough matches the obtained experimental data. The temperature profile result of the two dimensional model also estimates the experimental data fairly well. The few degree discrepancy between the model and experimental data is largely due to thermal conductivity profile estimation which has a strong effect on radial temperature profile. Trial and error must be used in order to obtain a corrected thermal conductivity equation. The IAST was used to predict the CO2/N2 mixture isotherm. A mass transfer coefficient of .017 ft/hr was used for the prediction of breakthrough curve.

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FIGURE 4-45 INPUT DATA SET "A" FOR 2DMOL COMPARISON WITH 01-27-94 TEST
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FIGURE 4-46 INPUT DATA SET "B" FOR 2DMOL COMPARISON WITH 01-27-94 TEST
FIGURE 4-47 CO₂ BREAKTHROUGH COMPARISONS FOR 01-27-94 TEST WITH 2DMOL RESULTS

FIGURE 4-48 CO₂ TEMPERATURE COMPARISONS FOR 01-27-94 TEST WITH 2DMOL RESULTS
4.7 Water Desorption

4.7.1 Molecular Sieve 5A

The test ran on 04-19-94 will be used to verify the FLOW1MOL and 2DMOL bed models for water desorption. Test specifications are shown in Figure 4-49. Breakthrough for H2O and temperatures will be shown in the comparative plots in the following sections.
4.7.1.1 FLOW1MOL Model Verification

The determination of mass transfer coefficients and verification of the single material flow-through desorption and desorption model, FLOW1MOL, is described in this section.

Model inputs are shown in Figures 4-50 and 4-51. Results of the model comparison are shown by the solid lines in Figures 4-52 and 4-53. The results of the partial pressure of H₂O and temperature profile of 1-D desorption model are not in good agreement with the test data. The model shows a fast reduction of H₂O partial pressure in the gas phase. A mass transfer coefficient as large as .04 ft/hr, in contrast with .0035 ft/hr in the case of H₂O adsorption, was used. However, there shouldn't be such a large difference mass transfer coefficients in adsorption versus desorption process for the same component. Even with this large mass transfer coefficient, the desorption of H₂O from the bed was not enough to increase the H₂O partial pressure in the gas phase. In contrast with adsorption process, any small discrepancy of H₂O partial pressure with test data will remain as an error throughout the completion of the test. In adsorption any small error at any point in the bed, if it caused by the isotherm at some partial pressure of the feed will be eliminated at a later time because of the correct value of isotherm at a larger partial pressure of the feed. This can be seen from the early breakthrough of most works done by previous researchers, (Hirpyuki, et al 1982, Rice, 1982). The obvious reason is that the equilibrium isotherm at low partial pressures are being underestimated. It is also possible that the adsorption/desorption of H₂O on 5A material could be modeled based on the assumption of equilibrium, where there is no resistance between the two phases. The other possible source of error is how the H₂O partial pressure was measured. Perhaps a more sensitive instrument should have been used in the test.
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<td>HE A T (1)</td>
<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-17000</td>
<td>-18000</td>
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<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
<td>-8988</td>
</tr>
<tr>
<td>HE A T (3)</td>
<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
<td>-8988</td>
</tr>
<tr>
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<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
<td>-8988</td>
</tr>
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<td>Mass Transfer Coefficient</td>
<td>ft/hr</td>
<td>0.025</td>
<td>0.017</td>
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<td>Mass Transfer Coefficient</td>
<td>ft/hr</td>
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<td>0.02</td>
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<td>Mass Transfer Coefficient</td>
<td>ft/hr</td>
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<td>0.05</td>
</tr>
<tr>
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<td>Mass Transfer Coefficient</td>
<td>ft/hr</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>IND (1)</td>
<td>Indicator for CO2 present</td>
<td></td>
<td>0</td>
<td></td>
</tr>
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<td>Indicator for H2O present</td>
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<td>Indicator for N2 present</td>
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<td></td>
</tr>
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<td>IND (4)</td>
<td>Indicator for O2 present</td>
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</tr>
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<td>IDES1</td>
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<td>Flag to indicate prior saturation of bed</td>
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FIGURE 4-50 INPUT DATA SET "A" FOR FLOW1MOL COMPARISON WITH 04-19-94 TEST
<table>
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<tr>
<th>LABEL(1) Output Labels</th>
<th>&quot;ppH2O&quot;</th>
<th>&quot;ppCO2&quot;</th>
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<tr>
<td>LABEL(2)</td>
<td>&quot;pp N2&quot;</td>
<td>&quot;ppN2&quot;</td>
</tr>
<tr>
<td>LABEL(3)</td>
<td>&quot;gas T&quot;</td>
<td>&quot;ppN2&quot;</td>
</tr>
<tr>
<td>LABEL(4)</td>
<td>&quot;tot P&quot;</td>
<td>&quot;gas T&quot;</td>
</tr>
<tr>
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<td>C array indices to output</td>
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</tr>
<tr>
<td>AOUT(2)</td>
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<td>2</td>
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<td>AOUT(3)</td>
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<td>6</td>
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<td>AOUT(4)</td>
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<td>5</td>
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<td>IOUT(3)</td>
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<td>IOUT(4)</td>
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<td>35</td>
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<td>IOUT(5)</td>
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<td>0.019175</td>
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<td>CON_WA</td>
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<td>32.875</td>
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<td>CON_WI K</td>
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<td>CP_WA</td>
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<tr>
<td>CP_WI Q</td>
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<td>0.21</td>
</tr>
<tr>
<td>CP_WI K</td>
<td></td>
<td>0.21</td>
</tr>
<tr>
<td>RO_WI Q</td>
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<td>3.5</td>
</tr>
<tr>
<td>RO_WI K</td>
<td></td>
<td>16</td>
</tr>
<tr>
<td>X_WA Canister Wall Thickness feet</td>
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<td>0.00541667</td>
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<td>557</td>
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<td></td>
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<td>D_P</td>
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<td>0.00944882</td>
</tr>
<tr>
<td>BC_L1 boundary temperature for fluid</td>
<td>532.5</td>
<td>531</td>
</tr>
<tr>
<td>BC_L2 boundary temperature for solid</td>
<td>532.5</td>
<td>531</td>
</tr>
<tr>
<td>BC_L3 boundary temperature for canister wall</td>
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<td>531</td>
</tr>
<tr>
<td>BC_L5 fluid pressure at each grid(?)</td>
<td>15.413</td>
<td>15.55</td>
</tr>
<tr>
<td>BC_L6 fluid pressure at each grid(?)</td>
<td>15.413</td>
<td>15.55</td>
</tr>
<tr>
<td>IN_L1 inlet temperature for fluid</td>
<td>532.5</td>
<td>531</td>
</tr>
<tr>
<td>IN_L2 inlet temperature for solid</td>
<td>532.5</td>
<td>531</td>
</tr>
<tr>
<td>IN_L3 inlet temperature for canister wall</td>
<td>532.5</td>
<td>531</td>
</tr>
<tr>
<td>IN_L5 fluid pressure at each grid(?)</td>
<td>15.413</td>
<td>15.55</td>
</tr>
<tr>
<td>IN_L6 fluid pressure at each grid(?)</td>
<td>15.413</td>
<td>15.55</td>
</tr>
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<td>0</td>
</tr>
<tr>
<td>ITEST1</td>
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</tr>
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**FIGURE 4-51 INPUT DATA SET "B" FOR FLOW1MOL COMPARISON WITH 04-19-94 TEST**
04-19-94 Comparison with FLOW1MOL
H2O desorption off zeolite 5A with N2 gas
Simulation results: solid lines
Experimental Results: symbols

FIGURE 4-52 H2O BREAKTHROUGH COMPARISONS FOR 04-19-94 TEST WITH FLOW1MOL RESULTS

04-19-94 Comparison with FLOW1MOL
H2O desorption off zeolite 5A with N2 gas
Simulation results: solid lines
Experimental Results: symbols

FIGURE 4-53 TEMPERATURE COMPARISONS FOR 04-19-94 TEST WITH FLOW1MOL RESULTS
4.7.1.2 2DMOL Model Verification

The determination of mass transfer coefficients and verification of the two-dimensional desorption and desorption model, 2DMOL, is described in this section.

Input data for the 2DMOL model for the 04-19-94 test are shown in Figures 4-54 and 4-55. Results of the model comparison are shown by the solid lines in Figures 4-56 and 4-57. The results of the partial pressure of H₂O and temperature profile of 2-D desorption model are better than the 1-D model. The model shows a fast reduction of H₂O partial pressure in gas phase as in 1-D model, but much closer to the test data. A mass transfer coefficient of 0.0035 ft/hr was chosen as in the case of H₂O adsorption. The same argument can be made as in 1-D on the discrepancies between model results and the test data. However, since the 2-D results are in better agreement with the test data, one can conclude the significant effect radial dispersion has on the adsorption/desorption of H₂O on the 5A material. More study and accurate testing are needed in the case of water desorption on 5A material.

<table>
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<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Current Value</th>
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<tr>
<td>END</td>
<td>final time</td>
<td>hours</td>
<td>9</td>
</tr>
<tr>
<td>DELT</td>
<td>time step</td>
<td>hours</td>
<td>0.00250</td>
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<tr>
<td>NJ</td>
<td>number of axial nodes</td>
<td>n/a</td>
<td>51</td>
</tr>
<tr>
<td>NJR</td>
<td>number of radial nodes</td>
<td>n/a</td>
<td>20</td>
</tr>
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<td>DELZ</td>
<td>distance between nodes</td>
<td>feet</td>
<td>0.0166666666</td>
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<td>TAMB</td>
<td>ambient temperature</td>
<td>°R</td>
<td>532</td>
</tr>
<tr>
<td>G F</td>
<td>volumetric flow rate</td>
<td>CFH</td>
<td>56.12</td>
</tr>
<tr>
<td>TI</td>
<td>inlet temperature</td>
<td>°R</td>
<td>532</td>
</tr>
<tr>
<td>N C</td>
<td>number of components</td>
<td></td>
<td>2</td>
</tr>
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<td>INERT</td>
<td>inert gas (1=N₂; 2=He)</td>
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<td>P TOT</td>
<td>total inlet pressure</td>
<td>mmHg</td>
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<td>inlet partial pressure</td>
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<td>inlet partial pressure</td>
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<td>P C(4)</td>
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<tr>
<td>D I</td>
<td>inside diameter</td>
<td>feet</td>
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<td>void fraction (eta)</td>
<td>dimless</td>
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<td>interfacial surface area</td>
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<td>CP S</td>
<td>pellet (solid) specific heat</td>
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<td>lb/lb-mol</td>
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<td>lb/lb-mol</td>
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<td>-18000</td>
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<td>BTU/lb-mole</td>
<td>-28000</td>
</tr>
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<td>heat of adsorption</td>
<td>BTU/lb-mole</td>
<td>-8988</td>
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<td>HEAT(4)</td>
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<td>-8988</td>
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<td>mass transfer coefficient</td>
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FIGURE 4-54 INPUT DATA SET "A" FOR 2DMOL COMPARISON WITH 04-19-94 TEST
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<th>Current Value</th>
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</thead>
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</tr>
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<td>not used</td>
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<td>65</td>
</tr>
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</table>

FIGURE 4-55 INPUT DATA SET "B" FOR 2DMOL COMPARISON WITH 04-19-94 TEST
FIGURE 4-56 BREAKTHROUGH COMPARISONS FOR 04-19-94 TEST WITH 2DMOL RESULTS

FIGURE 4-57 TEMPERATURE COMPARISONS FOR 04-19-94 TEST WITH 2DMOL RESULTS
4.8 FLOW3MOL MODEL RESULTS

The FLOW3MOL model represents the 4BMS desiccant beds, with the capability to model three different layers of sorbent material stacked in a single packed bed. The FLOW3MOL model was run for demonstration purposes configured for a packed column of the approximate size of the MSMBT apparatus. No reliable test data is currently available to compare these results with, so they are presented without comparison.

Figure 4-58 shows results from the FLOW3MOL model run for CO₂ breakthrough. The location of the breakthrough points are at the end of 13X, middle of Silica gel, end of Silica gel, middle of 13X, and end of 13X materials. As can be seen the CO₂ breakthrough occurs very fast for the first section of bed because of presence of water. No CO₂ adsorption takes place on Silica gel material. CO₂ is desorbed on the last section of the bed, 13X. Since for some period of time all of the H₂O would be adsorbed on Silica gel, flow passes to the last section of the bed without water. This gives the opportunity for CO₂ being adsorbed there. As silica gel is saturated with H₂O, water will pass to the 13X and this cause the roll-up of CO₂.

Figure 4-59 shows results from the FLOW3MOL model run for H₂O breakthrough. It can be seen the H₂O breakthrough at the exit of Silica Gel material is sharp at low partial pressure and disperse at higher partial pressure of H₂O. This is caused by the Silica gel equilibrium isotherm which dose not have high affinity for H₂O at low partial pressure in compare to 13X. However it has more capacity for adsorption at higher partial pressures of H₂O.

Figure 4-60 shows results from the FLOW3MOL model run for temperature. The figure shows the sharp increase and decrease of temperature at the beginning of the bed as it expected and a steady temperature for sometime on 13X section which is the same profile as in 13X-single bed.

**FIGURE 4-58 CARBON DIOXIDE BREAKTHROUGH RESULTS FOR FLOW3MOL**
FIGURE 4-59 WATER BREAKTHROUGH RESULTS FOR FLOW3MOL

FIGURE 4-60 TEMPERATURE RESULTS FOR FLOW3MOL
4.9 VACMOL Model Results

The VACMOL model represents the 4BMS 5A sorbent beds, with the capability to model thermal/vacuum desorption for a packed bed. The VACMOL model was run for demonstration purposes configured for a packed column of the approximate size of the 5A sorbent beds in the Life Test 4BMS. No reliable test data is currently available to compare these results with, so they are presented without comparison.

Figure 4-61 shows temperature prediction results from the VACMOL model. The constant heat input into the vacuum chamber causes a steady rise of temperature as time progresses.

Figure 4-62 shows results from the VACMOL model run for H₂O and CO₂ partial pressures. Initially the bed is saturated with CO₂, H₂O, and N₂ at atmospheric pressure and temperature. In order to simulate the actual bed performance a pressure boundary condition of 25 mm Hg was chosen. The sudden decrease in pressure is caused by outflow of N₂. The partial pressure of CO₂ and H₂O start rising as heat being input to the vacuum chamber. Since CO₂ is less adsorbent than H₂O, it starts coming off the bed sooner and depleted off the bed in very short time.

Figure 4-63 shows results from the VACMOL model run for total pressure. A sudden decrease in total pressure to the boundary condition value is an indication that pressure is being transferred along the bed in very short time. After a minima, the pressure start rising because of desorption of CO₂ and H₂O from the bed as temperature increases.

The model is written in a such a way that any velocity, caused by differential pressure, will not exceed the choke velocity. As shown in Figures 4-64 and 4-65, the velocity profile starts from a very high value, because of large pressure gradient along the bed, to a minima after a very short time. The minima corresponds to a minima of pressure gradient in the bed. The velocity starts rising as CO₂ and H₂O are desorbed off the bed. This makes the pressure increase inside of the bed, creating a differential pressure with the boundary pressure. Given the profile of pressure and velocity along the bed, it is reasonable to say that variation of these two variables along the bed is not significant. For simulation of the actual 4BMS a lumped velocity and pressure could be used.

![Figure 4-61 Temperature Results for VACMOL](image-url)
FIGURE 4-62 PARTIAL PRESSURE RESULTS FOR VACMOL

FIGURE 4-63 TOTAL PRESSURE RESULTS FOR VACMOL
FIGURE 4-64 VELOCITY RESULTS FOR VACMOL

FIGURE 4-65 VELOCITY RESULTS FOR VACMOL (FIRST 0.25 HOURS)
5.1 Conclusion

Based on analytical and experimental investigation of convective flows in porous media the following conclusions are drawn:

1. The experimental results from the laboratory scale-fixed bed adsorber are quantitatively consistent with the one-dimensional model at the column center. The average concentration of cross sectional bed obtained by test result deviates from the column center concentration appreciably. This indicates the strong effects of porosity variation along the radial direction of column bed on the temperature, concentration, and velocity field. These observations resulted in the decision to model the dynamic behavior of the column in two-dimensions.

2. The two-dimensional model demonstrates the importance of non-darcian momentum and porosity variation on the flow distribution, concentration, and temperature in the radial direction of the bed. The two-dimensional model not only predicts the concentration and temperature profile at the column center well, but it also predicts the average concentration reasonably well.

3. A linear driving force mass transfer model provides a reasonable fit to the experimental adsorption and desorption.

4. The concentration of a key component, CO₂, is affected by the presence of the non-key component, N₂, in CO₂/N₂ adsorption. CO₂ effluent concentration overshoots its inlet concentration because of H₂O displacement (more easily adsorbed) component. The height of this roll-up is increased with the inlet concentration of H₂O component.

5. Comparison of model results with test data shows the created models can be accurately used for modeling of the actual 4BMS.

6. The two-dimensional model can be used to simulate the actual 5A bed of 4BMS, which contains an array of approximately 1/2 inch square channels, for porosity variation.

7. The IAST equilibrium predicts the breakthrough curve much closer to the test data than the Lanmuir-Fredlich theory for mixtures of CO₂/N₂ and CO₂/H₂O.

5.2 Recommendations

1. Since the PDE's of the two-dimensional model are a strong function of porosity, research into the velocity variation is obviously important.

2. Because of transient behavior of adsorption processes, the CPU usage of the two-dimensional model is very large. Attempts should be made to convert the two-dimensional model to a one dimensional model by choosing the appropriate functions to describe the concentration, temperature, and velocity field in the radial direction of the column.

3. The solution to IAST functions relies on a ε-al and error type. This costs a large amount of CPU time. Further study should be done to eliminate this barrier.
4. Thermal vacuum description is the regenerative mode of the actual 4BMS 5A sorbent beds. Experimental data is needed to verify the model.

5. Literature shows that a pressure swing process which only uses two beds is more efficient than any other adsorption/desorption process. Research should be done to convert the 4BMS to a 2BMS.

6. More recent isotherm data, obtained from the same sorbent that is expected to be used for the actual flight 4BMS system, has recently become available. This sorbent data should be incorporated into the models developed in this study.

7. The models developed during this study have been shown to model the processes present in the 4BMS to a very reasonable degree of accuracy. Therefore, they should be incorporated into an integrated 4BMS for the purpose of analyzing and optimizing the 4BMS system.
SECTION 6
REFERENCES


"Davison Molecular Sieves Adsorption Equilibria", W. R. Grace & Co., Davison Chemical Division.


Newman, J., Numerical Solution Of Coupled, Ordinary Differential Equations (UCRL-17739), Lawrence Radiation Laboratory, University of California, Berkeley, August (1967).


Knowing that the spreading pressure is related to temperature and the amount adsorbed on the solid by
\[
\frac{\pi(p'_i)A}{RT} = \int_0^{p'_i} \frac{q'_i}{P'_i} dP'_i
\]
and assuming the adsorbed phase obeying Langmuir-Freundlich isotherm
\[
q'_i = \frac{q_{ml}B_iP_i^{n_i}}{1 + B_iP_i^{n_i}}
\]
the spreading pressure can be obtained as
\[
\frac{\pi(p'_i)A}{RT} = \int_0^{p'_i} \frac{q'_i}{P'_i} dP'_i = \int_0^{p'_i} \frac{q_iB_iP_i^{n_i}}{P_i(1 + B_iP_i^{n_i})} dP_i
\]
therefore \( \pi \) is
\[
\pi = \frac{RT q_{ml} \ln(1 + B_iP_i^{n_i})}{A n_i}
\]
solving for \( P_i \)
\[
P'_i = \left( \frac{\exp\left(\frac{\pi n_i A}{RT}\right) - 1}{B_i} \right)^{\frac{1}{n_i}}
\]
knowing the fact that
\[
P_i = P_y = p'_i(\pi)x_i
\]
substitution of eq 2.23 into 2.6, and solving for \( x_i \)
\[
x_i = \frac{P_y}{\left( \frac{\exp\left(\frac{\pi n_i A}{RT}\right) - 1}{B_i} \right)^{\frac{1}{n_i}}}
\]
knowing that
\[
\sum x_i = \sum y_i = 1
\]
equation 2.8 will result

\[ \sum_{i=1}^{n} \frac{P_y_i}{\left( \exp\left( \frac{\pi A_n_i}{RTq_{mi}} \right) - 1 \right)^{z_i} B_i} - 1 = 0 \]

eq 2.8
APPENDIX B

DERIVATION OF MOMENTUM, ENERGY, AND MOLAR CONCENTRATION BALANCES FOR TWO DIMENSIONS

In order to derive the mass, energy, and momentum balances for adsorption packed column in cylindrical coordinates, the conservation laws were set over a thin "shell" of fluid. In all of conservation laws the balances are:

\[
\text{time rate of change of } i = \text{rate of } i \text{ in } - \text{rate of } i \text{ out} + \text{rate production or dissipation of } i
\]

where \( i \) could be momentum, thermal heat, or molar mass of component \( i \). After a balance is made on a shell of finite thickness, the limit is taken as the spatial dimensions approach zero. As a result of this, a differential equation is generated which describes the time rate of change of a particular variable.

In this study, the diffusion of momentum, heat and molar mass was taken into account not only in the axial direction but also in the radial direction.

For developing the conservative equations the following assumptions were made:

1. The gas phase is dilute and follows ideal gas law
2. Axial and radial conduction within column wall is neglected
3. The adsorbent pellet can be modeled as sphere
4. The temperature within the pellet is uniform
5. The radial convection is negligible

**B.1 Conservation Of Molar Mass Of Component \( i \) In The Mixture**

In developing the molar mass balance of component \( i \) in the mixtures which is being adsorbed by pellet particles within the packed bed, the fluxes of component \( i \) take place by diffusion and convection in axial direction and only by diffusion in radial direction, since the radial convection is negligible. The rate of disappearance of component \( i \) in the mixture is by diffusion of \( i \) at the surface and into the pore and the solid part of the particles. Writing the molar mass conservation of component \( i \)

\[
\varepsilon 2\pi r \Delta r \Delta x \frac{\partial C_i}{\partial t} = \varepsilon 2\pi r \Delta r N_i |_{x+\Delta x} - \varepsilon 2\pi r \Delta r N_i |_{x} + \varepsilon 2\pi r \Delta x N_i |_{r+\Delta r} - \varepsilon 2\pi r \Delta x N_i |_{r} - (1-\varepsilon) 2\pi r \Delta r \Delta x r_i
\]

Collecting the terms and dividing by \( \varepsilon 2\pi r \Delta r \Delta x \)

\[
\frac{\partial C_i}{\partial t} = \frac{(N_i |_{x+\Delta x} - N_i |_{x})}{\Delta x} - \frac{(rN_i |_{r+\Delta r} - rN_i |_{r})}{r\Delta r} - \frac{(1-\varepsilon)}{\varepsilon} r_i
\]

Take the limit as \( \Delta x \) and \( \Delta r \) go to zero

\[
\frac{\partial C_i}{\partial t} = -\frac{\partial N_i}{\partial x} - \frac{\partial (rN_i)}{r \partial r} - \frac{(1-\varepsilon)}{\varepsilon} r_i
\]
Knowing that
\[
N_{i,x} = -D_{eff,x} \frac{\partial C_i}{\partial x} + u_x C_i
\]
\[
N_{i,r} = -D_{eff,r} \frac{\partial C_i}{\partial r} + u_r C_i
\]
eq B.5

where the second term, the convection term in the radial direction, is negligible. Substitution of fluxes into the above equation
\[
\frac{\partial C_i}{\partial t} = D_{eff,x} \frac{\partial^2 C_i}{\partial x^2} - \frac{\partial (u C_i)}{\partial x} + D_{eff,r} \frac{\partial}{\partial r} \left( \frac{r \partial C_i}{\partial r} \right) - \frac{(1 - \varepsilon)}{\varepsilon} r_i
\]
eq B.6

The derivation for one dimensional molar mass balance is the same as above except that the third term on the right hand side, flux due to radial diffusion, is not considered.

B.2 Conservation Of Energy Of Fluid Flow

Energy transfer in fluid phase is by convection in the axial direction and by diffusion in axial and radial directions. Energy is also being produced by heat of adsorption of components in the particle. Energy is also being transferred to the wall of column by an overall heat transfer coefficient. Writing the energy balance for the gas phase
\[
\varepsilon 2\pi r \Delta r \Delta x \rho \frac{\partial T_s}{\partial t} = \varepsilon 2\pi r \Delta r (q - \rho_s C_{pe} u_s T_s)_t - \varepsilon 2\pi r \Delta r (q - \rho_s C_{pe} u_s T_s)_t + \varepsilon 2\pi r \Delta x (q - \rho_s C_{pe} u_s T_s)_t - \varepsilon 2\pi r \Delta x (q - \rho_s C_{pe} u_s T_s)_t + (1 - \varepsilon) 2\pi r \Delta r \Delta x h_s a_s (T_s - T_s)
\]
eq B.7

Collecting the terms and dividing by \( \varepsilon 2\pi r \Delta r \Delta x \)
\[
\rho_s C_{pe} \frac{\partial T_s}{\partial t} = \frac{(q + \rho_s C_{pe} u_s T_s)_t}{\Delta x} - (q + \rho_s C_{pe} u_s T_s)_t - \frac{r (q + \rho_s C_{pe} u_s T_s)_t - r (q + \rho_s C_{pe} u_s T_s)_t}{r \Delta r} - \frac{(1 - \varepsilon)}{\varepsilon} h_s a_s (T_s - T_s)
\]
eq B.8

Take the limit as \( \Delta x \) and \( \Delta r \) go to zero and ignoring the radial convection
\[
\rho_s C_{pe} \frac{\partial T_s}{\partial t} = - \frac{\partial q_s}{\partial x} - \rho_s C_{pe} \frac{\partial (u_s T_s)}{\partial x} - \frac{\partial (r q_r)}{\partial r} - \frac{(1 - \varepsilon)}{\varepsilon} h_s a_s (T_s - T_s)
\]
eq B.9
Knowing the fluxes are
\[ q_x = -k_{s,x} \frac{\partial T_s}{\partial x} \]
\[ q_r = -k_{s,r} \frac{\partial T_s}{\partial r} \]  

eq B.10

Substitution of fluxes into the above equation
\[ \frac{\partial T_s}{\partial t} = k_{s,x} \frac{\partial^2 T_s}{\partial x^2} - \rho_s c_p \frac{\partial (u T_s)}{\partial x} + k_{s,r} \frac{\partial}{\partial r} \left( r \frac{\partial T_s}{\partial r} \right) - \frac{(1 - \varepsilon)}{\varepsilon} h_a a_s (T_s - T_i) \]  

eq B.11

The derivation for one dimensional heat balance is the same as above except that the third term on the right hand side, flux due to radial diffusion, is not being considered. And, a dissipation rate of energy to the column wall must be added to the above equation.

B.3 Conservation Of Energy Of Solid Phase

Energy transfers in solid phase by diffusion in axial and radial directions. Energy is also being produced by heat of adsorption of components in the particle. Energy is being transferred to the fluid phase by an overall heat transfer coefficient. Writing the energy balance for the solid phase

\[ 2\pi r \Delta r \Delta x \rho_s c_p \frac{\partial T_s}{\partial t} = 2\pi r \Delta r (q)_x - 2\pi r \Delta r (q)_{x+\Delta x} + 2\pi r \Delta x (q)_r - 2\pi r \Delta x (q)_{r+\Delta r} - \\
2\pi r \Delta r \Delta h_i a_s (T_s - T_i) - 2\pi r \Delta r \Delta x \sum_{i=1}^{n} \Delta H_i r_i \]  

eq B.13

Collecting the terms and dividing by \( \varepsilon 2\pi r \Delta r \Delta x \)

\[ \rho_s c_p \frac{\partial T_s}{\partial t} = \frac{(q)_x - (q)_{x+\Delta x}}{\Delta x} - \frac{r (q)_{r+\Delta r} - r (q)_r}{r \Delta r} - h_a a_s (T_s - T_i) - \sum_{i=1}^{n} \Delta H_i r_i \]  

eq 4.14

knowing the fluxes
\[ q_x = -k_{s,x} \frac{\partial T_s}{\partial x} \]
\[ q_r = -k_{s,r} \frac{\partial T_s}{\partial r} \]  

eq B.14

inserting fluxes in equation
\[ \rho_s c_p \frac{\partial T_s}{\partial t} = k_{s,x} \frac{\partial^2 T_s}{\partial x^2} + k_{s,r} \frac{\partial}{\partial r} \left( r \frac{\partial T_s}{\partial r} \right) - h_a a_s (T_s - T_i) - \sum_{i=1}^{n} \Delta H_i r_i \]  

eq B.15

The derivation for one dimensional heat balance for the solid phase is the same as above except that the second term on the right hand side, flux due to radial diffusion, is not being considered.
B.4 Conservation Of Energy Based On An Effective Conductivity

When the temperature difference between fluid and particle phases is neglected, column temperature can be derived by summation of eqs B-11 and 4.15.

\[
(\varepsilon \rho c_p + (1-\varepsilon)\rho c_p) \frac{\partial T}{\partial t} = \varepsilon k_{\text{eff},x} \frac{\partial^2 T}{\partial x^2} - \varepsilon \rho c_p \frac{\partial (uT)}{\partial x} + \varepsilon k_{\text{eff},r} (r \frac{\partial T}{\partial r}) - (1-\varepsilon) \sum_{i=1}^{n} \Delta H_{i} r_{i}
\]

where \( k_{x,\text{eff}} \) and \( k_{r,\text{eff}} \) are the effective thermal conductivity in the axial and radial direction in the packed column, which are

\[
k_{\text{eff},x} = k_{x} + k_{f, \text{eff}}
\]

\[
k_{\text{eff},r} = k_{r} + k_{f, \text{eff}}
\]

The derivation for one dimensional-homogeneous heat balance is the same as above except that the third term on the right hand side, flux due to radial diffusion, is not considered. And, a dissipation rate of energy to the column wall must be added to the above equation.

B.5 Total Mass Balance

Assuming ideal gas law \( C_i = \frac{p_i}{RT} \) and knowing \( \sum P_i = \rho \), the component mass balance equation can be recast into an overall mass balance equation, substitution of \( C_i \) into eq 2.10 and carrying out the derivatives yields to

\[
-\frac{D}{RT_g} \frac{\partial^2 P_i}{\partial x^2} - \frac{D}{RT_s} \frac{\partial P_i}{\partial x} \left( \frac{\partial T}{\partial x} \right)^2 - \frac{D}{RT_s} \frac{\partial^2 T}{\partial x^2} + \frac{1}{RT_s} \frac{\partial P_i}{\partial t} - \frac{P_i}{RT_s} \frac{\partial T}{\partial t} + \frac{u P_i}{RT_s} \frac{\partial T}{\partial x} + \frac{P_i}{RT_s} \frac{\partial u}{\partial x} + \frac{1-\varepsilon}{\varepsilon} \frac{\partial Q}{\partial t} = 0
\]

neglecting the second term and multiplying by \( RT_g \), the above equation reduces to

\[
\frac{\partial P}{\partial t} = D_i \frac{\partial^2 P}{\partial x^2} - u \frac{\partial P}{\partial x} - \frac{P_i}{T_s} \left( \frac{\partial T}{\partial t} - D_i \frac{\partial^2 T}{\partial x^2} + u \frac{\partial T}{\partial x} \right) - RT_s \frac{1-\varepsilon}{\varepsilon} \frac{\partial Q}{\partial t}
\]

summation of the above equation over all the components and knowing that \( \sum P_i = \rho \), the equation for total pressure is

\[
\frac{\partial P}{\partial t} = D_i \frac{\partial^2 P}{\partial x^2} - u \frac{\partial P}{\partial x} - \rho \frac{\partial u}{\partial x} + \frac{P}{T_s} \left( \frac{\partial T}{\partial t} - D_i \frac{\partial^2 T}{\partial x^2} + u \frac{\partial T}{\partial x} \right) - RT \frac{1-\varepsilon}{\varepsilon} \sum_{i=1}^{n} \frac{\partial Q_i}{\partial t}
\]
Four FORTRAN computer programs are presented in this report. The first is a two-dimensional model of flow adsorption/desorption in a packed bed. The second is a one-dimensional model of flow adsorption/desorption in a packed bed. The third is a model of the thermal vacuum desorption. And the last is a tri-sectional packed bed with two different sorbent materials. The programs are capable of simulating up to four gas constituents for each process. If it is necessary to simulate more constituents, minor changes are needed in a few subroutines.

C.1 Two Dimensional FORTRAN Program

A flow chart of the two-dimensional modeling of flow adsorption/desorption is shown in Figures C-1 and C-2. This program simulates the two-dimensional adsorption and desorption of a fixed-bed column 10 inches long and 1.87 inches in diameter. The model simulates four constituents with variations in radial velocity and porosity. The users supply initial and boundary condition in the INITIAL subroutine. If it is necessary to run the model with a larger diameter or length, the number of grids must be specified in the INITIAL subroutine.

For each time step the temperature dependent parameters (density, conductivity, viscosity, etc.) are recalculated. If the temperature change is not significant in the packed bed during the simulation, the user can specify that these parameters will not be recalculated.

Solid-gas equilibrium for the pure components are predicted by the Langmuir-Freundlich isotherm. For mixtures, two types of solid-gas equilibrium are implemented in the program. One is based on the Langmuir-Freundlich isotherm for mixtures. The second prediction uses the IAST isotherm. The IAST model has an iterative solution and is CPU time intensive. The user can switch an indicator to chose the desired isotherm method.

The energy balance includes the heat lost to the surroundings. For an adiabatic simulation of a packed bed, the heat transfer coefficient between the wall and the surroundings equal is set to zero.

Heat transfer is assumed between the solid, fluid flow, and the wall of the column. The program is also capable of simulating the heat transfer bed based on an effective conductivity. In this case a thermal equilibrium between solid and fluid flow is assumed. Axial and radial conductivity is included in the model. These parameters vary along the radial and axial direction based on the porosity variation. The program is also capable of making these parameters constant by switching the proper indicator.

Mass transfer is simulated with a lumped resistance model. This resistance is obtained by matching experimental breakthrough curves with the results of the model.

This model uses the UNDER-RELAXATION method for calculation of all variables in the PDE's, except the velocity and the pressure which are computed by the NEWMAN method. The total numbers of equations involved for four components is 13.
FIGURE C-1 THE FLOW CHART OF THE MAIN PROGRAM FOR THE 2-D MODEL
FIGURE C-2 THE FLOW CHART FOR THE SUBROUTINE PROGRAMS FOR THE 2-D MODEL
A list of program variables is given below with a brief description.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>LL</td>
<td>Time step index</td>
<td>none</td>
<td>Int</td>
</tr>
<tr>
<td>T_Time</td>
<td>current time</td>
<td>minutes</td>
<td>real</td>
</tr>
<tr>
<td>S(i,j,k)</td>
<td>matrix variable; i=variable ID; j=axial grid number; k=radial grid number</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>P(i,j,k)</td>
<td>Old of S array</td>
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<td>real*13</td>
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<td>real</td>
</tr>
<tr>
<td>L2</td>
<td>solid temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L3</td>
<td>wall temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
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<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
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<td>L5</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>L6</td>
<td>pressure</td>
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</tr>
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<td>pressure</td>
<td>mmHG</td>
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<td>int</td>
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<td>porosity</td>
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</tr>
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</tr>
<tr>
<td>D_E</td>
<td>outside bed diameter</td>
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A list of program variables is given below with a brief description (continued).

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<td>Total Pressure</td>
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<td>real</td>
</tr>
<tr>
<td>BC_L6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>W0</td>
<td>under relaxation coeff</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>L_SOL_FLO</td>
<td>indicator, no equilibrium between the gas indicator and solid temperature</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DP</td>
<td>particle diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>H_OW</td>
<td>heat transfer coefficient outside of the wall</td>
<td>Btu/sq ft</td>
<td>real</td>
</tr>
<tr>
<td>U(i,j)</td>
<td>velocity/Darcy velocity, center line velocity</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>UMAX</td>
<td>max velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>NUMAX</td>
<td>the grid where max velocity is</td>
<td>ft/hr</td>
<td>int</td>
</tr>
<tr>
<td>EPS(i)</td>
<td>porosity</td>
<td>sq ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>REY</td>
<td>Reynolds number</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>CP_P</td>
<td>specific heat</td>
<td>BTU/F/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>VISC_P</td>
<td>viscosity</td>
<td>lb/ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>H_FP</td>
<td>heat transfer coefficient fluid-particle</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>CON_Z</td>
<td>fluid axial conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>CON_R</td>
<td>fluid radial conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>CON_S</td>
<td>particle conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>EFF_CON_Z1</td>
<td>fluid axial effective conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>EFF_CON_R1</td>
<td>fluid radial effective conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>DIF</td>
<td>molecular diffusivity</td>
<td>sq ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>SC_N</td>
<td>Schmidt number</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>Eff_DIFF_R</td>
<td>fluid radial effective diffusivity</td>
<td>sq ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>EFF_DIFF_Z</td>
<td>fluid axial effective diffusivity</td>
<td>sq ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>H_W</td>
<td>heat transfer coefficient fluid-wall</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>V(i)</td>
<td>Langmuir constant</td>
<td>lb mol/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>B(i)</td>
<td>Langmuir constant</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>PO(i)</td>
<td>Langmuir constant</td>
<td>dimensionless</td>
<td>real</td>
</tr>
<tr>
<td>PP</td>
<td>component partial Pressure</td>
<td>mm Hg</td>
<td>real</td>
</tr>
<tr>
<td>Qt</td>
<td>adsorbed concentration</td>
<td>lb mol/solid</td>
<td>real</td>
</tr>
</tbody>
</table>

C-5
C.2 One-Dimensional Flow Adsorption/Desorption FORTRAN Program for Column Packed with One Section Material

A flow chart of the one-dimensional modeling of flow adsorption/desorption is shown in Figure C-3 and C-4. This program simulates the one-dimensional adsorption and desorption of a fixed-bed column 10 inches long and 1.87 inches in diameter. Users supply initial and boundary condition in the INITIAL subroutine. If it is necessary to run the model with larger diameter or length, the number of grids must be specified in the INITIAL subroutine.

For each time step the temperature dependent parameters (density, conductivity, viscosity, etc.) are recalculated. If the temperature change is not significant in the packed bed during the simulation, the user can specify that these parameters will not be recalculated.

Solid-gas equilibrium for the pure components are predicted by the Langmuir-Freundlich isotherm. For mixtures, two types of solid-gas equilibrium are implemented in the program. One is based on the Langmuir-Freundlich isotherm for mixtures. The second prediction uses the IAST isotherm. The IAST model has an iterative solution and is CPU time intensive. The user can switch an indicator to chose the desired isotherm method.

The energy balance includes the heat lost to the surroundings. For an adiabatic simulation of a packed bed, the heat transfer coefficient between the wall and the surroundings equal is set to zero.

Heat transfer is assumed between the solid, fluid flow, and the wall of the column.

Mass transfer is simulated with a lumped resistance model. This resistance is obtained by matching experimental breakthrough curves with the results of the model.

This model uses the UNDER-RELAXATION method for calculation of all variables in the PDE's, except the velocity and the pressure which are computed by the NEWMAN method. The total numbers of equations involved for four components is 13.
FIGURE C-3  THE FLOW CHART OF THE MAIN PROGRAM FOR THE 1-D MODEL
FIGURE C-4 THE FLOW CHART OF THE SUBROUTINES PROGRAM FOR THE 1-D MODEL
A list of program variables is given below with a brief description.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>LL</td>
<td>Time step index</td>
<td>none</td>
<td>Int</td>
</tr>
<tr>
<td>T_Time</td>
<td>current time</td>
<td>minutes</td>
<td>real</td>
</tr>
<tr>
<td>C(i,j)</td>
<td>matrix variable; i=variable ID; j=axial various grid number; k=radial grid number</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>P(i,j)</td>
<td>Old of C array</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>L1</td>
<td>gas temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L2</td>
<td>solid temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L3</td>
<td>wall temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L4</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>L5</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>L6</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>PT</td>
<td>pressure</td>
<td>mm HG</td>
<td>real</td>
</tr>
<tr>
<td>NCOMP</td>
<td>number of component</td>
<td>non dimensional</td>
<td>real</td>
</tr>
<tr>
<td>INERT</td>
<td>type of carrier gas</td>
<td>non dimensional</td>
<td>real</td>
</tr>
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<td>EPSX</td>
<td>porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>RHOS</td>
<td>particle density</td>
<td>lbs/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>Z</td>
<td>bed length</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>VOID_B</td>
<td>porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>D_I</td>
<td>inside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_E</td>
<td>outside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>S_B</td>
<td>cross sectional area of bed</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_WA</td>
<td>heat capacity of wall</td>
<td>BTU/F/LB</td>
<td>real</td>
</tr>
<tr>
<td>RO_WA</td>
<td>density of wall</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_S</td>
<td>heat capacity of particle</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>RO_S</td>
<td>density of particle</td>
<td>ft</td>
<td>real</td>
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<td>R_P</td>
<td>particle radius</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_P</td>
<td>particle diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>heat(i)</td>
<td>heat of adsorption for each component</td>
<td>BTU/lb mole</td>
<td>real</td>
</tr>
<tr>
<td>NC</td>
<td>number of component</td>
<td>non dimensional</td>
<td>int</td>
</tr>
<tr>
<td>G_F</td>
<td>volumetric flow rate</td>
<td>cu ft/min</td>
<td>real</td>
</tr>
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<td>T0</td>
<td>initial temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>R</td>
<td>ideal gas law constant</td>
<td>lbf/sq ft .lb</td>
<td>real</td>
</tr>
<tr>
<td>P1</td>
<td>constant</td>
<td>mol/cu ft/R</td>
<td>3.14 real</td>
</tr>
<tr>
<td>M_W</td>
<td>Molecular weight</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>D</td>
<td>constant</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>K_F</td>
<td>mass transfer coefficient</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>NJ</td>
<td>grids number in axial direction</td>
<td>non dimension</td>
<td>int</td>
</tr>
<tr>
<td>DELZ</td>
<td>grid size in axial direction</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>DLT</td>
<td>time step</td>
<td>hr</td>
<td>real</td>
</tr>
<tr>
<td>CON_S1</td>
<td>pellet conductivity</td>
<td>BTU/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>ERROR</td>
<td>convergence criteria</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>N</td>
<td>number of equation</td>
<td>non dimension</td>
<td>int</td>
</tr>
<tr>
<td>Y_F</td>
<td>component mole fraction</td>
<td>lb mole i/lb</td>
<td>real</td>
</tr>
</tbody>
</table>

C-9
A list of program variables is given below with a brief description (continued).

<table>
<thead>
<tr>
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<th>Description</th>
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<th>Type</th>
</tr>
</thead>
<tbody>
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<td>P_TOT</td>
<td>Total Pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>BC_L1 to BC_L6</td>
<td>boundary condition for L1 to L6</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>W0</td>
<td>under relaxation coeff</td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>H_OW</td>
<td>heat transfer coefficient outside of the wall</td>
<td>Btu/hr/F/sq</td>
<td>real</td>
</tr>
<tr>
<td>REY</td>
<td>Reynolds number</td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>CP_P</td>
<td>specific heat</td>
<td>BTU/F/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>VISC_P</td>
<td>viscosity</td>
<td>lb/ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>H_FP</td>
<td>heat transfer coefficient fluid-particle</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>CON_L</td>
<td>fluid axial conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>CON_S</td>
<td>particle conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>H_W</td>
<td>heat transfer coefficient fluid-wall</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>V(l)</td>
<td>Langmuir constant</td>
<td>lb mole/lb</td>
<td>real</td>
</tr>
<tr>
<td>B(i)</td>
<td>Langmuir constant</td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>P0(i)</td>
<td>Langmuir constant</td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>PP</td>
<td>component partial Pressure</td>
<td>mm Hg</td>
<td>real</td>
</tr>
<tr>
<td>Q1</td>
<td>adsorbed concentration</td>
<td>lb mol/lb</td>
<td>real</td>
</tr>
<tr>
<td>BC_C1(i)</td>
<td>boundary condition of molar concentration under relaxation for each component and temperature</td>
<td>lb mole/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>W0-W3</td>
<td></td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>F3-F8</td>
<td>PDE's coefficient</td>
<td>various</td>
<td>real</td>
</tr>
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<td>PE_N_M</td>
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<td>non- dimension</td>
<td>real</td>
</tr>
<tr>
<td>PE_N_H</td>
<td>heat Peclet number</td>
<td>non dimension</td>
<td>real</td>
</tr>
<tr>
<td>AINT</td>
<td>interfacial area</td>
<td>sq ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>U_F1</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
</tbody>
</table>
C.3 One-Dimensional Flow Adsorption/Desorption FORTRAN Program for Column Packed with Three Sections of Different Material

A flow chart of the one-dimensional modeling of flow adsorption/desorption for column packed with three sections of different materials is shown in Figure C-5 and C-6. This program simulates the one-dimensional adsorption and desorption of a fixed-bed column 10 inches long and 1.87 inches in diameter. Users supply initial and boundary condition in the INITIAL subroutine. If it is necessary to run the model with larger diameter or length, the number of grids must be specified in the INITIAL subroutine.

The first section of the column, about 3 inches, contains the 13X material, followed by about 10 inches of silica gel, and finally the rest of the bed is filled with 13X material.

For each time step the temperature dependent parameters (density, conductivity, viscosity, etc.) are recalculated. If the temperature change is not significant in the packed bed during the simulation, the user can specify that these parameters will not be recalculated.

Solid-gas equilibrium for the pure component is predicted by Langmuir-Freundlich isotherm for the 13X material. Silica gel is depicted from the literature as an exponential function of temperature and pressure. For mixtures, two types of solid-gas equilibrium are implemented in the program. One is based on the Langmuir-Freundlich isotherm for mixtures. The second prediction uses the IAST isotherm. The IAST model has an iterative solution and is CPU time intensive. The user can switch an indicator to choose the desired isotherm method.

The energy balance includes the heat lost to the surroundings. For an adiabatic simulation of a packed bed, the heat transfer coefficient between the wall and the surroundings equal is set to zero.

Heat transfer is assumed between the solid, fluid flow, and the wall of the column.

Mass transfer is presented as lumped resistance model for the 13X material. For silica gel, the flux of the adsorbate is considered to be a combination of solid and pore diffusion. This resistance is obtained by matching experimental breakthrough curves with the results of model.

The model uses UNDER-RELAXATION method for calculation of all variables in the PDE's, except the velocity and the pressure which are computed by NEWMAN method. The total numbers of equations involve for four components is 13.
FIGURE C-5 THE FLOW CHART OF THE MAIN PROGRAM FOR THE 1-D MODEL FOR BED PACKED WITH THREE DIFFERENT MATERIALS
FIGURE C-6 THE FLOW CHART OF THE SUBROUTINES PROGRAM FOR THE 2-D MODEL FOR BED PACKED WITH THREE DIFFERENT MATERIALS
A list of program variables is given below with a brief description.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>LL</td>
<td>Time step index</td>
<td>none</td>
<td>Int</td>
</tr>
<tr>
<td>T_Time</td>
<td>current time</td>
<td>minutes</td>
<td>real</td>
</tr>
<tr>
<td>C(i,j)</td>
<td>matrix variable; i=variable ID; j=axial grid number; k=radial grid number</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>P(i,j)</td>
<td>Old of S array</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>L1</td>
<td>gas temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L2</td>
<td>solid temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L3</td>
<td>wall temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L4</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>L5</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>L6</td>
<td>pressure</td>
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<td>real</td>
</tr>
<tr>
<td>PT</td>
<td>pressure</td>
<td>mm HG</td>
<td>real</td>
</tr>
<tr>
<td>NCOMP</td>
<td>number of component</td>
<td>nonedimension</td>
<td>int</td>
</tr>
<tr>
<td>INERT</td>
<td>type of carrier gas</td>
<td>nonedimension</td>
<td>real</td>
</tr>
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<td>EPSEX1,2</td>
<td>porosity, material type 1,2</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>RHOS1,2</td>
<td>particle density, material type 1, 2</td>
<td>lbs/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>Z</td>
<td>bed length</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>VOID_B</td>
<td>porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>D_I</td>
<td>inside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_E</td>
<td>outside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>S_B</td>
<td>cross sectional area of bed</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_WA</td>
<td>heat capacity of wall</td>
<td>BTU/F/LB</td>
<td>real</td>
</tr>
<tr>
<td>RO_WA</td>
<td>density of wall</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_S1,2</td>
<td>heat capacity of particle type 1,2</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>RO_S1,2</td>
<td>density of particle</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>R_P1,2</td>
<td>particle radius of type 1, 2</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_P1,2</td>
<td>particle diameter type 1, 2</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
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<td>heat of adsorption for each component of BTU/lb mole type 1,2</td>
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<td>real</td>
</tr>
<tr>
<td>NC</td>
<td>number of component</td>
<td>nonedimension</td>
<td>int</td>
</tr>
<tr>
<td>G_F</td>
<td>volumetric flow rate</td>
<td>cu ft/min</td>
<td>real</td>
</tr>
<tr>
<td>TO</td>
<td>initial temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>R</td>
<td>ideal gas law constant</td>
<td>lbf/sq ft</td>
<td>lb real</td>
</tr>
<tr>
<td>P1</td>
<td>constant</td>
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<td>3.14</td>
</tr>
<tr>
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<td>Molecular weight</td>
<td>lb/mole</td>
<td>real</td>
</tr>
<tr>
<td>GC</td>
<td>constant</td>
<td>in hr, ...</td>
<td>real</td>
</tr>
<tr>
<td>K_F</td>
<td>mass transfer coefficient</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>NJ</td>
<td>grids number in axial direction</td>
<td>nonedimension</td>
<td>int</td>
</tr>
<tr>
<td>DELZ</td>
<td>grid size in axial direction</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>DELT</td>
<td>time step</td>
<td>hr</td>
<td>real</td>
</tr>
<tr>
<td>CON_S1</td>
<td>pellet conductivity</td>
<td>BTU/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>ERROR</td>
<td>convergence criteria</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>N</td>
<td>number of equation</td>
<td>non-</td>
<td>int</td>
</tr>
<tr>
<td>dimension</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Y_F</td>
<td>component mole fraction</td>
<td>lb mole/lb</td>
<td>real</td>
</tr>
<tr>
<td></td>
<td></td>
<td>mol</td>
<td></td>
</tr>
</tbody>
</table>
A list of program variables is given below with a brief description (continued).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>P_TOT</td>
<td>Total Pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>BC_L1 to BC_L6</td>
<td>boundary condition for L1 to L6</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>W0</td>
<td>under relaxation coeff</td>
<td>Btu/hr/F/sq</td>
<td>real</td>
</tr>
<tr>
<td>H_OW</td>
<td>heat transfer coefficient outside of the wall</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>REY</td>
<td>Reynolds number</td>
<td>Btu/hr/ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_P</td>
<td>specific heat</td>
<td>lb/ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>VISC_P</td>
<td>viscosity</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>H_FP</td>
<td>heat transfer coefficient fluid-particle</td>
<td>ft/F</td>
<td></td>
</tr>
<tr>
<td>CON_L</td>
<td>fluid axial conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>CON_S1,2</td>
<td>particle conductivity of type 1 and 2</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>H_W</td>
<td>heat transfer coefficient fluid-wall</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>V(i)</td>
<td>Langmuir constant</td>
<td>lb mole/lb</td>
<td>solid</td>
</tr>
<tr>
<td>B(i)</td>
<td>Langmuir constant</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>PO(i)</td>
<td>Langmuir constant</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>PP</td>
<td>component partial Pressure</td>
<td>mm Hg</td>
<td>real</td>
</tr>
<tr>
<td>Q1</td>
<td>adsorbed concentration</td>
<td>lb mol/solid</td>
<td>real</td>
</tr>
<tr>
<td>BC_C1(i)</td>
<td>boundary condition of molar concentration</td>
<td>lb mole/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>W0-W3</td>
<td>under relaxation for each component and nonedimension</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>F(i)</td>
<td>PDE's variable</td>
<td>real</td>
<td></td>
</tr>
<tr>
<td>AINT</td>
<td>interfacial area</td>
<td>sq ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>U_F1</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>LAYER1,2</td>
<td>number of grids for first section, for the nonedimension</td>
<td>int</td>
<td></td>
</tr>
<tr>
<td>EPS</td>
<td>particle porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
</tbody>
</table>
C.4 One Dimensional Thermal Vacuum Desorption FORTRAN Program

A flow chart of the one-dimensional modeling of thermal vacuum desorption is shown in Figures C-7 and C-8. This program simulates a one-dimensional desorption of a fixed-bed column 10 inches long and 1.87 inches in diameter. The users supply initial and boundary conditions in INITIAL subroutine. If it is necessary to run the model with a larger diameter or length, the number of grids must be specified in the INITIAL subroutine.

For each time step the temperature dependent parameters (density, conductivity, viscosity, etc.) are recalculated. If the temperature change is not significant in the packed bed during the simulation, the user can specify that these parameters will not be recalculated.

Solid-gas equilibrium for the pure component is predicted by Langmuir-Freundlich isotherm for the 13X material. For mixtures, two types of solid-gas equilibrium are implemented in the program. One is based on the Langmuir-Freundlich isotherm for mixtures. The second prediction uses the IAST isotherm. The IAST model has an iterative solution and is CPU time intensive. The user can switch an indicator to choose the desired isotherm method.

The energy balance includes the heat lost to the surroundings. Adiabatic simulation of a packed bed can be done by setting the heat transfer coefficient between the wall and the surroundings equal zero.

Heat transfer is assumed between the solid, fluid flow, and the wall of the column. Axial conductivity is included in the model. These parameters vary along axial direction inside the bed. The program is also capable of making these parameters constant by switching the proper indicator.

Mass transfer is presented as lumped resistance model. This resistance is obtained by matching the experimental breakthrough curve with the result of model.

In this model the material balances are based on the partial pressure. The pressure and velocity gradient inside the column are steep. Because of this, the model uses NEWMAN method for calculation of all variables in the PDE's. The total numbers of equations involve for four components is 13.
FIGURE C-7 THE FLOW CHART OF THE MAIN PROGRAM FOR THE THERMAL VACUUM DESORPTION
FIGURE C-8 THE FLOW CHART OF THE SUBROUTINES PROGRAM FOR THE THERMAL VACUUM DESORPTION
A list of program variables is given below with a brief description.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>LL</td>
<td>Time step index</td>
<td>none</td>
<td>Int</td>
</tr>
<tr>
<td>T_Time</td>
<td>current time</td>
<td>minutes</td>
<td>real</td>
</tr>
<tr>
<td>C(i,j)</td>
<td>matrix variable; i=variable ID; j=axial grid number; k=radial grid number</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>P(i,j)</td>
<td>Old of C array</td>
<td>various</td>
<td>real*13</td>
</tr>
<tr>
<td>L1</td>
<td>gas temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L2</td>
<td>solid temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L3</td>
<td>wall temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>L4</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>L5</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>L6</td>
<td>pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>PT</td>
<td>pressure</td>
<td>mmHG</td>
<td>real</td>
</tr>
<tr>
<td>NCOMP</td>
<td>number of component</td>
<td>non-dimensional</td>
<td>real</td>
</tr>
<tr>
<td>INERT</td>
<td>type of carrier gas</td>
<td>non-dimensional</td>
<td>real</td>
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<tr>
<td>EPSEX</td>
<td>porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>RHOS</td>
<td>particle density</td>
<td>lbs/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>Z</td>
<td>bed length</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>VOID_B</td>
<td>porosity</td>
<td>cu ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>D_I</td>
<td>inside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_E</td>
<td>outside bed diameter</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>S_B</td>
<td>cross sectional area of bed</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_WA</td>
<td>heat capacity of wall</td>
<td>BTU/F/LB</td>
<td>real</td>
</tr>
<tr>
<td>RO_WA</td>
<td>density of wall</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>CP_S</td>
<td>heat capacity of particle</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>RO_S</td>
<td>density of particle</td>
<td>lb/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>R_P</td>
<td>particle radius</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>D_P</td>
<td>particle diameter</td>
<td>ft</td>
<td>real</td>
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<td>heat(i)</td>
<td>heat of adsorption for each component</td>
<td>BTU/lb mole</td>
<td>real</td>
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<tr>
<td>N_C</td>
<td>number of component</td>
<td>non-dimensional</td>
<td>real</td>
</tr>
<tr>
<td>G_F</td>
<td>volumetric flow rate</td>
<td>cu ft/min</td>
<td>real</td>
</tr>
<tr>
<td>TO</td>
<td>initial temperature</td>
<td>R</td>
<td>real</td>
</tr>
<tr>
<td>R</td>
<td>ideal gas law constant</td>
<td>lb/sq ft .lb</td>
<td>real</td>
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<tr>
<td>PI</td>
<td>constant</td>
<td>mol/cu ft/R</td>
<td>3.14</td>
</tr>
<tr>
<td>M_W</td>
<td>Molecular weight</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>G</td>
<td>constant</td>
<td>real</td>
<td>real</td>
</tr>
<tr>
<td>K_F</td>
<td>mass transfer coefficient</td>
<td>ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>NJ</td>
<td>grids number in axial direction</td>
<td>non-dimensional</td>
<td>real</td>
</tr>
<tr>
<td>DELZ</td>
<td>grid size in axial direction</td>
<td>ft</td>
<td>real</td>
</tr>
<tr>
<td>DELT</td>
<td>time step</td>
<td>hr</td>
<td>real</td>
</tr>
<tr>
<td>CON_S1</td>
<td>pellet conductivity</td>
<td>BTU/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>ERROR</td>
<td>convergence criteria</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>N</td>
<td>number of equation</td>
<td>non-dimensional</td>
<td>real</td>
</tr>
<tr>
<td>Y_F</td>
<td>component mole fraction</td>
<td>lb mole i/lb</td>
<td>real</td>
</tr>
</tbody>
</table>

C-19
A list of program variables is given below with a brief description (continued).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>P_TOT</td>
<td>Total Pressure</td>
<td>psia</td>
<td>real</td>
</tr>
<tr>
<td>BC_L1 to BC_L6</td>
<td>boundary condition for L1 to L6</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>W0</td>
<td>under relaxation coeff</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>H_OW</td>
<td>heat transfer coefficient outside of the wall</td>
<td>Btu/hr/F/sq</td>
<td>real</td>
</tr>
<tr>
<td>REY</td>
<td>Reynolds number</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>CP_P</td>
<td>specific heat</td>
<td>BTU/F/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>VISC_P</td>
<td>viscosity</td>
<td>lb/ft/hr</td>
<td>real</td>
</tr>
<tr>
<td>H_FP</td>
<td>heat transfer coefficient fluid-particle</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>CON_L</td>
<td>fluid axial conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>CON_S</td>
<td>particle conductivity</td>
<td>Btu/hr/ft/F</td>
<td>real</td>
</tr>
<tr>
<td>H_W</td>
<td>heat transfer coefficient fluid-wall</td>
<td>Btu/hr/sq</td>
<td>real</td>
</tr>
<tr>
<td>V(i)</td>
<td>Langmuir constant</td>
<td>lb mole/lb</td>
<td>solid</td>
</tr>
<tr>
<td>B(i)</td>
<td>Langmuir constant</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>PO(i)</td>
<td>Langmuir constant</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>PP</td>
<td>component partial Pressure</td>
<td>mm Hg</td>
<td>real</td>
</tr>
<tr>
<td>Q1</td>
<td>adsorbed concentration</td>
<td>lb mol/lb</td>
<td>solid</td>
</tr>
<tr>
<td>BC_C1(i)</td>
<td>boundary condition of molar concentration</td>
<td>lb mole/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>W0-W3</td>
<td>under relaxation for each component and temperature</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>F3-F8</td>
<td>PDE's coefficient</td>
<td>various</td>
<td>real</td>
</tr>
<tr>
<td>PE_N_M</td>
<td>mass Peclet number</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>PE_N_H</td>
<td>heat Peclet number</td>
<td>nonedimension</td>
<td>real</td>
</tr>
<tr>
<td>AINT</td>
<td>interfacial area</td>
<td>sq ft/cu ft</td>
<td>real</td>
</tr>
<tr>
<td>U_F1</td>
<td>velocity</td>
<td>ft/hr</td>
<td>real</td>
</tr>
</tbody>
</table>
APPENDIX D

FLOW1MOL FORTRAN CODE

C
C this is the main routine, the initial values of matrix C and parameters are
C called by 'INITIAL_Z' subroutine, the main routine then calls the 'FUNCT2_Z'
C subroutine to solve the discretized partial differential equations (pde's).
C after convergence, the routine calls the "DIFFEQI" subroutine, which is
C the main routine for solving the momentum and the pressure equations.
C if it is desire to solve these two equations as the time progresses.
C
C IMPLICIT REAL*8(A-H,O-Z)
INTEGER IOUT(5),AOUT(4)
CHARACTER*5 LABEL(4)
CHARACTER*8 DATE
CHARACTER*12 OUTFILE, VISFILE
REAL*8 PI(11,301),QP(14,301),T_TIME,K_F(4),END
REAL*8 C1(14,301),P1(14,301),C11(14,301),P11(14,301),C12(14,301)
COMMON/DATE/DATE
COMMON/PLOT/ISAT,LABEL,AOUT,IOUT
COMMON/BND_ZC(14,301),F(14,301),N,NJ
COMMON/PROP_D_Z/DELZ1,DEL,DELZU_F1,Z,END,NC,IL1,LL,K_F
COMMON/INDIC/L1,L2,L3,L4,L5,L6,TIME,PERERR,MT
COMMON/BOUN_CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC_C(4),TO
COMMON/PRO_IND/HTEST2,TEST1
COMMON/NUM_OF_ITR/ITCNT1
COMMON/INDIC1/IND(4)
WRITE(*.*)'DESIGNATE A DATE FOR THE INPUT/OUTPUT FILES'
WRITE(*.*)'FORMAT 00-00-00 WITH DOUBLE QUOTES'
READ*,DATE
OUTFILE = DATE // '.OUT'
VISFILE = DATE // '.VIS'
OPEN (50,FILE=OUTFILE,STATUS='NEW',RECL=32766)
OPEN (66,FILE=VISFILE,STATUS='NEW',RECL=32766)

C IOUT designates the 5 grid locations to be printed/ploted
C LABEL designates the 4 labels for printed/ploted data

C DATA IOUT(2,15,30,45,61)/
C DATA LABEL/ppH20',pp N2',pp N2',gas T/
C Initialize the c array with the initial guesses of the solution

CALL INITIAL_Z
T_TIME=0.
TIME=0.

C Write header data to ACSII file

WRITE(50,47X)(LABEL(I),IOUT(I),I=1,5),J=1,4)

CJK ICOT=1 not used again!
T_TIME=0
NLOOPS = END/DELTI1
IF (IND(2),EQ.0 .OR. ISAT.EQ.1) THEN
IND0=0
NEQ=2*NC+3
NA=NEQ+2
ELSE
IND0=1
NEQ=2*NC
NA=NEQ+5
END IF

D-1
C Begin looping through each time step;
C Call main routine for calculation of state conditions at current time step
DO 301 LL=1,NLOOPS
   ITRAT=0
   CALL diffeq subroutine to compute the pressure and the velocity
121   IF(ITRAT.GT.5)GO TO 201
   DO 30 IT=1,NA
      DO 30 II=1,NJ
         C(I1,I2)=C(I1,I2)
         C(I1..I2)=C(I1..I2)
         P(I1..I2)=P(I1..I2)
      30   CONTINUE
      ITRAT=ITRAT+1
   MT=1
   IF(ITRAT.EQ.1 .AND. LL.EQ.1)THEN
      ITCNT0 = 15
      ELSE IF(ITRAT.EQ.1) THEN
      ITCNT0 = 7
      ELSE
      ITCNT0 = 7
   END IF
   IF(INDO.EQ.1)THEN
      CALL diffeq(C1,P1,NJ,NEQ,1,ITCNT0)
   ELSE
      CALL diffeq(C1,P1,NJ,NEQ,1)
   END IF
   IF(IND0.EQ.1)THEN
      DO 35 IT=1,NEQ
         DO 35 II=1,NJ
            C(I1..I2)=C(I1..I2)
            P(I1..I2)=P(I1..I2)
         35   CONTINUE
         LI3=2*NC+1
      END DO
      DO 31 IT=1,NC
         DO 31 II=1,NJ
            C(I1..I2)=C(I1..I2)
            P(I1..I2)=P(I1..I2)
         31   CONTINUE
         LI3=L13+1
      END DO
      MT=0
   CALL diffeq(C1,P1,NJ,3,3,4)
   DO 31 IT=1,NC*2
      DO 31 II=1,NJ
         C(I1..I2)=C(I1..I2)
         P(I1..I2)=P(I1..I2)
      31   CONTINUE
      LI3=L13+1
      END DO
      DO MM1=1,NC
         DO MM2=1,NJ
            IF(C(MM1,MM2).GT.1.0E-15)THEN
               DIF=ABS(C(MM1,MM2)-C12(MM1,MM2))/C(MM1,MM2)
               IF(DIF.GT.1.0E-2)THEN
                  GO TO 121
               END IF
            END IF
         END DO
      END DO
D-2
END DO
ELSE
DO I = 1, NEQ
DO I2 = 1, NJ
C(I, I2) = C(I, I2) + P(I2)
END DO
END DO
ENDIF
ITESTI = I
IF(ISAT.EQ. 1) GO TO 303
DO 300 I2 = 1, NJ
C(I, I2) = C(L4, I2)
P(I, I2) = P(L4, I2)
C(2, I2) = C(L5, I2) * 760 / 14.696
P(2, I2) = P(L5, I2) * 760 / 14.696
C(3, I2) = C(L6, I2) * 760 / 14.696
P(3, I2) = P(L6, I2) * 760 / 14.696
C(4, I2) = C(L1, I2)
P(4, I2) = P(L1, I2)
300 CONTINUE
IF(IND0.EQ.1) THEN
CALL DIFEQ(C1, P1, NJ3, 2.5)
ELSE
CALL DIFEQ6(C1, P1, NJ3, 2.2)
ENDIF
DO 400 I2 = 1, NJ
C(L4, I2) = C(1, I2)
C(L6, I2) = C(3, I2) * 14.696/760.
400 CONTINUE
C Add time step (converted from dimless to minutes)
303 T_TIME = T_TIME + DELT * Z/U_F*60.
TIME = T_TIME/60.
ITESTI = 0
CJK Do we want to common DELT or DELT1 (both not needed)?
IF(LL.EQ.25) THEN
DELT1 = DELT1 * 2
DELT = 2
ENDIF
IF(LL.EQ.50) THEN
DELT1 = DELT1 * 2
DELT = DELT1 * 2
ENDIF
CJK Eliminate above?
C Convert to units used for plotting (psia to mmHg, R to F, R*8 to R*4)
DO 74 M2 = 1, NJ
DO I1 = 1, NC
QP(I1, M2) = C(I1, M2)*10.73D0*C(L1, M2)*760/14.696
END DO
DO I1 = NC + 1, 2*NC
QP(I1, M2) = C(I1, M2)
END DO
QP(L1, M2) = C(L1, M2) * 460.
QP(L2, M2) = C(L2, M2) * 460.
QP(L3, M2) = C(L3, M2) * 460.
QP(L4, M2) = C(L4, M2)
QP(L5, M2) = C(L5, M2)
QP(L6, M2) = C(L6, M2)
74 CONTINUE
C ISAMP is the sampling frequency, where "10" plots every 10th time step data

ISAMP=10
IF(T_TIME.LT.30) ISAMP=1

C Print runtime output headers every 4th and data every time step

IF(((LL/(ISAMP*4))=ISAMP*4.EQ.LL.OR.LL.LEQ.1) THEN
WRITE(6,49)
WRITE(6,41) ' GRID', IOUT(I), ', I=1,5)
ENDIF
WRITE(6,49)
WRITE(6,40) *** TIME =', T_TIME, ' LOOPS = ITCNT, ***
WRITE(6,42) LABEL(1),(QP(AOUT(1),IOUT(I)), I=1,5)
WRITE(6,42) LABEL(2),(QP(AOUT(2),IOUT(I)), I=1,5)
WRITE(6,43) LABEL(3),(QP(AOUT(3),IOUT(I)), I=1,5)
WRITE(6,43) LABEL(4),(QP(AOUT(4),IOUT(I)), I=1,5)

C Print time slice data 1/10 less often

IF(((LL/ISAMP=10)*ISAMP=10.EQ.LL) THEN
WRITE(66,44) (LABEL(I), I=1,4), T_TIME
WRITE(66,45) (QP(AOUT(I),IOUT(I)), I=1,4), T_TIME
ENDIF

C Print pp, temp output data every ISAMP

IF((LL/ISAMP=*ISAMP.EQ.LL) THEN
WRITE(50,46) T_TIME, (QP(AOUT(I),IOUT(I)), I=1,5), J=1,4)
ENDIF

DO 78 J=1,N
DO 78 I=1,J
P(I,J)=C(I,J)
78 CONTINUE

CONTINUE

FORMAT(1X,A12,G10.2,23X,A8,L4.A5,/,I)
FORMAT(1X,A7.5(A7,B3.A2))
FORMAT(1X,A5.5(2X,G10.2))
FORMAT(1X,A5.5(2X,F10.2))
FORMAT(1X,A5.5(2X,E15.3))
FORMAT(1X,A5.5(2X,E15.5,/,I))
FORMAT(1X,21(E15.5,/,I))
FORMAT(1X,20(A5,B3,/,))
FORMAT(1X,72(=))
STOP
END

C this subroutine is being called by main routine once to get the initial
C values and the neccessary parameters

C SUBROUTINE INITIAL_Z
IMPLICIT REAL*8(A-H,O-Z)
INTEGER IOUT(5), AOUT(4)
REAL*4 K_F(4), END
REAL*8 M_AVE,M_W(4), C_FO(4), IN_L1, IN_L2, IN_L3, IN_L4,
. IN_L5, IN_L6, ss(4), q2(4)
CHARACTER*5 LABEL(4)
CHARACTER*8 DATE
CHARACTER*14 INFILEA, INFILEB
COMMON/DATE/DAT
COMMON/PLOT/ISAT,LABEL,AOUT,IOUT

D-4
COMMON/BND_Z/C(14,301),P(14,301),N,NJ
COMMON/PROP_B/Z/D_E_S_B,CON_WA,CON_WI_Q,CON_WI_K,
   CP_WI,CP_WI_Q,CP_WI_K,RO_WA,RO_WI_Q,RO_WI_K,RO_WI_K,
   X_WI_K,RO_LMIA,RO_LMA,FP_H_OW
COMMON/PROP_S/Z/CP_S,RO_S,AINT,R,P_D_P,CON_S,G_F,HEAT(4),M_W
COMMON/PROP_D/Z/D_ELZ1,DEL_T1,DEL_T1,Z,F,LZ,END,NC,ILL_L,K_F
COMMON/BOUN_CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC_C(4),TO
COMMON/PRO_IN_DTEST2/TEST1
COMMON/INDIC/L12,L13,L14,L15,L6,TIME
COMMON/INDIC1/IND(4)
COMMON/NCY/NC1
COMMON/GAS/INERT,NCOMP
COMMON/PRIME/GNI

C WRITE(*,*)'SELECT FILE CONTAINING INPUT SET A'
INFILEA = DATE //'_A.DAT'
OPEN (UNIT=40,FILE=INFILEA,STATUS='OLD')
C WRITE(*,*)'SELECT FILE CONTAINING INPUT SET B'
INFILEB = DATE //'_B.DAT'
OPEN (UNIT=41,FILE=INFILEB,STATUS='OLD')
C
C INITIALIZATION
C
READ(UNIT=40,FMT=*)END,DEL_T1,NJ,DEL_Z1,TO,G_F,T_O,NC,INERT,P_TOT,
   BC_C(1),BC_C(2),BC_C(3),BC_C(4),Z,D_ELD,RO_WA,EPSEX,
   AINT,CON_S,CP_S,F_W,H_OW,RO_S,M_W(1),M_W(2),M_W(3),M_W(4),
   HEAT(1),HEAT(2),HEAT(3),HEAT(4),K_F(1),K_F(2),K_F(3),K_F(4),
   ind(1),ind(2),ind(3),ind(4),IDES,ISAT,
READ(UNIT=41,FMT=*)
   LABEL(1),LABEL(2),LABEL(3),LABEL(4),AOUT(1),AOUT(2),
   AOUT(3),AOUT(4),AOUT(1),AOUT(2),AOUT(3),AOUT(4),AOUT(5),
   S_B,CON_WA,CON_WI_Q,CON_WI_K,CP_WA,CP_WI_Q,CP_WI_K,
   RO_WI_Q,RO_WI_K,RO_WI_K,RO_WI_K,RO_WI_K,RO_WI_K,RO_WI_K,
   ALPHA1,R_P,D_P,BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,
   IN_L1,IN_L2,IN_L3,IN_L5,IN_L6,P,PL,TEST2,TEST1
C number of component
NC1=NC
c number of equation
N=NC*2+6
ALF=(1.0D0-EPSEX)/EPSEX
PT=P_TOT*760./14.696
N1=1
DO 11=1,4
IF(INDEX(1).EQ.1)THEN
   IF(11,EQ.3)N2=N1
   M_W(N1)=M_W(11)
   BC_C(N1)=BC_C(11)
   HEAT(N1)=HEAT(11)
   K_F(N1)=K_F(11)
   IF(11,EQ.3)THEN
      IDES=N1
      IND3=N1
   ELSE IF(11,EQ.4)THEN
      IN_D4=N1
   END IF
   N1=N1+1
   END IF
END DO
SUM_Y=0
M_AVE=0.
YO=0
C compute the initial mole fraction and average molecular weight
DO 10 I=1,NC
   Y_F=BC_C(I)/P_TOT
   Y_O=Y_F+YO

D-5
SUM_Y = SUM_Y + Y_F

BC_C(I) = P_TOT * Y_F / BC_L1
M_AVE = M_AVE + Y_F * M_W(I)
C_FO(I) = BC_C(I)

10 CONTINUE
M_AVE = M_AVE + (1 - YO) * 28.0
RO_VO = P_TOT / (BC_L1 * R)
G_F = G_F / RO_VO / S_B / 60.
U_F1 = G_F / (S_B * EPSEX)
BC_L4 = U_F1

c make the grid size and the time step dimensionless
DELT_Z = DELZ1 / Z
DELT_U = U_F1 * DELT1 / Z

c L1 is the gas temp, L2 is the solid temp, L3 is the wall temp, L4 is the c velocity, L5 is the total pressure, and L6 is the total pressure without c thermal effect

c
L1 = 2 * NC + 1
L2 = L1 + 1
L3 = L2 + 1
L4 = L3 + 1
L5 = L4 + 1
L6 = L5 + 1

DO 20 I = 1, N
DO 20 I2 = 1, NJ
P(I, I2) = 0.0
C(I, I2) = 0.0

20 CONTINUE

C set the first grid equal to the initial condition
C
DO 22 I = 1, NC
C(I, I) = C_FO(I)

22 CONTINUE

DO 24 I = 1, NJ
C(I1, I2) = 0.0

24 CONTINUE

DO 30 I = 1, NJ
P(L1, I) = IN_L1
P(L2, I) = IN_L2
P(L3, I) = IN_L3
P(L4, I) = BC_L4
P(L5, I) = BC_L5
P(L6, I) = BC_L6
C(L1, I) = BC_L1
C(L2, I) = BC_L2
C(L3, I) = BC_L3
C(L4, I) = BC_L4
C(L5, I) = BC_L5
C(L6, I) = BC_L6

30 CONTINUE
IF (ND2.EQ.1) THEN
DO I = 1, NJ
C(N2(I1)) = C_FO(N2)
END DO
END IF
IF (IDES .EQ. 1) THEN
SS(IDES) = C(IDES, 1)
CALL IST_Z(1, C(L2, 1), BC_L1, SS, Q2)
DO I = 1, NC
Q2(I) = Q2(I) * RO_S
END DO
DO I=1,NJ
C(IDES,I)=C_FO(IDES)
P(IDES,I)=Q2(IDES)
C(IDES+NC,I)=Q2(IDES)
P(IDES+NC,I)=Q2(IDES)
END DO
END IF
IF(ISAT.EQ.1)THEN
DO I=1,NC
SS(I)=BC_C(I)
END DO
CALL IST_Z(1,BC_L1,BC_L2,SS,Q2)
END DO
DO I=1,NC
Q2(I)=Q2(I)*RO_S
END DO
DO II=I,NC
DO 12=I,NJ
C01,12)=BC_C(I)
C(II+NC,12)=Q2(II)
P(II,12)=BC_C(I)
END DO
END DO
DO II=I,NC
BC_C(II)=0
END DO
BC_C(IND3)=c_fo(IND3)
RETURN
END

SUBROUTINE FUNCT1(I)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4),END
REAL*8 M,AVE,M_W(4),KGAS,K_FP(4,301),C1(14,301),
P1(14,301),REY_P(301),KEFF,D_L(4),H(4),YO(4),SS(4),
DIMENSION Q2(4),C2(14,301),PE_N_M(4),RATE_C2(301)
COMMON/PR_OLZ/RO_P(301),CP_P(301),CONN,FPP(301),
CON_LPP(301),D_LPP(4,301),H_FP(301),H_TTPP(301),H_PP(301),
H_OWPP(301),H_FWPP(301),Q(4,301),VISC_P(301),RATE_C(301)
COMMON/BND/A(14,14),B(14,14),C(14,301),D(14,29),X(14,14),
Y(14,14),P(14,301),N,NTPTT,ITCNY(14),P(14,301)
COMMON/PROP_B/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_G/NOP,NOP,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_B/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_G/NOP,NOP,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_B/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
X_W1_K,D_LM,LM_H,FW,H_OW
COMMON/PROP_S/ZIPP,NOZ,CON,WA,CON_WI_Q,CON_W1_K,
CP_WA,CP_W1_Q,CP_W1_K,RO_WA,RO_W1_Q,RO_W1_K,W_X,W1_Q,
C  BC_L1=TEMPIN(TIME)
C  ICOM=LL+1
C  END IF
  IF(ITEST.1.EQ.1)THEN
   D_T=D_E+D_J
   X_W=D_E-D_J
 c calculate the area for the heat transfer, inside and outside
  A_C=2*D_J/(D_I+D_E)*X_W
  A_INS=2*D_E/(D_I+D_E)*X_W
  RO_F=C(L5,I)/(C(L1,1)*R)
c calculate superficial mass velocity
  GN2=G_F*RO_F/S_B/60.
  IF(ITEST1.EQ.1 OR ITTEST2.EQ.1)THEN
    DO 199 J1=1,NJ
    RO_F=C(L5,J1)/(C(L1,1)*R)
    YTOT=0.
c calculate the mole fraction
    DO J1=1,NC-1
    YO(J1)=C(J1,J1)/RO_F
    YTOT=YO(J1)+YTOT
   END DO
    YO(NC)=1-YTOT
    M_AVE=0.
c calculate the average molecular weight
    DO J1=1,NC
    M_AVE=M_AVE+M_W(J1)*YO(J1)
   END DO
    M_AVE=M_AVE/(1-YTOT)*28.0
    TEMP=C(L1,J1)
    GN=GN2
c calculate the viscosity
    VISC_P(J1)=VIS(TEMP)*60
 c calculate reynold's number
    REY=RE(GN,TEMP)
c calculate the heat capacity of the fluid flow
    CP_P(J1)=CPAS(TEMP,YO)
c calculate the film coefficient between the particle and fluid
    H_FP(J1)=HFILM(M_AVE,TEMP,REY,CP_P(J1))*60.
c change the unit on pressure
    PP=C(L5,J1)*760/14.77
 c calculate the axial effective conductivity
    CON_LPP(J1)=EFFK(GN,TEMP,CP_P(J1),RO_F,PP,YO)*60.
c calculate axial mass dispersion for each component
    DO J1=1,NC
    D_LPP(J1,J1)=EFFD(J1,GN,TEMP,RO_F,PP,YO)*60.
    IF(D_LPP(J1,J1),LT.0) THEN
      D_LPP(J1,J1)=D_LPP(J1,J1-1)
    END IF
   END DO
199 CONTINUE
  END IF
 END IF
 c start iteration for each time step
 IF(MT.EQ.1)THEN
  DO J1=1,NC
  D_L(J1)=D_LPP(J1,J)
  END DO
  DO J1=1,NC
  SS(J1)=C(J1,J)
  END DO
 c calculate the equilibrium 2=IST theory; 1=Langmuir theory
 CALL IST_Z(1,J,C(L2,J),BC_L1,SS,Q2)
 DO 40 J1=1,NC

CONTINUE

c compute the C array for the first grid
IF(J.EQ.1) THEN

DO 85 M1 = 1, NC
PE_N_M(M1) = U_F1 * Z / D_L(M1)
85 CONTINUE

CONTINUE
C_TOT = 0
DO 90 M1 = 1, NC - 1
F2 = ALP * K_F(M1) * AINT * Z / U_F1
F(M1) = 1.0D0 / PE_N_M(M1) / DELZ ** 2 * (BC(C(M1,1)) - 2*C(M1,1) -
C(M1,1) - 1) * 1.0D0 / U_F1 / DELZ * (C(M1,1) - BC(C(M1))) * C(L4,1) -
F2 * (Q(M1,1) - C(NC + M1,1)) - (C(M1,1) - P(M1,1)) / DELT
C_TOT = C_TOT + C(M1,1)
90 CONTINUE

F(NC) = C(L5,1) - C_TOT * C(L1,1) * R / (C(L1,1) * R) - C(NC,1)

CONTINUE

C compute amount adsorbed on the pellet
DO 70 M1 = 1, NC
F1 = K_F0 * AINT * Z / U_F1
F(NC + M1) = F1 * (Q(M1,1) - C(M1 + NC,1) - (C(M1 + NC,1) - P(NC + M1,1)) / DELT
70 CONTINUE

CONTINUE
FLUX1 = 0.
FLUX2 = 0.
DO 100 M1 = 1, NC

CONTINUE

C compute total amount adsorbed
FLUX0 = AINT * K_F(M1) * (Q(M1,1) - C(NC + M1,1))
FLUX2 = FLUX2 + FLUX0
FLUX1 = FLUX1 + FLUX0 * HEAT(M1)
100 CONTINUE

C compute the amount adsorbed on the bed
DO 110 M1 = 1, NC
F1 = K_F(M1) * AINT * Z / U_F1
F(NC + M1) = F1 * (Q(M1,1) - C(M1 + NC,1) - (C(M1 + NC,1) - P(NC + M1,1)) / DELT
110 CONTINUE

C compute the molar concentration of each component
DO 130 M1 = 1, NC - 1
F2 = ALP * K_F(M1) * AINT * Z / U_F1
F(M1) = 1.0D0 / PE_N_M(M1) / DELZ ** 2 * (Q * C(M1,1 - 1) - 2 * C(M1,1) -
1.0D0 / U_F1 / DELZ * (C(M1,1) - C(M1,1 - 1)) * C(L4,1) - F2 * (Q(M1,1) -
C(NC + M1,1) - (C(M1,1) - P(M1,1)) / DELT
C_TOT = C_TOT + C(M1,1)
130 CONTINUE

F(NC) = C(L5,1) - C_TOT * C(L1,1) * R / (C(L1,1) * R) - C(NC,1)

CONTINUE

C compute the amount adsorbed on the particle
DO 140 M1 = 1, NC
F1 = K_F(M1) * AINT * Z / U_F1
F(NC + M1) = F1 * (Q(M1,1) - C(NC + M1,1)) - (C(M1 + NC,1) - P(NC + M1,1)) / DELT
140 CONTINUE

CONTINUE
RATE\_C1(J)=FLUX2
RATE\_C2(J)=FLUX1
C
C INTERIOR ROWS
C computation of C array for interior grids
ELSE
DO 165 M1=1,NC
PE\_N\_M(M1)=U\_F1\_Z/D\_L(M1)
165 CONTINUE
C\_TOT=0.
c compute the molar concentration
DO 170 M1=1,NC-1
FLUX2=ALF*K\_F(M1)*AINT*Z/U\_F1
FLUX1=(1.0D0/PE\_N\_M(M1)/DELZ)**2*(C(M1,J-1)-2*C(M1,J)+
C(M1,J+1))-1.0D0/U\_F1/DELZ*(C(M1,J)-C(M1,J-1))*C(L4,J)-
FLUX2*(Q(M1,J)-C(NC+M1,J))-(C(M1,J)-P(NC+M1,J))/DELT
C\_TOT=C\_TOT+C(M1,J)
170 CONTINUE

F(\_NC)=(C(L5,J)-C\_TOT*C(L1,J)*R)/(C(L1,J)*R)-C(NC,J)
c compute the amount adsorbed on
DO 150 M1=1,NC
FLUX1=K\_F(M1)*AINT*Z/U\_F1
F(NC+M1)=FLUX1*(Q(M1,J)-C(NC+M1,J))/FLUX1+FLUX1*HEAT(M1)
150 CONTINUE

RATE\_C1(J)=FLUX2
RATE\_C2(J)=FLUX1
C
END IF
ELSE
C compute the C array for the first grid
C
RO\_F=C(L5,J)/(C(L1,J)*R)
CP\_F=CP\_P(J)
H\_FS=H\_FP(J)
CON\_L=CON\_LPP(J)
c Peclet number for the solid
PE\_N\_S=U\_F1*RO\_S*CP\_S*Z/CON\_S
C Peclet number for the heat
PE\_N\_H=U\_F1*RO\_P*CP\_P*Z/CON\_L
C these are coefficient the Discretized PDE's
F3=ALP*H\_FS*Z/AINT/(RO\_P*CP\_P*U\_F1)
F4=H\_FW*Z*4/(U\_F1*D\_J)*EPSEX*RO\_P*CP\_P
F5=H\_FS*AINT*Z/(U\_F1*RO\_S*CP\_S)
F6=Z/(RO\_S*CP\_S)
F7=Z*H\_FW*A\_C/U\_F1/RO\_WA/CP\_WA
F8=Z*H\_OW*A\_INS/U\_F1/RO\_WA/CP\_WA
IF(J.EQ.1)THEN
C compute gas temperature
F(1)=1.0D0/PE\_N\_H/DELZ**2*(BC\_L1-2*C(1,J)+C(1,J+1))-
1.0D0/(DELZ*U\_F1)*(C(1,J)-BC\_L1)*C(L4,J)-F3*(C(1,J)-C(2,J))-
-F4*(C(1,J)-C(3,J)-C(1,J)-P(1,J))/DELT
C compute the solid temperature
F(2)=1.0D0/PE\_N\_S/DELZ**2*(BC\_L1-2*C(2,J)+C(2,J+1))+
SUBROUTINE FUNCTION(F)
IMPLICIT REAL*8(A-H,O-Z)
REAL*4 K_F(4),END
REAL*8 M_AVE,M,W(4),KGAS,K_FP(4,301),C1(14,301),
P1(14,301),REY_P(301),K_EFF,D_L(4),H(4),YO(4),SS(4)
DIMENSION Q(4),C2(14,301),PE_N_M(4)
COMMON/PR_OLD Z/RO P(301 _CP_P(301 ),CON_FPP(301 ),
CON_LPPO01).D_LPP(4,301).H_FPO01).H_T_O01).H_.I_(301),
H_OWPPO01).H_FWPP(301),Q(4,301).VISC_PO01).RATE_C1(301)
COMMON/BND/A(14,14),B(14,14),C(14,.301),D(14,29),X(I
4,14),y( 14,14),G(14),N,NArI'PRTXI'L_T,F(14),P(14,301)
COMMON/PROP_B_TdD_LD_E,S_B,CON_WA, CON_WI_Q,CON_WI_K,
CP_WA,CP_WI_Q,CP_WI_K,RO_WA,RO_WI_Q,RO_WI_K,X_WA,X_WI_Q,
X_WI_KD_LMLD_LMAH_FW,H_OW
COMMON/PROP_S_Z/CP_S,RO_SAI.NT,R_P.D_P,P,CON_S G,F,HEAT(4),M_W
COMMON/PROP_D_Z/DELT1,DELT,DELZ,U_F1,Z_END,NC,ILL,K_F
IF(LL.EQ.JCOM) THEN
  BC_L1 = TEMPIN(TIME)
  ICOM = LL+1
ENDIF

IF(ITEST1.EQ.1) THEN
  D_T = D_E + D_J
  X_W = D_E - D_J
endif

calculate the area for the heat transfer, inside and outside
A_C = 2*D_I/((D_I + D_E)*X_W)
A_INS = 2*D_E/((D_I + D_E)*X_W)
RO_F = C(L5,1)/(C(L1,1)*R)
calculate superficial mass velocity
GN2 = G_F * RO_F / S_B / 60.
ENDIF

IFDEF (TEST1.EQ.1.OR. ITEST2.EQ.1) THEN
  DO 199 J1 = 1,NJ
    RO_F = C(L5,J1)/(C(L1,J1)*R)
    YTOT = 0.
    YO(J1) = C(L1,J1)/RO_F
    END DO
    YO(NC) = 1 - YTOT
  M_AVE = 0.
calculate the average molecular weight
  DO 11 = 1,NC
    M_AVE = M_AVE + M_W(J1)*YO(J1)
  END DO
  M_AVE = M_AVE / (1 - YTOT) * 28.0
  TEMP_C = C(L1,J1)
  GN = GN2
calculate the viscosity
  VISC_P(J1) = VIS(TEMP)*60
  c calculate reynold's number
  REY = RE(GN,TEMP)
calculate the heat capacity of the fluid flow
  CP_P(J1) = CPAS(TMP,YO)
calculate the film coefficient between the particle and fluid
  H_FP(J1) = HFILM(M_AVE,TEMP,REY,CP_P(J1))*60.
calculate the unit on pressure
  PP = C(L5,J1)*760 /14.77
  c calculate the axial effective conductivity
  CON_LPP(J1) = EFFK(GN,TEMP,CP_P(J1),RO_F,PP,YO)*60.
calculate the axial mass dispersion for each component
  DO II = 1,NC
    D_LPP(II,J1) = EFFD(II,GN,TEMP,RO_F,PP,YO)*60.
    IF (D_LPP(II,J1) LT 0) THEN
      D_LPP(II,J1) = D_LPP(II,J1 - 1)
    END IF
  END DO
END IF
199 CONTINUE
ENDIF
ITEST1 = 0
ENDIF
RO_F = CP_J(Y/C(L, J)*R)
CP_F = CP_J
H_FS = H_FP(J)
CON_L = CON_LPP(J)
DO I=1, NC
D_L(I) = D_LPP(I, J)
END DO
c Peclet number for the solid
PE_N_S = U_F1*RO_S*CP_S*Z/CON_S
PE_N_H = U_F1*RO_P*CP_P*Z/CON_L
c these are coefficient the Discretized PDE's
F3 = AINT*(RO_F*CP_F*U_F1)
F4 = H_FW*M*4/(U_F1*D_I*EPSEX*RO_F*CP_F)
F5 = AINT*Z/(RO_S*CP_S*U_F1)
F6 = AINT*(RO_P*CP_P*U_F1)
F7 = Z*H_FW*A/CON/RO_WA*CP_WA
F8 = A/CON/RO_WA/CP_WA
DO I=1, NC
SS(I) = C(I, J)
END DO
c calculate the equilbrium 2=IST theory; 1=Langmuir theory
CALL IST_Z(1, C(L, J), BC_L, SS, Q, 2)
DO 40 I=1, NC
Q(L) = Q(I)*RO_S
40 CONTINUE
c compute the C array for the first grid
IF(J.EQ.1) THEN
DO 85 M = 1, NC
PE_N_M = U_F1*Z/D_L(M)
H(M) = 1.0D0/DELZ+2/PE_N_M(DLZ**2+1)/U_F1/DELZ*C(L, J)
85 CONTINUE
C_TOT = 0
DO 90 M = 1, NC-1
F2 = A*RO_F(M)*AINT*Z/U_F1
F(M) = C(M, J)*+1.0D0/PE_N_M(DLZ**2*(BC_C(M)+C(M, J)+2+1.0D0/U_F1/DELZ*(-BC_C(M)*C(M, J)-F2*(Q(M, J)-C0..C+M, J))+P(M, J))
C_TOT = C_TOT+C(M, J)
90 CONTINUE
F(NC) = (C(L, J)-C_TOT*C(M, J)*R)/(C(L, J)*R)-C(NC, J)
c compute amount adsorbed on the pellet
DO 70 M = 1, NC
F1 = K_F(M)*AINT*Z/U_F1
A2 = 1/DELZ+F1
F(NC+M) = C(NC+M, J)+1/A2*(F1*Q(M, J)+P(NC+M, J))/DELZ)
70 CONTINUE
FLUX1 = 0
FLUX2 = 0
DO 100 M = 1, NC
100 CONTINUE
RATE_C1(J) = FLUX2
c compute gas temperature
AL1 = 1/DELZ+2/PE_N_H(DLZ**2+(C(L, J)+DELZ/U_F1+F3+F4)
F(L1) = C(L1)+1*0.0D0/PE_N_H(DLZ**2*(BC_L1+C(L1)+1)+
1.0D0/DELZ*(U_F1)*(-BC_L1+C(L, J)-F3*(-C(L2, J)-F4*(-C(L3, J)+
P(L1, J))/DELZ)
c compute solid temperature
F(L2) = C(L2)+DELZ*(1.0D0/PE_N_S/DELZ**2*(3*BC_L1-2*C(L, J)+

d-13
C(I.2, 1)F5 , (C(L1)j')...C(L2_j)-F6*FLUX

\[ \text{compute wall} \]

\[ F(L3)=-(C(L3)_j+DELT*(F7*(C(L1)_j-C(L3)_j)-F8*(C(L3)_j-TO))+P(L3)_j) \]

C

C

C

THE LAST ROW

C

c compute the C_array for the last grid

ELSE IF(J.EQ. NJ) THEN

DO 125 M1=1, NC

PE N M(M1)=U_FI*Z/D_L(M1)

H(M1)=1.0/D DELT+2.0/PE N M(M1)/DELT**2+1/U_FI/DELZ*C(L4j)

125 CONTINUE

C_TOT=0.

c compute the molar concentration of each component

DO 130 M1=1,NC-1

Fi2=ALF*K_F(M1)*AINT*Z/U_FI

F(M1)=C(M1)_j+1.0/H(M1)*(1.0/PE N M(M1)/DELT**2*

. (C(M1j-1)+C(M1j-1))-1.0/U_FI/DELZ*(C(M1j-1)*

. C(L4j)-F2*(Q(M1j, C(NC+M1j))+P(M1j)/DELT)

TOT_C=C(M1j)*TOT_C

C_TOT=C_TOT+C(M1j)

130 CONTINUE

F(NC)=(C(L5j)-C_TOT*C(L1j)*R)/(C(L1j)*R)-C(NCj)

c compute the amount adsorbed on the bed

DO 110 M1=1,NC

Fi=K_F(M1)*AINT*Z/U_FI

A2=1/DELT+F1

F(NC+M1)=C(NC+M1j)+I/A2*(Fi*Q(M1j)+P(NC+M1j)/DELT)

110 CONTINUE

FLUX1=0.

FLUX2=0.

DO 140 M1=1,NC

c compute total heat of adsorption

FLUX1=FLUX1+HEAT(M1)*(K_F(M1)*Q(M1j)-C(NC+M1j))

c compute total amount adsorbed on the particle

FLUX2=FLUX2+AINT*K_F(M1)*Q(M1j)-C(NC+M1j)

140 CONTINUE

RATE_C1(J)=FLUX2

c compute the gas temperature

AL1=1/DELT+2.0/PE N H/DELZ**2+C(L4j)/DELT/U_FI+F3+F4

F(L1)=-C(L1j)+1.0/H(L1j)*(1.0/DELT*U_FI)*(-C(L1j-1)*C(L4j)-

F3*(-C(L4j))-F4*(-C(L3j))+P(L1)/DELT)

c compute the solid temperature

FLUX1=FLUX1+HEAT(M1)*(K_F(M1)*Q(M1j)-C(NC+M1j))

FLUX1=FLUX1+HEAT(M1)*(K_F(M1)*Q(M1j)-C(NC+M1j))

2*C(L2j)+F2*(C(L2j)-C(L2j-1))=F5*(C(L1j)-C(L2j))-F6*FLUX1)+P(L2j)

c compute the wall temperature

FLUX1=FLUX1+HEAT(M1)*(K_F(M1)*Q(M1j)-C(NC+M1j))

FLUX1=FLUX1+HEAT(M1)*(K_F(M1)*Q(M1j)-C(NC+M1j))

. P(L3j)

C

C

C

INTERIOR ROWS

C computation of C_array for interior grids

ELSE

DO 165 M1=1, NC

PE N M(M1)=U_FI*Z/D_L(M1)

H(M1)=1.0/D DELT+2.0/PE N M(M1)/DELT**2+1.0/U_FI/DELZ*

C(L4j)

165 CONTINUE

C_TOT=0.
c compute the molar concentration
  DO 170 M1=1,NC-1
    F2=ALF*K(F(M1)+AINT*Z/U_F1
    F(M1)=C(M1,J)+1.0D0/H(M1)*(1.0D0/PE_N_M(M1)/DELZ**2)*
      (C(M1,J-1)+C(M1,J+1)-1.0D0/U_F1/DELZ**2*C(M1,J-1)+
      C(L4,J)-F2*(Q(M1,J)-C(NC+M1,J)+P(M1,J)/DELZ)
    C_TOT=C_TOT+C(M1,J)
  CONTINUE
  F(NC)=(C(L5,J)-C_TOT*C(L1,J)*R)/(C(L1,J)*R)-C(NC,J)

C compute the amount adsorbed on
  DO 150 M1=1,NC
    F1=K_F(M1)*AINT*Z/U_F1
    A2=1/DELTA+F1
    F(NC+M1)=C(NC+M1,J)+1.0D0/A2*(F1*Q(M1,J)+P(NC+M1,J)/DELZ)
  CONTINUE
  FLUX1=0.
  FLUX2=0.
  DO 180 M1=1,NC

  c compute total heat of adsorption
    FLUX1=FLUX1+HEAT(M1)*K_F(M1)*(Q(M1,J)-C(NC+M1,J))
  c compute total amount adsorbed
    FLUX2=FLUX2+AIN'T*K_F(M1)*(Q(M1,J)-C(NC+M1,J))
  180 CONTINUE
  RATE_CI(.D)=FLUX2

  c compute gas temperature
    A1=1./DELTA**2.*PE_N_H/DELZ**2+C(L4,J)/DELZ/U_F1+F3+F4
    F(L1)=C(L1,J)+1./A1]*(1.0D0/PE_N_H/DELZ**2*(C(L1,J)-1.0D0/PE_N_S/DELZ**2*(C(L2,J)-2.0D0/PE_N_M/DELZ**2*(C(L1,J)-1.0D0/PE_N_P/DELZ**2*(C(L3,J)-F3*
      (-C(L2,J))-F4*(-C(L3,J))+P(L1,J)/DELZ)
  c compute solid temperature
    F(L2)=C(L2,J)+DELTA*1.0D0/PE_N_S/DELZ**2*(C(L2,J)-2.0D0/PE_N_M/DELZ**2*(C(L2,J)-2.0D0/PE_N_P/DELZ**2*(C(L2,J)-2.0D0/PE_N_S/DELZ**2*(C(L2,J)-2.0D0/PE_N_P/DELZ**2*(C(L2,J)-2.0D0/PE_N_P/DELZ**2*(C(L2,J)-2.0D0/PE_N_P/DELZ**2*(C(L2,J)-F3*
      (-C(L2,J))-F4*(-C(L3,J))+P(L2,J)
  c compute wall temperature
    F(L3)=(-C(L3,J)+DELTA*(F7*(C(L1,J)-C(L3,J))-F8*(C(L3,J)-TO)
    P(L3,J)
  END IF
  210 RETURN
END

C

C THIS SUBROUTINE IS BEING CALLED BY DIFFEQ1 WHICH IS ALSO BEING CALLED BY
C SUBROUTINE FUNCT2_Z TO COMPUTE THE VELOCITY AND THE PRESSURE DROP IN THE BED.
C THE EQUATIONS ARE BEING SOLVED BY NEWMAN'S METHOD.

C SUBROUTINE FUNCT2(J)

IMPLICIT REAL*8(A-H,O-Z)
REAL*8 D_L(4),M_AVE
COMMON/OLD/ AA(14),SUM(14),COLD(14,301)
COMMON/BND/A(14,14),B(14,14),C(14,301),D(14,301),X(14,14),
  Y(14,14),G(14,14),N,N,IT,P,T,F(14,14,301)
COMMON/PP_0LD/Z, RO_P(301), CP_P(301),CON_FPP(301),
  CON_LPP(301),D_LPP(4,301),H_FP(301),H_TTP(301),H_IIP(301),
  H_OWPP(301),H_FWPP(301),Q(301),VISC_P(301),RATE_CI(301)
COMMON/BOUN_CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC_L7,BC_L8,
  BC_L9,BC_L10,BC_L11,BC_L12,BC_L13,BC_L14,BC_L15,BC_L16,BC_L17,BC_L18,
  BC_L69,BC_L70,BC_L71,BC_L72,BC_L73,BC_L74,BC_L75,BC_L76,BC_L77,BC_L78,
  BC_L79,BC_L80,BC_L81,BC_L82,BC_L83,BC_L84,BC_L85,BC_L86,BC_L87,BC_L88,
  BC_L89,BC_L90,BC_L91,BC_L92,BC_L93,BC_L94,BC_L95,BC_L96,BC_L97,BC_L98,
  BC_L117,BC_L118,BC_L119,BC_L120,BC_L121,BC_L122,BC_L123,BC_L124,BC_L125,
  BC_L144,BC_L145,BC_L146,BC_L147,BC_L148,BC_L149,BC_L150,BC_L151,BC_L152,
  BC_L171,BC_L172,BC_L173,BC_L174,BC_L175,BC_L176,BC_L177,BC_L178,BC_L179,
  BC_L198,BC_L199,BC_L200,BC_L201,BC_L202,BC_L203,BC_L204,BC_L205,BC_L206,
C MASS TRANSFER FROM THE BULK OF GAS STREAM TO THE SURFACE OF ABSORBENT
C
C ESTABLISHED COEFFICIENT MATRIX
C
C THE FIRST ROW
C
C set parameters, total adsorbed, viscosity, density
NC=NC1
RATE=C-RATE_C(I(J)
VISC_F=VISC_P(J)
KK=0
SUM1=0.
DO I=1,NC
D_L(I)=D_LPP(I)
IF(D_L(I).GT.0).THEN
KK=KK+1
SUM1=SUM1+D_L(I)
ENDIF
END DO
D_L_AVE=SUM1/KK
RO_F=2(C(L5.J)/(C(L1.J)**R1)
IF(J.EQ.1).THEN
C compute the velocity for the first grid
F(L4)=FAC*(C(L5,J)-BC_L5*CONV)/DELZ1+1/GC*(RO_F*M_AVE*C(L4,J)*
. (C(L4.J)-BC_L4)/DELZ1+150*(1-EPSEX)**2*VISC_F*C(L4,J)/
. D_P/D_P/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
. D_P/EPSEX+RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELZ1)
C compute the pressure without the heat effect
F(L5)=(C(L5,J)-P(L5,J)/DELZ1-D_L_AVE/DELZ1**2*(BC_L5*CONV-
. 2*(C(L5,J)+C(L5,J+1))-C(L4,J)**C(L5,J)-BC_L5*CONV)/DELZ1+
. C(L5,J)**C(L4.J)-BC_L4)/DELZ1+R1*C(L1.J)*ALF*RATE_C
C compute the pressure with heat effect
F(L6)=(C(L6,J)-P(L6,J)/DELZ1-D_L_AVE/DELZ1**2*(BC_L6*CONV-
. 2*(C(L6,J)+C(L6,J+1))-C(L4,J)**C(L6,J)-BC_L6*CONV)/DELZ1+
. C(L6,J)**C(L4.J)-BC_L4)/DELZ1-C(L6,J)/C(L1.J)**C(L1.J-
. P(L1,J)/DELZ1-D_L_AVE/DELZ1**2*(C(L1,J+1)-2*C(L1,J)+BC_L1)+
. C(L4,J)**C(L1,J+1)-BC_L1)/(2*DELZ1)+R1*C(L1.J)*ALF*RATE_C
C the last grid
ELSE IF(J.EQ.N).THEN
C compute the velocity
F(L4)=FAC*(C(L5,J)-C(L5,J-1))/DELZ1+1/GC*(RO_F*M_AVE*C(L4,J)*
. (C(L4.J)-C(L4,J-1))/DELZ1+150*(1-EPSEX)**2*VISC_F*C(L4,J)/
. D_P/D_P/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/D_P/
. EPSEX+RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELZ1)
C compute the pressure without the heat effect
F(L5)=(C(L5,J)-P(L5,J)/DELZ1-D_L_AVE/DELZ1**2*(C(L5,J-1)-
. 2*(C(L5,J)+C(L5,J-1))-C(L4,J)**C(L5,J)-C(L5,J-1))/DELZ1+
. C(L5,J)**C(L4.J)-C(L4,J-1))/DELZ1+R1*C(L1.J)*ALF*RATE_C
C compute the pressure with the heat effect
F(L6)=(C(L6,J)-P(L6,J)/DELZ1-D_L_AVE/DELZ1**2*(C(L6,J-1)-
. 2*(C(L6,J)+C(L6,J-1))-C(L4,J)**C(L6,J)-C(L6,J-1))/DELZ1+
. C(L6,J)**C(L4.J)-C(L4,J-1))/DELZ1-C(L6,J)/C(L1.J)**C(L1,J-
. P(L1,J)/DELZ1-D_L_AVE/DELZ1**2*(C(L1,J-1)-2*C(L1,J)+C(L1,J-1))+
. C(L4,J)**C(L1,J-1)-C(L1,J-1)/(2*DELZ1)+R1*C(L1.J)*ALF*RATE_C
C
C
C interior grids
ELSE
C
C
D-16
c compute velocity

\[
F(L4) = \frac{F(L5, J) - C(L5, J - 1)}{DELZ1} + 1.0C*G\cdot C(L4, J)\cdot (RO_F M\_AVE C(L4, J) - C(L4, J - 1)) / DELZ1 + 1.75(1 - EPSEX)**2*VISC_F\cdot C(L4, J) / D_P + D_P / EPSEX / EPSEX + 1.75(1 - EPSEX)*RO_F M\_AVE C(L4, J) + R1 C(L4, J) ALF\_RATE\_C
\]

c compute pressure without the effect

\[
F(NO) = \frac{C(L5, J - P(L5, J))}{DELZ1} - D_L_AVE / DELZ1**2*(C(L5, J - 1) - 2*C(L5, J) + C(L5, J + 1)) + C(L5, J)\cdot C(L5, J - 1) / DELZ1 - C(L5, J)/C(L5, J)\cdot ((C(L5, J) - P(L5, J)) / DELT1 - D_L_AVE / DELZ1**2*(C(L5, J) - 2*C(L5, J) + C(L5, J + 1)) + C(L5, J)\cdot C(L5, J - 1)) / (2*DELZ1) + R1 C(L5, J) ALF\_RATE\_C
\]

END IF

C---------------------------------------------------------------------
210 RETURN

END

C---------------------------------------------------------------------
SUBROUTINE DIFFEQ(C1, P1, N1, N1, N1, IND1)
IMPLICIT REAL*8(A-H, O-Z)
C***************************************************************
C GENERALIZED CALLING PROGRAM FOR BAND(J) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY
C***************************************************************
C CALLED BY: MAIN CALLING PROGRAM
C***************************************************************
C***************************************************************
C SUBROUTINES CALLED:
C WRTOUT (FOR DATA OUTPUT)
C BAND (TO SOLVE BANDED TRIDIAGONAL COEFFICIENT MATRIX)
C FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
C FOR A VARIABLE)
C***************************************************************
C***************************************************************
C LIST OF IMPORTANT VARIABLES:
C A A coefficient described in Newman, Appendix C
C AA first AA is F(WORKC*CU). Later AA is the
C value of the derivative df/dc used in Newton's
C method
C B A coefficient described in Newman, Appendix C
C C variables to be solved for
C CD multiplication factor used in obtaining
C numerical derivatives
C COLD value of C from previous iteration
C CU 2.0 - CD
C D D coefficient described in Newman, Appendix C
C ERR convergence criterion
C F value of function f(C), calculated in FUNCT
C G residual of f(C) calculated with updated C value
C I index used for equation number
C ITCNT index for iteration number
C ITPRT flag used for determining whether intermediate
C calculations are output; for ITPRT=0, only
C converged results are output; for
C ITPRT=1, results of each iteration are printed.
C***************************************************************
C***************************************************************

D-17
CONTINUE

LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F(I).

DO 60 J=1,NJ
   IF(IND1.EQ.1) THEN
      CALL FUNCT0(J)
   ELSE
      CALL FUNCT2(J)
   END IF
   DO 15 I=1,N
      SUM(I)=0.0
      G(I)=-F(I)
   CONTINUE

THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
(IN RELATION TO J).

IF (J.EQ.1) THEN
   MM=0
ELSE IF (J.LT.NJ) THEN
   MM=-1
ELSE
   MM=-2
   END IF
   DO 50 M=MM,MM+2

ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC

DO 50 K=1,N
   SAVEC=C(KJ+M)
   WORKC=SAVEC

DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)

IF (ABS(WORKC).LT.TINY) THEN
   IF (ABS(WORKC).LT.TINIER) WORKC=SIGN(TINIER,WORKC)
   C(KJ+M)=1.2*WORKC
   ELSE
   CALL FUNCT0(J)
   END IF
   DO 20 I=1,N
      AA(I)=-F(I)
   CONTINUE

C(KJ+M)=1.1*WORKC
IF (IND1.EQ.1) THEN
   CALL FUNCT0(J)
ELSE
   CALL FUNCT2(J)
END IF
   DO 25 I=1,N
      AA(I)=AA(I)+4.0*F(I)
   CONTINUE
C(KJ+M)=WORKC
IF (IND1.EQ.1) THEN
   CALL FUNCT0(J)
ELSE
   CALL FUNCT2(J)
   END IF
   DO 30 I=1,N
AA(I)=(AA(I)-3.0*F(I))/(0.2*WORKC)

CONTINUE

C
C DERIVATIVES CALCULATED FOR LARGER VALUES OF C (GREATER THAN TINY)
C
ELSE
C(KJ+M)=WORKC*CU
IF(IND1.EQ.1)THEN
   CALL FUNCT0(I)
ELSE
   CALL FUNCT2(I)
END IF
DO 35 I=1,N
   AA(I)=F(I)
35 CONTINUE
C(KJ+M)=WORKC*CD
IF(IND1.EQ.1)THEN
   CALL FUNCT0(I)
ELSE
   CALL FUNCT2(I)
END IF
DO 40 I=1,N
   AA(I)=(AA(I)-F(I))/((CU-CD)*WORKC)
40 CONTINUE
ENDIF
C(KJ+M)=SAVEC
C
VALUES FOR A, B, D, X AND Y GIVEN. SUM IS ALSO INCREMENTED
C
DO 45 I=1,N
   SUM(I)=SUM(I)+AA(I)*C(KJ+M)
   IF (M.EQ.-2) Y(IK)=AA(I)
   IF (M.EQ.-1) A(IK)=AA(I)
   IF (M.EQ.0) B(IK)=AA(I)
   IF (M.EQ.1) D(IK)=AA(I)
   IF (M.EQ.2) X(IK)=AA(I)
45 CONTINUE

CONTINUE
50 CONTINUE
G(I)=G(I)-SUM(I)
55 CONTINUE
C
BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(I)
60 CONTINUE
C
CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO 65 K=1,N
   DO 65 J=1,NJ
      IF(DABS((C(KJ)-COLD(KJ))/C(KJ))GT.ERR) GO TO 70
   ENDIF
65 CONTINUE
GO TO 80
70 IF(ITPRT GT 0) CALL WRTOUT2
75 CONTINUE
80 CONTINUE
DO 95 II=1,N1
   DO 95 I2=1,NJ1
      CI(I1,I2)=C(I1,I2)
95 CONTINUE

D-20
SUBROUTINE DIFFEQ(C1,P1,N1,NJ1,IND1,ITCNT0)
IMPLICIT REAL*8(A-H,O-Z)

C GENERALIZED CALLING PROGRAM FOR BAND(J) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY
C
C CALLED BY: MAIN CALLING PROGRAM
C
C SUBROUTINES CALLED:
C WRITOUT (FOR DATA OUTPUT)
C BAND (TO SOLVE BANDED TRIDIAGONAL COEFFICIENT MATRIX)
C FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
C FOR A VARIABLE)
C
C
C LIST OF IMPORTANT VARIABLES:
C
A A coefficient described in Newman, Appendix C
AA first, AA is F(WORKC*CU). Later AA is the
value of the derivative df/dc used in Newton's
method
B B coefficient described in Newman, Appendix C
C C variables to be solved for
CD multiplication factor used in obtaining
numerical derivatives
COLD value of C from previous iteration
CU 2.0 - CD
D D coefficient described in Newman, Appendix C
ERR convergence criterion
F value of function f(C), calculated in FUNCT
G residual of f(C) calculated with updated C value
I index used for equation number
ITCNT index for iteration number
ITPRT flag used for determining whether intermediate
calculations are output; for ITPRT=0, only
converged results are output; for
ITPRT=1, results of each iteration are printed.
J index for node number
K index for equation number
M index used in working through nodes used to
calculate numerical derivatives
MM used to determine starting node (in relation to
J) for estimation of numerical derivatives
N number of equations (no. of variables)
NJ number of node points
SAVEC saved value of C
SUM intermediate value used in calculating G
TINIER criterion used to avoid working with small numbers
TINY criterion used to avoid working with small numbers
TNIEST criterion used to avoid working with small numbers
WORKC saved value of C; modified when C less than Tinier
X X value described in Newman, Appendix C
Y Y value described in Newman, Appendix C
DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
WHATEVER YOU WANT.

REAL*8 C1(14,301),P1(14,301)
COMMON/INDIC/L1,L2,L3,L4,L5,L6
COMMON/OLD/AA(14),SUM(14),COLD(14,301)
COMMON/BND/A(14),B(14,14),C(14,301),D(14,29),X(14,14),
Y(14,14),G(14),N,NJ,ITPRT,ITCNT,P(14),P(14,301)
COMMON/NUM_OF_JTR/ITCNT
COMMON/NCY/NCI

DATA TINY0,TINIER0,TNIE0,ERR/1.0D-10,1.0D-15,1.0D-20,1.0D-3/
DATA TINY1,TINIER1,TNIE1,ERR/1.0D-10,1.0D-15,1.0D-20,1.0D-3/
DATA TINY2,TINIER2,TNIE2,ERR/1.0D-10,1.0D-15,1.0D-20,1.0D-3/
DATA CU,CD/I.0001,.9999/

ITCNT INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT
IF ITPRT=1.

ITPRT=0
N1=N1
N=N1
IF (ITPRT.GT.0) CALL WRTOUT2
IF(IND1.EQ.1)THEN
  DO 2 I=1,N1+5
  DO 2 J=1,NJ1
  C(I,J)=C(I,J-1)
  P(I,J)=P(I,J-1)
  2 CONTINUE
ELSE IF(IND1.EQ.2)THEN
  DO 5 I=1,N1+1
  DO 5 J=1,NJ1
  C(I,J)=C(I,J-1)
  P(I,J)=P(I,J-1)
  5 CONTINUE
ELSE IF(IND1.EQ.3)THEN
  ITR=5+NC1*2
  DO 7 I=1,ITR
  DO 7 J=1,N1
  C(I,J)=C(I,J-1)
  P(I,J)=P(I,J-1)
  7 CONTINUE
END IF

LOOP BEGUN FOR ITERATIONS
IF(ITCNT0.GT.7)ITCNT0=ITCNT0-1
DO 75 ITCNT=1,ITCNT0
COLD ARRAY SET UP
ITCNT=ITCNT
DO 10 K=1,N
  DO 10 J=1,NJ
  COLD(K,J)=C(K,J)
  10 CONTINUE

LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -P(I).
DO 60 J=1,NJ

D-22
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 15 I=1,N
SUM(I)=0.0
G(I)=F(I)
CONTINUE
15

C
C THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
C TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
C (IN RELATION TO J).
C
IF (J.EQ.1) THEN
MM=0
ELSE IF (J.LT.NJ) THEN
MM=-1
ELSE
MM=-2
ENDIF
DO 50 M=MM,MM+2

C
C ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC
C
DO 50 K=1,N
SAVEC=C(K,J+M)
WORKC=SAVEC

C
C DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)
C
IF(N.EQ.1)THEN
TINY=TINY0
TINIER=TINIER0
TNIEST=TNIEST0
ELSE IF(N.GE.L1)THEN
TINY=TINY2
TINIER=TINIER2
TNIEST=TNIEST2
ELSE
TINY=TINY1
TINIER=TINIER1
TNIEST=TNIEST1
ENDIF
IF (ABS(WORKC).LT.TINY) THEN
IF (ABS(WORKC).LT.TINIER) WORKC=SIGN(TINIER,WORKC)
C(K,J+M)=1.2*WORKC
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 20 I=1,N
AA(I)=F(I)
CONTINUE
20
C(K,J+M)=4.0*F(I)
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 25 I=1,N
AA(I)=AA(I)+4.0*F(I)
CONTINUE
C(K+M)=WORKC
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 30 I=1,N
AA(I)=(AA(I)-3.0*F(I))/(0.2*WORKC)
30 CONTINUE
C
C DERIVATIVES CALCULATED FOR LARGER VALUES OF C (GREATER THAN TINY)
C
ELSE
C(K+M)=WORKC*CU
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 35 I=1,N
AA(I)=F(I)
35 CONTINUE
C(K+M)=WORKC*CD
IF(IND1.EQ.1 .OR. IND1.EQ.3)THEN
CALL FUNCT1(J)
ELSE
CALL FUNCT2(J)
ENDIF
DO 40 I=1,N
AA(I)=(AA(I)-F(I))/((CU*CD)*WORKC)
40 CONTINUE
ENDIF
C(K+M)=SAVEC
C
C VALUES FOR A,B,D,X AND Y GIVEN. SUM IS ALSO INCREMENTED
C
DO 45 I=1,N
SUM(I)=SUM(I)+AA(I)*C(K+M)
IF (M.EQ.-2) Y(LK)=AA(I)
IF (M.EQ.-1) A(LK)=AA(I)
IF (M.EQ.0) B(LK)=AA(I)
IF (M.EQ.1) D(LK)=AA(I)
IF (M.EQ.2) X(LK)=AA(I)
45 CONTINUE
50 CONTINUE
DO 55 I=1,N
G(I)=G(I)+SUM(I)
55 CONTINUE
C
C BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(J)
60 CONTINUE
C
C CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO 65 K=1,N
DO 65 J=1,NJ
IF(DABS(C(K,J)).GT.TNIEST) THEN
IF(DABS((C(K,J)-COLD(K,J))/C(K,J)).GT.ERR) GO TO 70
ENDIF
65 CONTINUE
GO TO 80
70 IF(ITPRT.GT.0) CALL WRTOUT2
75 CONTINUE
80 CONTINUE
DO 95 II=1,N1
DO 95 I2=1,NJ1
C 1 (II,/2)=C('II,/2)
95 CONTINUE
RETURN
END

SUBROUTINE WRTOUT2

IMPLICIT REAL*8(A-H,O-Z)
COMMON/BND/A(14,14),B(14,14),C(14,301),D(14,29),X(14,14),Y(14,14),G(14),N,ITPRT,ITCNT,F(14)
IF (ITCNT.NE.0) WRITE (*,99)ITCNT
WRITE (*,100)
DO 1 K=1,N1
WRITE(*,101)K,(C(I,K),I=1,N)
1 CONTINUE
99 FORMAT('ITCNT=',I2)
100 FORMAT(C4,C2,C3)
101 FORMAT((I3,1PE16.8))
RETURN
END

C BLOCK TRIDIAGONAL MATRIX SUBROUTINE
SUBROUTINE BAND2(J)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION E(14,14)
COMMON/BND/A(14,14),B(14,14),C(14,301),D(14,29),X(14,14),Y(14,14),G(14),N,ITPRT,ITCNT,F(14)
101 FORMAT('0DETHERM=0 AT J=',I4)
IF(J.EQ.1) THEN
  NP1=N+1
  DO 2 I=1,N
    D(I,NP1)=G(I)
    DO 2 L=1,N
      D(L,NP1)=X(L)
      2 CONTINUE
    CALL MATINV2(N,2*N+I,DETERM)
    IF(DETERM.EQ.0) WRITE (1101)
    DO 5 K=1,N
      E(K,NP1)=D(K,NP1)
      DO 5 L=1,N
        E(K,L)=D(K,L)
        X(K,L)=D(K,L)
        5 CONTINUE
      RETURN
ELSE IF(J.EQ.2) THEN
  DO 7 I=1,N
    D(I,N)=NPI=N+1
    DO 7 L=1,N
      D(L)=G(I)-Y(I,L)*E(N,M)
      DO 7 M=1,N
        A(M)=E(M,L)
        7 CONTINUE
      RETURN
ELSE IF(J.EQ.NJ) THEN
  DO 10 I=1,N
    D(I)=G(I)-Y(I,L)*E(N,M)
    DO 10 M=1,N
      A(M)=E(M,L)
      10 CONTINUE
ENDIF
DO 12 I=1,N
D(I,NP1)=G(I)
DO 12 L=1,N
D(I,N)=D(L,NP1)*A(LL)*E(L,NP1,1)
DO 12 K=1,N
B(LK)=B(LK)+A(LL)*E(L,KJ)
12 CONTINUE
CALL MATINV2(N,NP1,DETERM)
IF(DETERM.EQ.0) WRITE(2,101) J
DO 15 K=I,N
DO 15 M=1,NP1
E(K,MJ)=D(K.M)
15 CONTINUE
IF(J.EQ.N) THEN
DO 17 K=1,N
C(K,J)=E(K,NP1,J)
17 CONTINUE
DO 18 M=NJ-1,1,-1
DO 18 K=1,N
C(K,MJ)=E(K,NP1,M)
DO 18 L=1,N
C(K,M)=C(K,M)+E(K,L,M)*C(L,M+1)
18 CONTINUE
DO 19 K=1,N
DO 19 M=1,N
C(K,M)=C(K,1)+X(K,L)*C(L,3)
19 CONTINUE
ENDIF
RETURN
END

MATRIX INVERSION SUBROUTINE
SUBROUTINE MATINV2(N,M,DETERM)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION ID(14)
COMMON/BND/A(14,14),B(14,14),C(14,30 I),D(14,29)
DETERM=1.0
DO 1 I=LN
DO 18 NN=1,N
BMAX=0.0
DO 6 I=1,N
IF(ID(I).EQ.0) THEN
DO 5 J=1,N
IF(ID(J).EQ.0) THEN
IF(DABS(B(LJ)).GT.BMAX) THEN
BMAX=DABS(B(LJ))
IROW=I
JCOL=J
ENDIF
ENDIF
5 CONTINUE
ENDIF
6 CONTINUE
IF(BMAX.EQ.0.0) THEN
DETERM=0.0
RETURN
ENDIF
ID(JCOL)=1
IF(JCOL.NE.IROW) THEN
DO 10 J=1,N
SAVE=B(IROW,J)
B(IROW,J)=B(JCOL,J)
B(JCOL,J)=SAVE
10 CONTINUE
ENDIF
9 CONTINUE
RETURN
END
I 0 CONTINUE
DO 11 K=1,M
SAVE=D(IROW,K)
D(IROW,K)=D(JCOL,K)
D(JCOL,K)=SAVE
11 CONTINUE
ENDIF
FF = 1.0/B(JCOL,JCOL)
DO 13 J=1,N
13 B(JCOLJ)=B(JCOLJ)*FF
DO 14 K=1,M
14 D(JCOL,K)=D(JCOL,K)*FF
DO 18 I=1,N
IF(I.NE.JCOL)THEN
15 FF = B(IJCOL)
DO 16 J=1,N
16 B(IJ)=B(IJ)-FF*B(JCOLJ)
DO 17 K=1,M
17 D(LK) = D(LK) -FF*D(JCOL,K)
ENDIF
18 CONTINUE
RETURN
END
C
C
C
C this subroutine compute the amount of adsorbed gas in equilibrium with gas
molar density, for single component uses Langmuir-Fredrich isotherm. the
computation of equilibrium for multi component uses the Ideal Solution Theory
IST. since the equations are non linear and implicit a numerical method
was used to compute the adsorbed equilibrium amount. the method is by Foythe,
Computer Methods for Mathematical Computation. it is a bisection method with
a quadratic convergence.
C
B,V,PO arrays are single equilibrium constant
SUBROUTINE IST_ZI (METHOD,T,SS,QI)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4),XI(4),Y(4)
COMMON/NCY/NC1
COMMON/INDIC1/IND(4)
REAL*8 Q1(4),SS(4)
INTEGER LNLIM
EXTERNAL FCN1
DATA XTOL,FTOL,CLIM/1.0E-5,1.0E-5,0.50/
DATA R,555/
T_G=T
NC=NC1
C the partial pressure
DO 11 I=1,NC
Y1(I)=SS(I1)
11 END DO
DO I=1,NC
PP(I)=Y1(I)*T_G*R
13 END DO
C no mole fraction return
Z=1.0E-32
DO I=1,NC
Q1(I)=0.
END DO
RETURN
END IF
N1=1

D-27
c set the constant as a function of temperature

IF(IND(1).EQ.1)THEN
   V(N1)=-(8.2983138-21118560043*T+1.587732293D-4*T*T)/441100
   B(N1)=6864.9000131*EXP(-.019625791466*T)
   V(N1)=5.323235056e-6*T**(-5)*EXP(13948.544244/1.987/T)
   PO(N1)=.8
   N1=N1+1
END IF

IF(IND(2).EQ.1)THEN
   V(N1)=1.69.035
   B(N1)=1.879094E-4*EXP(5467.4817024/T)
   IF(T.LT.610.) THEN
      B(N1)=5.5597278759E-7*EXP(9628.9655743/T)
   ELSE
      B(N1)=5.8089066B84E-7*EXP(9115.734593/T)
   END IF
   PO(N1)=1.0
   N1=N1+1
END IF

IF(IND(3).EQ.1)THEN
   V(N1)=1.637879912E-5*T+.00961297026
   IF(T.LE.532) THEN
      B(N1)=3.2694515539E-7*T+.4.59988799E-4
   ELSE
      B(N1)=7.90864008E-5*T-4.14400420E-2
   END IF
   PO(N1)=1.0
   N1=N1+1
END IF

IF(IND(4).EQ.1)THEN
   V(N1)=1.637879912E-5*T+.00961297026
   IF(T.LE.532) THEN
      B(N1)=3.2694515539E-7*T+.4.59988799E-4
   ELSE
      B(N1)=7.90864008E-5*T-4.14400420E-2
   END IF
   PO(N1)=1.0
   END IF

ENDIF

IF(NC.EQ.1)THEN
   Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0) THEN
   Q1(1)=V(2)*B(1)*PP(2)**PO(2)/(1+B(1)*PP(2)**PO(2))
ENDIF
ELSE IF(NC.EQ.2 .AND. PP(2).EQ.0) THEN
   Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
END IF

ENDIF
TERM1=.

c calculate the equilibrium isotherm by Langmuir method

DO I=1,N
   IF(PP(I).GT.0) THEN
      TERM1=B(I)*PP(I)**PO(I)-TERM1
   END IF
END DO
SUM=.
DO I=1,N
   IF(PP(I).LE.0.) THEN
      Q1(I)=.
   ELSE
      Q1(I)=V(I)*B(I)*PP(I)**PO(I)/(1+TERM1)
   END IF
END DO
SUM=SUM+Q(I)
END IF
END DO

if the Langmuir method is asked for then returned
IF(METHOD.EQ.1) THEN
RETURN
END IF

if not, take the result as the first guess for IST theory
DO I=1,NC
X1(I)=Q(I)/SUM
IF(X1(I).GT.0) THEN
P(I)=PI(I)/X1(I)
ELSE
P(I)=0.
ENDIF
END DO

calculate the spread pressure
DO I=1,NC
IF(PP(I).LE.0.) THEN
X1(I)=0
ELSE
X1(I)=V(I)*PO(I)*LOG(1+B(I)*PI(I)**PO1))
ENDIF
END DO
X=X1(IF)
DO I=1,NC
IF(X1(I).LT.X .AND. X1(I).GT.0) THEN
X=X1(I)
ENDIF
END DO
AX=X
DELX=AX
BX=AX
c call ZeroIn subroutine to find the root to the IST equation
DO I=1,100
BX=BX+DELX
FUN=FCN1(BX)
IF(FUN.LT.0) GO TO 113
END DO

113 X=ZEROIN(FCN1,AX,BX,TOL)
c root was found
DO I=1,NC
IF(PP(I).LE.0) THEN
PP(I)=1.0E-32
ENDIF

c calculate the fraction in the solid phase
PART1=PO(I)*X/V(I)
IF(PART1.GT.73) PART1=73
PI(I)=(EXP(PART1)-1)/B(I)
X1(I)=PI(I)/P(I)
END DO
TOT_Q=0
c calculate the total amount adsorbed
DO I=1,NC
Q1(I)=V(I)*B(I)*PI(I)**PO1/(1+B(I)*PI(I)**PO(I))
TOT_Q=TOT_Q+X1(I)*Q1(I)
END DO
c calculate the amount adsorbed for each component
DO I=1,NC
Q1(I)=1/TOT_Q*X1(I)
ENDIF
END DO

RETURN
END
c ISF function

REAL FUNCTION FCN1(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
IF(PP(I).GT.0) THEN
PART1=PO(I)*X/V(I)
IF(PART1.GT.73) PART1=73
SUM=SUM+PP(I)/((EXP(PART1)-1)/B(I))*((1./PO(I))
ENDIF
C C C C
IF(PP(I).LE.0)PP(I)=1.0E-32
PART1=PO(I)*X/V(I)
IF(PART1.GT.73) PART1=73
SUM=SUM+PP(I)/((EXP(PART1)-1)/B(I))*((1./PO(I))
END DO
FCN1=SUM-1
RETURN
END

C subroutine to find the root of equation by bisect method

REAL FUNCTION ZEROIN(_CN1,AX,BX,TOL)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 AX,BX,FCN1,TOL,
REAL*8 A,B,C,D,E,FP,FB,FC,TOL1,EPS,FA,FB,FC,TOL1,XM,P,R,S
EPS=1.0
10 EPS=EPS/2.
TOL1=1.0+EPS
IF(TOL1.GT.1.0) GO TO 10
 initialization
A=AX
B=BX
FA=FCN1(A)
FB=FCN1(B)
 begin step
20 C=A
FC=FA
D=B-A
E=D
30 IF(ABS(FC).LE.ABS(FB)) GO TO 40
A=B
B=C
C=A
FA=FB
FB=FC
FC=FA
 c convergence test
40 TOL1=2.*EPS*ABS(B)+.5*TOL
XM=.5*(C-B)
IF(ABS(XM).LE.TOL1)GO TO 90
IF(FBEQ0.0) GO TO 90
 c is bisection necessary
IF(ABS(E).LE.TOL1)GO TO 70
IF(ABS(FA).LE.ABS(FB)) GO TO 70
 c is quadratic interpolation possible
IF(FA.EQ.0.0)GO TO 50
 c linear interpolation
S=FB/FA
P = 2.0 * XM * S
Q = 1.0 - S
GO TO 60

C inverse quadratic interpolation
50  Q = FA / FC
R = FB / FC
S = FB / FA
P = S * (2.0 * XM * Q * (Q - R) - (B - A) * (R - 1.0))
Q = (Q - 1.0) * (R - 1.0) * (S - 1.0)

C adjust signs
60  IF (P GT 0.0) P = -Q
   P = ABS (P)

C is interpolation acceptable
   IF (P GE (2.0 * P) GE (3.0 * XM * Q - ABS (TOL1 * Q))) GO TO 70
   IF (P GE ABS (5.0 * P * Q)) GO TO 70
   E = D
   D = P / Q
   GO TO 80

C bisection
70  D = XM
   E = D
   C complete step
80  A = B
   FA = FB
   IF (ABS (D) GT TOL1) B = B + D
   IF (ABS (D) LE TOL1) B = B + SIGN (TOL1, XM)
   FB = FCN (B)
   IF ((FB * FCN (FC)) GT 0) C TO 20
   GO TO 30

C done
90  ZEROIN = B
   RETURN
   END

C-------------------------------------------------------------------
C
C the second method, this method is faster but the initial guess must be near
C the root of the equation.
C
C this subroutine compute the amount of adsorbed gas in equilibrium with gas
C molar density, for single component uses Langmuir-fredrich isotherm, the
C computation of equilibrium for multi component uses the Ideal Solution Theory
C (IST), since the equations are none linear and implicit a numerical method
C was used to compute the adsorbed equilibrium amount, the method is Newton.
C
C B, V, PO arrays are single equilibrium constant
SUBROUTINE IST_Z (METHOD, T, TT, SS, Q1)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON/EQLIB/PP(4), B(4), V(4), PO(4), PI(4), XI(4), X1(4), Y1(4)
COMMON/NCY/NC1
COMMON/INDIC1/IND(4)
REAL*8 Q1(4), SS(4)
INTEGER LNLM
EXTERNAL FCN, FDER
DATA XTOL, FTOL, I, NLIMI1.0E-5, 1.0E-5, 0, 50/
DATA R, 555.0/
T_G = T
NC = NC1
DO II = 1, NC
   Y1(II) = SS(II)
END DO
DO I = 1, NC
   PP(I) = Y1(I) * T_G * R
END

D-31
END DO

c no mole fraction return

Z=1.0E-32
DO I=1,NC
Q(I)=0.
END DO
RETURN
ENDIF
N1=1

c set the constant as a function of temperature
IF(IND(1),EQ.1)THEN

13x by l granting
point=-1567.1205874+9.00256903*T-.01723474*T*T+1.1008056e-5*T*T*T

if(pp(n1).gt.poin or. T.gt.627)then
V(N1)=(81.2983138-21118360043*T+1.587732293D4*T*T)/44/100
B(N1)=6864.9000131*EXP(-.019625791466*T)
p0(n1)=1.0
else
V(N1)=23.3222844/100
B(n1)=4.9639763e-4*T**(-5)*EXP(9233.33778/1.987/T)
p0(n1)=-2.9138991288+.017181761178*T-2.549083257e-5*T**T+
1.622511757e-8*T**T+T
end if

from Finn data 5A
if(pp(n1).le.1.0) then
b(N1)=2.37022397e-6*T**(-5)*EXP(14907.6535/1.987/T)
v(n1)=16.6/44/100
p0(n1)=80.
else
V(n1)=(25.97135006-6.084518e-3*T-2.179951646e-5*T**T)/44/100
b(n1)=1.88853393e-5*T**(-5)*EXP(12170.875335/1.987/T)
p0(n1)=1.
end if

5A BY GRACE, BY L_F
v(N1)=17.0/100/44
B(N1)=2.341477E-4*T**(-5)*EXP(10257.166145/1.987/T)
p0(N1)=3.830450111E-4*T**1.188379596

5A BY GRACE, BY L
v(N1)=-4.27886889+.087218022*T-9.101071580E-5*T**T)/44/100
B(N1)=9.253309123E-5*T**(-5)*EXP(10719.0/1.987/T)
p0(N1)=1.

5A BY GRACE, BY L_F BETWEEN 0-75 C
v(N1)=(-4.999421-1.93842896*T+3.2540511E-3*T**T-
1.822611899E-6*T**T)44/100
B(N1)=35.358072159-.70181735*T+2.7458762E-4*T**T-
1.484116035E-7*T**3
p0(1)=1.478184694E-7*T**3

linde 5a
v(n1)=.005
b(n1)=1.129015193e-5*EXP(5055.015089A)
p0(n1)=.6
N1=N1+1
END IF

c h2o on 5a by grace Lf
IF(IND(2),EQ.1)THEN
IF(IND(1),EQ.1)THEN
if(pp(n1).le.1.0) then
v(n1)=(39.914452-8.87103e-2*T+6.839502987e-5*T**T)/100/18
else
v(nl)=(873.44464-3.867834937*t+5.80375049e-3*t*t+2.9346685e-6*t^t)/100/18
end if
b(n)=29690.66923-137.837129*T+2.8346126*t*t
po(nl)=1
else
b(n)=48.56639771-2.262023975e-1*t+3.9101703168e-4*t*t-2.379098497e-7*t^t
v(nl)=(95.093824733-.21725775358*t+1.4628603e-4*t*t)/100/18
end if
ELSE
C h2o on 5a grace by L_F
b(n)=24.573259-5.885278e-2*t+3.473682438e-5*t*t
v(nl)=(66.62520167-.2299345*t+7.1897316221e-5*t*t)/100/18
if(t.le.600)then
po(nl)=8.219911486-3.3519986e-3*t+4.679276479e-6*t^t
else
po(nl)=6.0926707634+2.043004e-2*t-2.924858439e-5*t^t+1.1746734108e-8*t^t^t
end if
ENDIF
b(n)=22.47292664**(-.5)*exp(7858.45996/1.987/T)
v(nl)=172.54446-.66643613*t+9.738449e-4*t^t-.4.986888e-7**t^t)/18
po(nl)=1.
ELSE
V(NI)=22.0/18./100.
B(N1)=78.33485-.14255*T
PO(N1)=1.
ENDIF
IF(IND(3).EQ.1)THEN
V(N1)=-1.637879912E-5*T+.00961297026
IF(T.LE.532)THEN
B(N1)=3.2694515539E-7*T+.4.599887999E-4
ELSE
B(N1)=7.90864008E-5*T-.4.14400420E-2
ENDIF
PO(N1)=1.0
N1=N1+1
ENDIF
IF(IND(4).EQ.1)THEN
V(N1)=-1.637879912E-5*T+.00961297026
IF(T.LE.532)THEN
B(N1)=3.2694515539E-7*T+.4.599887999E-4
ELSE
B(N1)=7.90864008E-5*T-.4.14400420E-2
ENDIF
PO(N1)=1.0
ENDIF
IF(NC.EQ.1)THEN
Q1(1)=V(1)*B(1)**PP(1)**PO(1)/(1+B(1)**PP(1)**PO(1))
RETURN
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0)THEN
Q1(2)=V(2)*B(2)**PP(2)**PO(2)/(1+B(2)**PP(2)**PO(2))
Q1(1)=0
RETURN
ELSE IF(NC.EQ.2 .AND. PP(2).EQ.0)THEN
Q1(1)=V(1)*B(1)**PP(1)**PO(1)/(1+B(1)**PP(1)**PO(1))
Q1(2)=0
RETURN
ELSE IF(NC.EQ.3)THEN
if(pp(1)>0 .and. pp(2).le.0)
Q1(3)=V(3)*B(3)**PP(3)**PO(3)/(1+B(3)**PP(3)**PO(3))
RETURN
ENDIF
Q1(1) = 0
Q1(2) = 0
return
else if (pp(1) .le. 0 .and. pp(3) .le. 0) then
    Q1(2) = V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
    Q1(1) = 0
    Q1(3) = 0
    return
else if (pp(2) .le. 0 .and. pp(3) .le. 0) then
    Q1(1) = V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
    Q1(2) = 0
    Q1(3) = 0
    return
end if
END IF
TERM1 = 0.
c calculate the equilibrium by Langmuir isotherm
DO I=1,NC
    IF (PP(I) .GT. 0) THEN
        TERM1 = B(I)*PP(I)**PO(I)+TERM1
    END IF
END DO
SUM = 0.
DO I=1,NC
    IF (PP(I) .LE. 0) THEN
        Q1(I) = 0.
    ELSE
        Q1(I) = V(I)*B(I)*PP(I)**PO(I)/(1+TERM1)
        SUM = SUM + Q1(I)
    END IF
END DO
c if the Langmuir method is asked for, then return. If not use it as first guess
for IST theory
IF (METHOD .EQ. 1) THEN
    RETURN
END IF
DO I=1,NC
    X1(I) = Q1(I)/SUM
    IF (X1(I) .GT. 0) THEN
        PI(I) = PP(I)/X1(I)
    ELSE
        PI(I) = 0.
    END IF
END DO
c set the initial guess for the spreading pressure
DO I=1,NC
    IF (PP(I) .LE. 0) THEN
        X1(I) = 0
    ELSE
        X1(I) = V(I)/PO(I)*LOG(1+B(I)*PI(I)**PO(I))
    END IF
END DO
DO I=2,NC
    IF (X1(I) .LT. X .AND. X1(I) .GT. 0) THEN
        X = X1(I)
    END IF
END DO
c call newton method to the rout to IST equation
IF (X .LE. 1.0E-17) GO TO 80
CALL NEWTN(PCN,FDER,X,XTOL,FTOL,NLIM,J)
c rout was found, calculate the fraction in the solid phase
DO I=1,NC
IF(PP(1).LE.0) THEN
  XI(1)=0.
ELSE
  PART1=PO(1)*X/V(1)
  IF(PART1.GT.73) PART1=73
  PI(I)=(EXP(PART1)-1)/B(I)
  XI(1)=PP(1)/PI(I)
ENDIF
END DO

c calculate the total amount in the solid phase
TQT_Q=0
DO I=1,NC
  IF(PP(I).LE.0) THEN
    QI(I)=0.
  ELSE
    QI(I)=V(I)*B(I)*PI(I)**PO(I)/(1+B(I)*PI(I)**PO(I))
    TQT_Q=TQT_Q+XI(I)*Q(I)
  END IF
END DO

C c calculate the amount in equilibrium with the gas phase for each component
DO I=1,NC
  QI(I)=TOT_Q*XI(I)
END DO
80 RETURN
END

C c IST final equation
C
REAL FUNCTION FCN(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART1=PO(I)*X/V(I)
    IF(PART1.GT.73) PART1=73
    SUM=SUM+PP(I)/(EXP(PART1)-1/B(I)**PO(I))
  END IF
END DO
FCN=SUM-1
RETURN
END

C c IST final derivative
C
REAL FUNCTION FDER(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART1=PO(I)*X/V(I)
    IF(PART1.GT.35) PART1=-PP(I)/B(I)*EXP(PART1)
    PART2=((EXP(PART1)-1/B(I)**(1+PO(I))/PO(I))
    SUM=SUM+PART1/PART2
  ELSE IF(PART1.GT.73) THEN
    SUM=SUM-B(I)**(1+PO(I))/PO(I)*PP(I)/B(I)*V(I)*EXP(-PART1/B(I))
  ELSE
    D-35
PART3=-73
SUM=SUM-B(D**(1+PO(I))/PO(I))**PP(I)/B(I)/V(I)*
   EXP(-PART3)
END IF
END IF
END DO
FDER=SUM
RETURN
END

c

! this subroutine finds the root to a nonlinear equation using the Newton method
SUBROUTINE NEWTN(FCN,FDER,X,XTOL,FIDL,NLIM,I)
IMPLICIT REAL*8(A-H,O-Z)
INTEGER NLIM,I
FX=FCN(X)
X1=X
DO I=1,NLIM
DEI..X=FX/FDER(X)
X=X-DELX
FX=FCN(X)
IF (ABS(X-X1)/X.LE.XTOL) THEN
   RETURN
ENDIF
IF(FX.NE.0)THEN
   IF(ABS(FX-FX1)/FX.LE.FIDL) THEN
      RETURN
   ENDIF
ENDIF
X1=X
FX1=FX
END DO
I=-1
PRINT 200, NLIM,X,FX
200 FORMAT(/'TOLERANCE NOT MET ','4,' ITERATIONS X=',E12.5,' F(X)=',E12.5)
RETURN
END

FUNCTION CPGAS(TEM,Y)
C THIS FUNCTION CALCULATES THE HEAT CAPACITIES OF CMRIER GAS IN BTU/#MOLE/R
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 A(4),B(4),C(4),D(4),Y(4)
COMMON/GAS/INERT.NCOMP
COMMON/INDIC1/IND(4)
COMMON/NCYI/NC1
C CO2
DATA A/36.11,33.46,29.2,29.1/
C H2O
DATA B/4.233E-2,.6880E-2,.2199E-2,1.158E-2/
C N2
DATA C/-2.887E-5,.7604E-5,.5723E-5,-.6076E-5/
C O2
DATA D/7.464E-9,-3.593E-9,-2.871E-9,1.311E-9/
NC=NC1
CPGAS=0.
YO=0.
N1=1
T=TEM/1.8-273.15
IF (INERT.EQ.1) THEN
   DO I=1,4
      IF(IND(I).EQ.1)THEN

FUNCTION CPS(TEMP)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE HEAT CAPACITY
C BTU/LB/R.
   CPS=0.2
RETURN
END

FUNCTION KGAS (TEMP)
C THIS FUNCTION CALCULATES THE THERMAL CONDUCTIVITY OF CARRIER GAS ASSUMING
C A LINEAR FUNCTION OF TEMPERATURE AND BASED ON VALUES AT 492 AND 672 R.
C BTU/MIN/FT/R
IMPLICIT REAL*8(A-H,O-Z)
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
   KGAS=3.88E-7*TEMP+0.052E_-
ELSE
   KGAS=1.667E-6*TEMP+6.1E-4
ENDIF
RETURN
END

FUNCTION RE (G,TEMP)
C THIS FUNCTION CALCULATES THE PARTICLE REYNOLDS NUMBER ASSUMING THAT
C THE MOLECULAR WEIGHT OF THE GAS IS EQUAL TO THAT OF CARRIER GAS.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN,MW
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
COMMON/GAS/INERT,NCOMP
DATA IFLAG/0/
IF (INERT.EQ.1) THEN
   MW=28.0
ENDIF
IF (INERT.EQ.2) MW=4.
IF (IFLAG.EQ.0)THEN
   CONST=2.*RA
   IFLAG=1
ENDIF
RE=CONST*MW*ABS(G)/VIS(TEMP)
RETURN
END

FUNCTION VIS(TEMP)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE VISCOSITY OF CARRIER GAS AS A LINEAR FUNCTION
C OF TEMPERATURE (LB/MIN/FT).
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
   VIS=1.0E-6*TEMP+1.65E-4
   VIS=.010200712+5.384663937E-5*TEMP-8.7973727E-8*TEMP*TEMP+
2   4.811387495E-11*TEMP*TEMP*TEMP
ELSE
   VIS=0.9446E-6*TEMP+2.863E-4
ENDIF
FUNCTION RHOG(TR,T)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
C THIS FUNCTION CALCULATES THE MOLAR DENSITY OF AN IDEAL GAS IN
C LBMOLES/CV FS.
COMMON/PRIME/GN2,R2A,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
DATA R/555.9/
RHOG=PR/TR
RETURN
END

FUNCTION EFFD(IMP,G,TEMP,RHO,P,YO)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL DIFFUSIVITIES IN A PACKED BED
C USING THE EDWARDS AND RICHARDSON CORROLATION. (FT^2/FT/MIN)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LAMBDA1,LAMBDA2,LEN,YO(4)
COMMON/PRIME/GN2,RA,RAY,EPSEX,EPSIN,ALF,RHOS,ALPHA1
DATA IFLAG/0,LAMBDA1/0.73/
IF(IFLAG.EQ.0).THEN
CONST=2.*RA/EPSEX
IFLAG=1
ENDIF
DIF=DIFF(IMP,TEMP,P,YO)
EFFD=LAMBDA1*DIF+CONST*ABS(G)*LAMBDA2(DIF,RHO)/RHO
RETURN
END

FUNCTION EFFK(G,T,CP,RHO,P,YO)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL THERMAL CONDUCTIVITY OF A
C PACKED BED IN BTU/FT/MIN/F.
COMMON/NCY/NC1
REAL*8 YO(4)
NC=NC1
EFFK=0.
KK=0
DO II=1,NC
SUM=CP*RHO*EFFD(II,G,T,RHO,P,YO)
IF(SUM.GT.0)KK=KK+1
EFFK=SUM+EFFK
END DO
EFFK=EFFK/KK
RETURN
END

REAL FUNCTION LAMBDA2(G,DIF,RHO)
C THIS FUNCTION CALCULATES THE DIMENSIONLESS PARAMETER OF THE EDWARDS AND
C RICHARDS CORRELATION MODIFIED FOR SMALL DIAMETER PARTICLES.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
DATA IFLAG/0/
COMMON/PRIME/GN2,RA,RAY,EPSEX,EPSIN,ALF,RHOS,ALPHA1
IF(IFLAG.EQ.0).THEN
IF(RA.GT.0.00492)THEN
PE=.2.
ELSE
PE=406.4*RA
ENDIF
CONST=2.*RA/EPSEX
IFLAG=1
FUNCTION DIl_(ICOMP, TEM, YO)

C THIS FUNCTION CALCULATES THE MOLECULAR DIFFUSION COEFFICIENTS BY CORRECTING FOR PRESSURE AND TEMPERATURE (FT*FT/MIN).

IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN, YO(4), V(4), V1(4), MW(4), DIF(4)
COMMON/GAS/NERT, NCOMP
COMMON/NCTY,NC1
COMMON/INDIC1/IND(4)
COMMON/PRIME/GN2, RA, RAV, EPSX, EPSIN, ALF, RHOS, ALPHA1
DATA V1/26.9, 12.7, 17.9, 16.6/
DATA MW I/44.01, 18.0162, &013, 31.999/
NC=NC1
K=ICOMP
P=P1/760.
T=TEM/1.8
N1=1
DO 11=1, 4
 IF(IND(11).EQ.1) THEN
 MW(N1)=MW1(11)
 V(N1)=V1(11)
 N1=N1+1
 END IF
 END DO
 DO I=1, NC
 IF(NC.EQ.1) THEN
 MW(I)=MW(K)
 V(I)=V(K)
 END IF
 PART1=((MW(K)+MW(I))/MW(K)/MW(1))**.5
 PART2=(V(K)**(1./3)+V(I)**(1./3))**2
 DIF(I)=PART1/PART2*T**1.75/P**1.0E-3
 END DO
 IF(NC.EQ.1) THEN
 DIFF=DIF(1)*3.8745
 RETURN
 END IF
 IF(NC.EQ.2) THEN
 IF(K.EQ.1) DIFF=DIF(2)*3.8745
 IF(K.EQ.2) DIFF=DIF(1)*3.8745
 RETURN
 END IF
 SUM=0.
 DO I=1, NC
 IF(I.NE.K) THEN
 SUM=SUM+YO(I)/DIF(I)
 END IF
 END DO
 IF(SUM.NE.0) THEN
 DIFF=(1.-YO(K))/SUM*3.8745
 ELSE
 DIFF=1
 END IF
 RETURN
END

FUNCTION HFILM(MW, TEMP, REY, CP)
C THIS FUNCTION CALCULATES THE FLUID FILM HEAT TRANSFER COEFFICIENT 
C IN BTU/SQ FT/MIN/F USING THE CORRELATION OF PETROY AND THODOS.

IMPLICIT REAL*8(A-H,O-Z)
REAL*8 ID,KGAS,KG,LEN,MW
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
COMMON/GAS/INERT,NCOMP
Kg=KGAS(TEMP)
PR=CP/MW*VIS(TEMP)/KG
HFLM=0.357/EPSEX*REY**0.64*PR**0.33*KG**0.5/RA
RETURN
END

FUNCTION DHCAR(TMP,P)
C THIS SUBROUTINE CALCULATES HEAT OF ADSORPTION OF CARRIER GAS ONTO THE
C ACTIVATED CARBON TIMES THE TEMPERATURE DERIVATIVE OF THE SOLID PHASE
C CARRIER GAS CONCENTRATION AT THE BED PRESSURE (BTU/# SOLID/R).
C IMPLICIT REAL*8(A-H,O-Z)
C REAL*8 LEN
C COMMON/GAS/INERT,NCOMP
C COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
C DATA R/1.9872/A/1.28E-9/B/3151/
C
C IF(INERT.EQ.1) THEN
  DH=R*B
  DHN2=DH*A*B*EXP(B/TEMP)*P/TEMP/TEMP
ELSE
  DHN2=0.
ENDIF
RETURN
C END

FUNCTION DHADS(ICOMP.T)
C THIS FUNCTION CALCULATES THE ISOTERIC HEAT OF ADSORPTION. (BTU/#MOLE)

IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
IF(iCOMP.EQ.1) THEN
  DHADS=20400.0
ELSE
  DHADS=20000.0
ENDIF
RETURN
END

REAL*8 FUNCTION TEMPIN(TIME)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES CURRENT INLET TEMPERATURE
C BASED ON THE TIME FOR A TEMPERATURE CHARACTERIZATION
C COMPARISON RUN
C
IF(TIME.LT.0.2) THEN
  T0 = 71.776
  T1 = 13.611
  T2 = -25.775
  T3 = -7529.2
  T4 = 84821.0
  T5 = -1.9364E+5
ELSE
  T0 = 74.358
  T1 = 154.04
  T2 = -77.999
  T3 = 20.167
  T4 = -2.5737
  T5 = .12789
ENDIF
X = TIME
TEMPIN = T0+T1*X+T2*X**2.+T3*X**3.+T4*X**4.+T5*X**5.
TEMPIN = TEMPIN+460.
RETURN
END
APPENDIX E

2DMOL FORTRAN CODE

C this is the main routine, the initial values of matrix S and parameters are
C called by "INITIAL_Z" subroutine, the main routine then calls the "FUNCT1"
C subroutine to solve the discretized partial differential equations (pde's).
C after convergence, the routine calls the "DIFFEQ1" subroutine, which is
C the main routine for solving the momentum and the pressure equations,
C if it is desire to solve these two equations as the time progresses.
C
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 C2(14,201,101),CI(14,201),P(14,201),RP(101),RP(101),
, Y1(33),Y2(33),Y3(33)
REAL*4 QP(14,201,101),C_AVE(2,101),P_TIME,aa,bb,cc,dd
INTEGER IOUT(5)
CHARACTER*5 COUT(3)
CHARACTER*5 LABEL(4)
CHARACTER*8 DATE
COMMON/DATE/DATF.,IS
COMMON/NEW_GRID/DEL0(101),ALF(101),NGR1,NGR2
COMMON/BND3/S(14,201,101),P(14,201,101)
COMMON/BND2/NJ2,NJTPRT,NJNT,NJ1
COMMON/PROP_D/Z/DELZ,DEL,T,M,EDEL1,DEL2,IZJT,NC,NJ,RP
COMMON/INDIC/L1,L2,L3,L4,L5,L6,L7,L8,L9,L10,L11,L12,L13,L14,L15,
COMMON/RADIAZ/RD
READ*,DATE
RADFILE = DATE//'_RAD.OUT'
AVGFILE = DATE//'_AVG.OUT'
CTLFILE = DATE//'_CTL.OUT'
OPEN (50,FILE=RADFILE,STATUS='NEW',RECL=32766)
OPEN (60,FILE=AVGFILE,STATUS='NEW',RECL=32766)
OPEN (70,FILE=CTLFILE,STATUS='NEW',RECL=32766)
DATA IOUT/5,25,50,75,101/
DATA IOUT/5,15,25,35,51/
DATA COUT/'pCO2_','pN2_','rgas_'/
WRITE(50,48X(COUT(I),IOUT(/),J= 15),I= 1,3)
WRITE(60,47X(COUT(I),IOUT0)J= 1,5),J= 1,3)
WRITE(70,47X(COUT(I),IOUT(J)= 1,5),J= 1,3)

C WRITE HEADER DATA TO ASCII FILE

WRITE(50,48X(COUT(I),IOUT(J),I= 1,5),J= 1,3)
WRITE(60,47X(COUT(I),IOUT(J)= 1,5),J= 1,3)
WRITE(70,47X(COUT(I),IOUT(J)= 1,5),J= 1,3)

C INITIALIZE THE C ARRAY WITH THE INITIAL GUESSES OF THE SOLUTION

C
CALL INITIAL_Z
T_TIME=0.
TIME=0.
C start marching through time, LL is the number of time steps
IF(IND(2),EQ.0.OR. ISAT.EQ.1)THEN
IND0=0
NEQ=2*NC+3
NA=NEQ
ELSE
IND0=1
NEQ=2*NC

E-1
NA=NEQ+3
END IF
NEQ1=2*NC+5
IVEL=1
NJ_OR_1=1
LL2=15
DO LL=1,1800
IF(LL2.GT.5) THEN
   LL2=LL2-1
END IF
DO 20 LL1=1,LL2
DO II=1,NEQ1
   DO I2=1,NJ1
      DO I3=1,NJR
         C2(I1,12,13)=S(I1,12,13)
      END DO
   END DO
   END DO
DO 5 II=1,NJ1
IF(IVEL.EQ.1) THEN
   CALL VEL_POR(I1, NJ OR_1, IVEL_1)
   IVEL=2
END IF
DO I2=1,NA
   DO I3=1,NJR
      C1(I2,13)=S(I2,11,13)
      P1(I2,13)=P(I2,11,13)
   END DO
END DO
II=11
MT=1
IF(LL1.EQ.1 .AND. LL2.EQ.1) THEN
   ITCNT0=13
ELSE IF(LL2.EQ.1) THEN
   ITCNT0=7
ELSE
   ITCNT0=5
END IF
IF(IND0.EQ.1) THEN
   CALL DIFEQ2(C1,P1,NEQ,NJR,1,ITCNT0)
ELSE
   CALL DIFEQ1(C1,P1,NEQ,NJR,1,ITCNT0)
END IF
DO M1=1,NEQ
   DO M2=1,NJR
      S(M1,M2)=C1(M1,M2)
   END DO
END DO
CONTINUE
DO 10 II=1,NC
DO 10 I2=1,NJ1
DO 10 I3=1,NJR
IF(S(I1,12,13).GE.1.0E-15) THEN
   IF(ABS(S(I1,12,13)-C2(I1,12,13))/
      S(I1,12,13).GT.1.0E-2) THEN
      GO TO 25
   END IF
END IF
END IF
END IF
CONTINUE
IF(LL1.GE.2) GO TO 205
25 IF(IND0.EQ.1) THEN
   DO 35 LL1=1,5
   DO 15 II=1,NJ1
   JJ=11
   "E-2"
L13=2*NC+1
DO M1=1,3
  DO M2=1,NJR
    C1(M1,M2)=S(L13,I1,M2)
    P1(M1,M2)=P(L13,I1,M2)
  END DO
L13=L13+1
END DO
CALL DIFFEQ2(C1,P1,3,NJR,2,4)
L13=2*NC+1
L31=L13
DO M1=1,3
  DO M2=1,NJR
    S(L13,I1,M2)=C1(M1,M2)
  END DO
L13=L13+1
END DO
CONTINUE
DO 17 II=L31,L31+3
  DO 17 I2=1,NJ1
    DO 17 I3=1,NJR
      IF(S(I1,I2,J3).GE.1.0E-15)THEN
        IF(ABS(S(I1,I2,J3)-C2(I1,I2,J3)).GT.1.0E-2)THEN
          GOTO 35
        END IF
      ELSE
        GO TO 15
      END IF
    END DO
    IF(LLL.GE.2)GO TO 20
  CONTINUE
END DO
DO 17 I2=1,NJ1
  DO 17 I1=1,3
    C1(I1,I2)=S(L4,I1,I2)
    P1(I1,I2)=P(L4,I1,I2)
  END DO
END DO
CALL DIFFEQ1(C1,P1,3,NJ1,1,5)
DO I2=1,NJ1
  DO I1=1,NJR
    P(L5,I2,I1)=S(L5,I2,I1)
    S(L5,I2,I1)=C1(I1,I2)
  END DO
END DO
T_TIME=T_TIME+DELT*60.
TIME = TIME + DELT

c increase the time step after some initial time steps, since the equations
c are more stable

IF(LL.LE.2.5) DELT = DELT * 2
IF(LL.LE.50) DELT = DELT * 2

c convert the variable for printing the data

DO 74 M1 = 1, N1
    DO 74 M2 = 1, N2
        DO II = 1, NC
            QP(II, M1, M2) = S(II, M1, M2) * 10.73D0 * S(LI, M1, M2) * 760 / 14.696
        END DO
        DO II = NC + 1, 2 * NC
            QP(II, M1, M2) = S(II, M1, M2) * 10.73D0 * S(LI, M2) * 760 / 14.696 / 75
        END DO
    QP(I, M1) = S(LI, M1) - 460.
    QP(I, M2) = S(LI, M2) - 460.
    QP(L3, M1) = S(L3, M1) - 460.
    QP(L4, M1) = S(L4, M1) - 460.
    QP(L5, M1) = S(L5, M1) - 460.
    QP(L6, M1) = S(L6, M1) - 460.

    CONTINUE

74    CONTINUE

c compute the inverse of bed radios, the RP variables are calculated in FUNCT1

IF(LL.LE.1) THEN
    DO K1 = 1, N1
        IF(K1.NE.1) THEN
            RP1(K1) = 1. / RP(K1)
        ELSE
            RP1(1) = 0.
        END IF
    END DO
END IF

the average concentration is being computed by numerical integration for
c every 'ISAMP' time steps

ISAMP = 10
IF(LL.LT.130) ISAMP = 1
IF((LL.ISAMP).EQ.LL)) THEN

the average is taken at 5 points in the axial direction, KK is the grid point
c in axial direction, k1 is component number

N_AXIAL = 5
    DO K1 = 1, NC
        KK = K1
        KK = 5
        DO K2 = 1, N_AXIAL
            the integration is done numerically by cubic spline; or by Simpson method
            IFICU_SIM.EQ.1 THEN
                DO K3 = 1, NJR
                    Y1(K3) = S(K1, KK, K3) * S(L1, KK, K3) * 555. * RP1(K3)
                END DO
                CALL CUBSPL(RP1, Y1, NJR, IC, AVE(K1, KK))
                C_AVE(K1, KK) = C_AVE(K1, KK) * 2 / RP1(NJR) * RP1(NJR)
            ELSE
                DO K3 = 1, 5
                    Y2(K3) = S(K1, KK, K3) * S(L1, KK, K3) * 555. * RP1(K3)
                END DO
                CALL SIMPS(Y2, DELR0(NJR), RESULT1)
                PART1 = RESULT1 * 2
                DO K3 = 5, NJR
                    Y3(K3 - 4) = S(K1, KK, K3) * S(L1, KK, K3) * 555. * RP1(K3)
                END DO
                CALL SIMPS(Y3, NJR, DELR0(NJR), RESULT2)
                PART2 = RESULT2 * 2
                C_AVE(K1, KK) = (PART1 + PART2) / RP1(NJR) * RP1(NJR)
            END IF
END IF

IF(K2.EQ.1) THEN
C     KK=25
     KK=15
     ELSE IF(K2.EQ.4)THEN
C     KK=101
     KK=51
     ELSE
C     KK=KK+25
     KK=KK+10
     END IF
     END DO
     END DO
C printing the variables
P_TIME=T_TIME
IF((LL/(ISAMP*4))>ISAMP*4.EQ.LL.OR.LLEQ.I) THEN
WRITE(6,49)
WRITE(6,41) '(', 'GRID ',IOUT(I), ' ', J=1,5)
ENDIF
AA=S(1.25,1)*S(L1.25,1)*555
BB=S(1.51,1)*S(L1.51,1)*555
cc=S(2.25,1)*S(L1.25,1)*555
dd=S(2.51,1)*S(L1.51,1)*555
WRITE(*,*)AA, BB, cc, dd
WRITE(6,49)
WRITE(6,40)**** TIME = P_TIME, 'LOOPS = ', LL, '; ***
WRITE(6,43)PCCO2, ',(C_AVE(1,IOUT(I)),J=1,5)
WRITE(6,44)PPN2, ',(C_AVE(2,IOUT(I)),J=1,5)
WRITE(6,44)GAS TEMPS, (QP(L1,IOUT(I),1),J=1,5)

IF((LL/(ISAMP*10))>ISAMP*10.EQ.LL) THEN
WRITE(50,46)(P_TIME,RP1(I),
& '(QP(1,IOUT(K),J),K=1,3,J=1,33,2)
ENDIF
WRITE(60,45)P_TIME,((C_AVE(IOUT(J)),J=1,5),J=1,2),
& (QP(L1,IOUT(I),1),J=1,5)
WRITE(70,45)P_TIME,((QP(1,IOUT(J),1),J=1,5),J=1,2),
& (QP(L1,IOUT(I),1),J=1,5)

ENDIF
DO I1=1,NEQ+2
DO I2=1,N11
DO I3=1,NJR
P(I1,I2,I3)=S(I1,I2,I3)
END DO
END DO
END DO

40 FORMAT('1X,A12,G10.2,32X,A8,J4,A5,/)
41 FORMAT('1X,A12,5(A7,J4,A2))
42 FORMAT('1X,6(A12))
43 FORMAT('1X,A10.5(2X,G10.2))
44 FORMAT('1X,A10.5(2X,F10.2))
45 FORMAT('1X,16(E15.5,''))
46 FORMAT('1X,17(E15.5,''))
47 FORMAT('1X,TIME,15(',',A5,I3))
48 FORMAT('1X,TIME,R INCHES,15(',',A5,I3))
49 FORMAT('1X,70(',')
STOP
END
C
C this subroutine is being called by maine routine once to get the initial
c values and the necessary parameters
C
SUBROUTINE INITIAL_Z
IMPLICIT REAL*(A-H,O-Z)
REAL*8 K_F(4),K_FO(4),MOL(4),M_AVE,M_W(4),BC_1(4),MW,Q1(4),
SS(4),Q2(4)

CHARACTER*8 DATE
CHARACTER*14 INFILEA,INFILEB
COMMON/DATFJDATE,ISAT
COMMON/BND3/S(14,201,101),P(14,201,101)
COMMON/BND2/N,J2,NJ,ITPRT,ITCNT,NJ1
COMMON/PROP_B_Z/REC Void_B_ID_E_S_B_ALF,GZ,M_W
COMMON/PROP_D_Z/DELZ,DELT,TIME,DEL1,DEL2,JZ,TJ,NC,NJR,NP
COMMON/PROP_S_Z/CP_S,RO_S,AINT,R,P,D,P,CON,S1,HEAT(4)
COMMON/PROP_W/AWP,CP_WA,RO_WA,ERROR0,ERROR1
COMMON/INV_2/R,F,O,F1,CP_F,T,F1,TO,C_FO(4),K_F,P_C(4)
COMMON/MISC_Z/R,G,F,PLP,TOT,BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_1
COMMON/INDIC/L1,L2,L3,L4,L5,L6,L7
COMMON/INDIC1/IND(4)
COMMON/PRIM_2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UINS,HWALL,LEN
COMMON/NCY/NCl
COMMON/MISC_B_Z/DELT_Z,T,J2,JS2,J1,L1,J2,J1
COMMON/INDICI/IND(4)
COMMON/INF_T/NCOMP,W
COMMON/MISC_B_Z/CP_W,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UINS,HWALL,LEN
COMMON/MISC_B_Z/DELT_Z,T,J2,JS2,J1,L1,J2,J1
COMMON/INDICI/IND(4)
COMMON/INF_T/NCOMP,W

C INITIALIZATION
C
C SELECT FILE CONTAINING INPUT SET A
INFILEA = DATE /// _A.DAT
OPEN (UNIT=40,FILE=INFILEA,STATUS='OLD')

C SELECT FILE CONTAINING INPUT SET B
INFILEB = DATE /// _B.DAT
OPEN (UNIT=41,FILE=INFILEB,STATUS='OLD')

C Initialization

READ(UNIT=40,FMT=*)END,DEL,T,NJ,NJR,DELZ,TAMB,G,F,T0,NCOMP,INERT,
.P_TOT,P_C(1),P_C(2),P_C(3),P_C(4),ZD_ED,ED_LRO,WA,EPSEX,
.AINT,CP_S,RO_S,M_W(1),M_W(2),M_W(3),M_W(4),HEAT(1),HEAT(2),
.HEAT(3),HEAT(4),K_F(1),K_F(2),K_F(3),K_F(4),ERROR0,ERROR1
READ(UNIT=41,FMT=*)S_B,CP_WA,RA,RAV,RHOS,ALPHA1,R_P,D_P,P,P_F,
.UINS,HWALL,NC_T,S,GC,CON_S1,NC,PT,LEN,VOID_B,IND(1),IND(2),
.IND(3),IND(4),IDES,ISAT

c the number of component
NJ1=NJ
NC1=NC

c number of equations
N=N*2+3

c number of grids
NJ2=NJR

c number of grids in radial directions, variable grids were used for efficiency
A1=21
A2=104

c 90 percent of the radius was used for the first 49 grids and 10 percent

c for 71 remainder
DEL1 = .99*D_J/2/(A1-1)
DEL2 = .07*D_J/2/(A2)

C volume of solid/volume of porosity
ALF=(1.0D0-VOID_B)/VOID_B
N1=1
IND3=0
IND4=0
DO 11=1,4
IF(IND(11),EQ,1)THEN
M_W(N1)=M_W(N1)
P_C(N1)=P_C(N1)
HEAT(N1)=HEAT(N1)

E-6
K_F(NI)=K_F(I I)

IF(I I.EQ.3)THEN
    IDES=N1
    IND3=N1
ELSE IF(I I.EQ.4)THEN
    IND4=N1
END IF
N1=N1+1
END IF
END DO
SUM_Y=0

c find the partial pressures and average molecular weight
DO I=1,NC
    Y_F=P_C(I)/P_TOT
    SUM_Y=SUM_Y+Y_F
    M_AVE=M_AVE+Y_F*M_W(I)
END DO
M_AVE=M_AVE+(1-SUM_Y)*28.
MW=M_AVE

c L1 is the gas temp, L2 is the solid temp, L3 is the wall temp, L4 is the
c velocity, L5 is the total pressure, and L6 is the total pressure without

c thermal effect:
c
    L1=2*NC+1
    L2=L1+1
    L3=L2+1
    L4=L3+1
    L5=L4+1
    L6=L5+1

C
BOUNDARY CONDITIONS
C
DO I=1,NC
    BC_L(I)=P_C(I)*555.0/T0
END DO
BC_L1=T0
BC_L2=T0
BC_L3=T0
BC_L4=G_F/D_INI/4./VOID_B
BC_L5=P_TOT
BC_L6=BC_L5

C
INITIALIZATION OF VARIABLES
C
DO I=1,NJ
DO J=1,NJR
    P(L1,LJ)=BC_L1
    P(L2,LJ)=BC_L2
    P(L3,LJ)=BC_L3
    P(L4,LJ)=BC_L4
    P(L5,LJ)=BC_L5
    P(L6,LJ)=BC_L6
    S(L1,LJ)=BC_L1
    S(L2,LJ)=BC_L2
    S(L3,LJ)=BC_L3
    S(L4,LJ)=BC_L4
    S(L5,LJ)=BC_L5
    S(L6,LJ)=BC_L6
END DO
END DO
DO I=1,NC
DO J=1,NJR
DO K=1,NJ
    P(I,J,K)=0.
END DO
END
SCII...I2.I3 )_.
ENDDO
ENDDO
ENDDO
DO I=I,NC
DO J=I,NJR
S(I,J)=BC_1(I)
END DO
END DO
IF(IND3.NE.0)THEN
DO I2=1,NJ
DO I3=1,NJR
S(IND3,I2,I3)=BC_1(IND3)
END DO
END IF
IF(IDES1.EQ.1)THEN
SS(IDES)=S(IDES,1,1)
CALL IST_Z(1.S(L2,1,1),SS,Q2)
DO I=1,NC
Q2(I)=Q2(I)*RO_S
END DO
DO I2=1,NJR
S(IDES,1,12)=BC_1(IDES)
P(IDES,1,12)=BC_1(IDES)
S(NC+IDES,1,12)=Q2(IDES)
P(NC+IDES,1,12)=Q2(IDES)
END DO
END IF
IF(INDM.NE.0)THEN
DO I1=1,NJ
DO I2=1,NJR
S(IDES+1,1,12)=BC_1(IDES+1)
P(IDES+1,1,12)=BC_1(IDES+1)
S(NC+IDES+1,1,12)=Q2(IDES+1)
P(NC+IDES+1,1,12)=Q2(IDES+1)
END DO
END DO
END IF
IF(SAT.EQ.1)THEN
DO I1=1,NC
SS(I1)=BC_1(I1)
END DO
CALL IST_Z(1.S(L2,1,1),SS,Q2)
DO I=1,NC
Q2(I)=Q2(I)*RO_S
END DO
DO I1=1,NC
DO I2=1,NJ
DO I3=1,NJR
S(I1,I2,I3)=BC_1(I1)
S(I1+NC,I2,I3)=Q2(I1)
P(I1,I2,I3)=BC_1(I1)
P(I1+NC,I2,I3)=Q2(I1)
END DO
END DO
END IF
END DO
END DO
DO I1=1,NC
BC_1(I1)=0
END DO
BC_1(IND3)=P_C(ind3)/555.0/TO
end if
SUBROUTINE VEL_POR(JJ,NJ,OR_1.IVEL_1)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 U(14,201),EPS(1000),U1(101,201),A1(14,201),V(30),
VS(30),RP(30),EPS1(1000)
COMMON/UG/U_GUESS,EPS
COMMON/OLD/AA(I 4).SUM(14).COLD(14,201,101)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),G1(F14),P1(14,201)
COMMON/NEW_GRID/DELR0(101),ALF1(101),NGR1,NGR2
COMMON/BND2/NJ2,NJ1,ITPRT,ITCNT,NJ1
COMMON/BND3/S(14,201,101)
COMMON/PROP_D..Z/DELZ,DELT,TIME,DELR1,DELX2,TTJ,NC,NJR,NP
COMMON/PROP_S_Z/Z/CP_S,RO_S,AINT.R,P,D_P,CON_S1,HEAT(4)
COMMON/INDIC/L1,L2,L3,L4,L5,L6,LL
COMMON/NZY/NC1
COMMON/PRIMF..GN2.RAj_V,EPSEX.RHOS,TAMB,ALPHA1,UINS,HWALL,LEN

DATA R1/555.

c a number to make the division of grids correctly
IF(IVEL_1.EQ.0)THEN
  III=2
ENDIF

c there is a temperature difference between the gas and solid phases
  EC=1./VOID_B-1.
  DP=R.P*2.

c grid number for velocity distribution
  NP=125
  TR=D1/DP

c grid fraction for almost-constant velocity section in the radial direction
  FRAC1=.93

c grid fraction for variable velocity section in the radial direction
  FRAC2=.07

c number of grids in the bulk section
  K1=21

c number of grids close to the wall
  K2=104
  K11=K1
  K22=K2
  IR=5

c start computing the velocity profile
c guess the velocity at the center of the column
  U_GUESS=1.0

133 IF(U_GUESS.EQ.1.0)THEN
  DO JJ=1,NP-1
    U(JJ,1)=U_GUESS
  END DO
  ELSE
  DO JJ=2,NP-1
    U(JJ,1)=C(1,1)
  END DO
  U(1,1)=U_GUESS
  END IF

IF(U_GUESS.EQ.1.0)THEN
  GN=S(L5,JJ,1)/S1(JJ,1)/R1
ENDIF

c at wall no-slip flow, therefore velocity is zero
U(JJ,NP)=0.

RO_F=S(L5,JJ,1)/S1(JJ,1)/R1
IF(U_GUESS.EQ.1.0)THEN
  GN=S(L4,JJ,1)*RO_F/60.*VOID_B
ELSE
  GN=UD*RO_F

RETURN
END
ENDIF
T_GAS=S(L1,J1,1)
REY_D=RE(GN,T_GAS)
REC=1.75/150.*REY_D/(1.-VOID_B)
US=(1.+4.*REC)**.5-1.)/(2.*REC)
c "DIFFEQ1" is the main routine to compute the velocity profile
CALL DIFFEQ1(U.A,1.1,NP,3.5)
c if converged go out
IF(ABS(U.GUESS-C(1,2)).GT.1.0E-7)THEN
U.GUESS=C(1,2)
UD=S(L4,J1,1)**VOID_B/C(1,2)/60.
GO TO 133
ENDIF

c the velocity obtained is an intrinsic velocity multiplying by porosity

c gives seepage velocity, here c(1,11) is array of variable velocity which

c is being calculated in one of the subroutine of DIFFEQ1 routine
DO I=1,NP
U(J1,J1)=C(1,11)*UD*60.
U1(J1,J1)=C(1,11)
END DO
DO I=1,NP
EPS(I)=EPS(I)
END DO
ide_1=5
ide_2=7
k=1
del0(1)=delr1*5
eps(1)=eps(1)
alf1(1)=1.-eps(1))/eps(1)
if(nj_or_1.eq.1)then
do i6=1,nj
s(4,i6,1)=u(jj,i6)/eps(1)
end do
else
s(4,i6,1)=u(jj,i6)/eps(1)
end if
do i8=5,20,5
n1=n1+1
del0(1)=delr1*5
eps(1)=eps(1)
alf1(1)=1.-eps(1))/eps(1)
if(nj_or_1.eq.1)then
do i6=1,nj
s(4,i6,1)=u(jj,i6)/eps(1)
end do
else
s(4,i6,1)=u(jj,i6)/eps(1)
end if
end do
ng1=n1
do i8=27,125,7
n1=n1+1
del0(1)=delr2*7
eps(1)=eps(1)
alf1(1)=1.-eps(1))/eps(1)
if(nj_or_1.eq.1)then
do i6=1,nj
s(4,i6,1)=u(jj,i6)/eps(1)
end do
else
s(4,i6,1)=u(jj,i6)/eps(1)
end if
end do
if(nj_or_1.eq.1)then
do i6=1,nj
  s(4,i6,N1)=u(jj,124)/eps(124)
end do
else
  s(4,i6,N1)=u(jj,124)/eps(124)
end if
ngr2=n1-ngr1
ELSE IF(VEL_1.EQ.1)THEN
  C1=1.4
  NJR1=6
  NJR2=NJR-10
  DELR11=8.*D_I/(2*(NJR1-1))
  DELR12=2.*D_I/(2*(NJR-NJR1))
  DELR0(1)=DELR11
  DELR0(NJR)=DELR12
  EPS(1)=VOID_B
  EPS(NJR)=VOID_B*(1+C1)
  ALF1(1)=(1-EPS(1))/EPS(1)
  ALF1(NJR)=(1-EPS(NJR))/EPS(NJR)
else
  ALF1(1)=(1-EPS(1))/EPS(1)
  ALF1(NJR)=(1-EPS(NJR))/EPS(NJR)
endif

DO K=NJR-2,1,-1
  IF(K.LE.NJR1)THEN
    Y1=(NJR1-1)*DELR11+NJR2*DELR12
    DELR0(K)=DELR11
  ELSE
    Y1=DELR12*K
    DELR0(K)=DELR12
  END IF
  CALL COEF2(Y1,VOID_B,D_P,C1,POR)
  EPS(1)=POR
  ALF1(1)=(1-EPS(1))/EPS(1)
i1=i1+1
END DO
RP(1)=0.
RP(NJR)=1.
DO K=2,NJR-1
  RP(K)=2*DELR0(K)/D_I+RP(K-1)
END DO
VAV=5(*4,1,1)*EPS(1)
NJ=1
RMS=1.-2.*D_P/D_I
BO=16.*(D_P/(D_I))**(-3./2.)
AO=1./(BO+2.)-RMS/(BO+1.)
A2=RMS/(BO+1.)
A3=1./(BO+2.)
D1=AO/2.+A2/(BO+3.)-A3/(BO+4.)
DO I=1,NJ
  V(I)=VS(I)*VAV
  do i6=1,nj
    s(4,i6,i)=v(i)/eps(i)
  end do
end do
END DO
END IF
RETURN
END

C
C
C this subroutine is being called by main routine to compute the variable in
C matrix. In this routine first velocity profile is being determined. the
C conductivity, diffusivity, porosity....... are being calculated in this

E-11
c routine by calling the appropriate subroutine. The routine obtained the
C matrix in axial and radial directions. It iterates till it converges to the
allowable error
C
C SUBROUTINE FUNCT(J1)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4),K_FO(4),MOL(4),MAVE,M_W(4),NU_NP,NU_NW,KGAS,
K_FP(4,201,201),BC_L(4),D_L(4),Q2(4),MW,A1(4,201),
C1(4,201,101),D_FP(4),U(4,201),EPS(1000),E30,AKT(30),
C2(4,201,101),F01(101),F11(101),F21(101),F02(101),
F1(101),F22(101),R(101),DR(101),RR(101),D_LP(4,201,101),
D_LP_R(4,201,101),U1(101,201),Y(4),SS(4),RATE_H1(201,33)
COMMON/UG/U_GUESS,EPS
COMMON/OLD/AA(14,14),SUM(14),COLD(14,201,101)
COMMON/BOND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),G(14),F(14),P(14),P(14)
COMMON/BOND/S(14,201,101)
COMMON/NEW_GRID/DEL(101),ALP(101),NGR1,NGR2
COMMON/BOND2/A,NJ2,NQRT,ITCNT,NJ1
COMMON/PR_OLD/Z/CON_Z(201,101),CON_R(201,101),CON_S(201,101),
H_W(201,101),CP_P(201,101),H_FP(201,101),Q(4,201,101),
VISC_P(201,101),D_LP(4,201),RATE_H(101,101)
COMMON/PROP_WAL/CP_WA,RO_WA,
COMMON/PROP_B_Z/REC,VOID_B,D_E,B,ALF,C,GZ,M_W
COMMON/PROP_B_Z/DELZ,TIME,DEL1,DEL2,EZ,T,NC,NU_NP
COMMON/PROP_S_Z/CP_S,RO_S,ADT,R,P,D_P,CON_S1,HEAT(4)
COMMON/INT_Z/RO_F0,UG_F0,F1,F1,CP_F0,T,F0,CF_F0(4),K_FP,C(4)
COMMON/MISC_Z/R,F,CP_FL,TOT,BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,
COMMON/INDIC/L1,L2,L3,L4,L5,L6,L7,L8,L9,L10,L11,L12,L13,L14,L15,L16,
COMMON/INDIC1/IND(4)
COMMON/RADIAL/R
COMMON/GAS/I,COMP,MW
COMMON/NCY/NC1
COMMON/PRIME/G2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UINS,HWALL,LEN
DATA EMIS,R1,/,ONCE,J1,COND,1,COM/.9,555.,0.0,0,1,1/ 
c there is a temperature difference between the gas and solid phases
C IF(L.LE.I.COM) THEN
C BC_L=TEMPF(TIME)
C I.COM=I.L+1
C END IF
C IF(J1.EQ.1 .AND. IONCE.EQ.0) THEN
C IONCE=1
C NU.OR=1
C I_SOL=0
C END IF 
c an indication number for type of gas to compute the gas conductivity
C I=2,N2, 2=air, 3=co2
C IGAS=1
C DP=!R_P2.
C IF(TVEL.I.EQ.1) THEN
C IR=10
C ELSE
C IR=5
C END IF
C calculating the area for heat transfer to the wall or from the wall
C D_T=D_E+D_1
C X_W=D_E-D_1
C D_L=2*D_L1/(D_1+D_E)*X_W
C D_INS=2*D_E/(D_1+D_E)*X_W)*1.4
C heat transfer coefficient outside of the wall
C H_OW=0.1
C END IF 
c call vel_pos to compute velocity and porosity profile
C IF(J1.EQ.1 .AND. IONCE.EQ.0) THEN
C IONCE=1
C
c compute the ratio of distance from the center to each grid over the pellet
c diameter
RR=0.
RR0(NJR)=0.
DO 15=1,NJR
RR=RR+DELR0(I5+1)/|P
RR(I5)=RR
END DO
c this section calculates the coefficients to the discretized PDE's
c

c compute the inverse of distance from the center to each grid
RR=0.
DO 15=1,NJR
IF(I5.NE.1)THEN
RR=RR+DELR0(I5)
RP(I5)=1./RR
ELSE
RP(I5)=0.
ENDIF
IF(I5.LT.IR) THEN
DELR=DELR0(I5)
DR(I5)=DELR
ELSE IF(I5.eq.IR) THEN
DELR1=DELR0(I5)
DELR2=DELR0(I5+1)
DELR=DELR1
DR(I5)=DELR
FR=DELR2/DELR1
ENDIF
ENDIF

these variables are being computed at the point where two adjacent grids are
c not the same size

IF(15.LT.IR) THEN
DELR=DELR0(I5)
DR(I5)=DELR
ENDIF
ENDIF

c this section calls the proper subroutine to compute the parameters such as
c diffusivity, conductivity......

IF(15.NE.1) THEN

DO 16=1,NC
YO(M1)=C(M1,16)*R1*C(L1,16)/S(L5,15,16)
END DO

TEMP=C(L1,16)
M_AVE=0
SUM_Y=0.
DO M1=1,NC
M_AVE=M_AVE+YO(M1)*M_W(M1)
SUM_Y=SUM_Y+YO(M1)
END DO

M_AVE=M_AVE+(1.-SUM_Y)*28.
RO_F=S(L5,15,16)/(C(L1,16)*R1)
IF(RO_F.LE.0) RO_F=P_TOT/(C(L1,16)*R1)
GN=S(L4,15,16)*RO_F/60.* VOID_B

c calculate Reynolds number:
REY=RE(GN,TEMP)
c calculate specific heat of gas phase
CP_P(IS,16)=CPGAS(TEMP,YO)
c calc viscosity
VISC_P(IS,16)=VIS(TEMP)*60.
c calc heat transfer coeff
H_FP(IS,16)=HFILM(MW,TEMP,REY,CP_P(IS,16))*60.
  iest11=0
IF((TEST11.EQ.0) MN=2
c this section compute the conductivity of gas and solid in axial and
cradial directions
  CALL PHI_CONDIR(GAS,TEMP,CON_S1,EPS(1),PHI,PHIW)
  CALL CONDUC(MNJ,GAS,PHLD_P,CON_S1,RO(16),U1(1,16),REY,TEMP,EPS(1),EFF_CON_R1,CON_R1,EFF_CON_Z1,
  CON_Z1,CON_P1,NJR,NGR1,NGR2,16)
c if there is a temperature difference between the gas and solid
  IF((SOL_FLO.EQ.1)THEN
  CON_Z(IS,16)=CON_Z1
  CON_S(IS,16)=CON_P1
  END IF
  c if there is no temperature difference between the gas and solid
  ELSE
  CON_Z(IS,16)=EFF_CON_Z1
  END IF
c computation for number of component
  DO M1=1,NC
  c calc the molecular diffusivity of each component in the mixture
  DIF=DIF(M1,TEMP,S(L5,1,16),YO)*60
  c calc Schmidt number
  SC_N=VISC_P(IS,16)/DIF/RO_F/M_AVE
  c calc axial diffusion
  CALL AXDIFF_R_Z(MNJ,GAS,PHLD_P,DIF,RO(16),U1(1,16),
  REY,SC_N,T,EP(1),EFF_DIFF_R,EFF_DIFF_Z,
  ngr,ngr1,NGR2,16)
  D_L_P_R(M1,15,16)=EFF_DIFF_R
  D_L_P_Z(M1,15,16)=EFF_DIFF_Z
  D_LP_R(M1,15,16)=CON_Z(IS,16)/RO_F/CP_P(IS,16)
  END DO
  c calc the heat transfer coefficient between the gas phase and the wall
  IF((16.EQ.NJR) THEN
  IF(GN.EQ.0)GN=S(L4,1,1)*RO_F/60.*VOID_B
  REY=RE(GN,TEMP)
  CALL HEAT_WALL(GAS,PHIW,D_P,CON_S1,RO(16),U1(1,16),
  REY,TEMP,VOID_B,H_W1)
  H_W1(NJ)=H_W1
  END IF
  IF((COND1.EQ.1) THEN
  VAV=G_F/D1/D_PI*4
  GA=G_F/D2/D_PI*4.*RO_F
  TAV=S(L1,1,1)/1.8
  RO=S(L5,1,1)/S(L1,1,1)/R1
  CP=CP_P(1,1)
  AVIS=VISC_P(1,1)
  AKC=0.000358895+3.0026706379E-5*S(L1,1,1)-5.3528942E-9*S(L1,1,1)*S(L1,1,1)
  CALL CONDUC(EMIS,CON_S1,D_P,D1,G1A,VAV,TAV,RO,CP,AVIS,
  AKC,NJR,EPSEX,EPS(1),EPS(NJR),DELR0,E,AKT)
  ICOND1=0
  END IF
  CON_R(IS,16)=AKT(IS)
  IF(E(IS).LE.0)E(IS)=E(IS-1)
  DO M1=1,NC
  D_L_P_R(M1,15,16)=AKT(IS)/RO_F
  D_LP_R(M1,15,16)=E(IS)
  END DO

E-14
END DO
IF(CON_Z(15,NJR).EQ.0)THEN
  CON_Z(15,NJR)=CON_Z(15,NJR-1)
  DO M1=1,NC
    D_LP_Z(M1,15,NJR)=CON_Z(15,NJR)/RO_F/CP_P(15,NJR)
  END DO
END IF
DO I1=1,NJ
  DO M1=1,NC
    D_LP_PP(M1,I1)=D_LP_Z(M1,I1,1)
  END DO
DO II=IojNJ
  DO MI=I,NC
    D_LP_Z(MI,I)=D_LP_Z(MI,II)
  END DO
END DO
ENDIF
DO II=I,NC
  DO MI=I,NC
    D_LP_Z(MI,I)=D_LP_Z(MI,II)
  END DO
END DO

c set the parameters to new variables
J=II
RO_F=S(L5,IIJ)/(C(L1,JJ1)*R1)
DO M1=1,NC
  D_L(M1)=D_LP_Z(M1,II)
END DO
DO M1=1,NC
  D_RF(M1)=D_LP_R(M1,II)
END DO
DO II=I,NC
  SS(II)=C(II,J1)
END DO

c call the isotherm to compute the equilibriium concentration
IF(I_SOL)==.F.)THEN
  CALL IST_Z(I,C(1,II),SS,Q2)
ELSE
  CALL IST_Z(I,C(L1,J1),SS,02)
ENDIF

c based the equilibriium per unit volume of pellet
DO I=1,NC
  Q(I,JJ1)=Q2(I)*RO_S
END DO

C this is the boundary, the first grids in axial direction
IF(I.EQ.1)THEN
  RATE_C=0
ENDIF

C compute the total amount is being adsorbed
DO M1=1,NC
  RATE_C=RATE_C+K_F(M1)*AIN_T*(Q(M1,II1)-C(M1+NC,J1))
END DO

RATE_H=0

C compute the total heat of adsorption
HEAT(2)=-(411.93585-57470.2733*C(3,J1)/RO_S+3971259.2258*
C . C(J1)=*2/RO_S/RO_S)*.44
DO M1=1,NC
  RATE_H=RATE_H+HEAT(M1)*K_F(M1)*AIN_T*(Q(M1,II1)-C(M1+NC,J1))
END DO

C this "if" calculates the first grid in radial direction, center of the bed
IF(J,J1.EQ.1)THEN
  RATE_C=0
ENDIF

C computation of moiar density component
TOT_C=0
DO M1=1,NC-1
  A2=1/(2*D_L(M1)/DELZ**2+S(L4,JJ1)/DELZ-4*D_RF(M1)/
   DR(J1)/DR(J1)+1./DELZ)
  P1=D_L(M1)/DELZ**2*(BC_1(M1)+S(M1+1,J1))
  P2=-(S(L4,JJ1)/DELZ)**(BC_1(M1))
  P3=-ALF1(JJ1)*AIN_T*K_F(M1)*(Q(M1,II1)-C(M1+NC,J1))
  P4=4*D_RF(M1)*(C(M1,J1)+1.)/DR(J1)/DR(J1)
  P5=(-P(M1,J1))/DELZ

E-15
F(M) = -C(I) + A2*(P1 + P2 + P3 + P4 + P5)
TOT_C = TOT_C + C(M)
END DO
F(NC) = (S(L,S,J,J) - TOT_C*R1*S(L,S,J,J))/R1/S(L,S,J,J) - C(NC)

The computation of molar adsorption for each component:
DO M = 1, NC
A2 = 1/(K_F(M)*AINT + 1./DEL)
F(M + NC) = -C(M + NC) + A2*(K_F(M)*AINT*(Q(M,J,J) + P(M + NC,J))/DEL)
END DO

The same computation as above except it is now for the grid at the wall
ELSE IF(J,J,E,Q,N,J) THEN
TOT_C = 0.
END DO
F(NC) = (S(L,S,J,J) - TOT_C*R1*S(L,S,J,J))/R1/S(L,S,J,J) - C(NC)

The computation of molar adsorption:
DO M = 1, NC
A2 = 1/(K_F(M)*AINT + 1./DEL)
F(M) = -C(M) + A2*(K_F(M)*AINT*(Q(M,J,J) + P(M,J,J))/DEL)
END DO

The same computation as above except it is now for the grid at the wall
ELSE IF(J, E Q, N, J) THEN
TOT_C = 0.
END DO
F(NC) = (S(L,S,J,J) - TOT_C*R1*S(L,S,J,J))/R1/S(L,S,J,J) - C(NC)

The computation of molar density of each component:
DO M = 1, NC
A2 = 1/(2*D_L(M)/DELZ**2 + S(L,S,J,J)/DELZ + 2*D_RF(M)/DR(J))
F(M + NC) = -C(M + NC) + A2*(K_F(M)*AINT*(Q(M,J,J) + P(M + NC,J))/DEL)
END DO

The same computation as above except it is now for the grids from the center to the point where the velocity starts to change
ELSE IF(J, E Q, N, J) THEN
TOT_C = 0.
END DO
F(NC) = (S(L,S,J,J) - TOT_C*R1*S(L,S,J,J))/R1/S(L,S,J,J) - C(NC)

The same computation as above except it is now for the grids from the point where the velocity starts to change to the wall.
ELSE

    TOT_C=0.

c compute molar density of each component
    DO MI=1,NC-1
      A2=J/(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+F11(J1)**D_RF(M1)**
      RP(J1)/DR(J1)+2*D_RF(M1)**F12(J1)/DR(J1)/DR(J1)+1./DELT)
      P1=J/(2*D_L(M1)/DELZ**2+S(M1,J1+1)+BC_1(M1))
      P2=-(S(L4,J1)/DELZ)**(-BC_1(M1))
      P3=-ALF1(J1)**AINT*K_F(M1)**Q(M1,J1)/C(M1+NC,J1))
      P4=J/(2*D_L(M1)/DELZ**2+S(M1,J1+1)+BC_1(M1))
      P5=-(S(L4,J1)/DELZ)**(-BC_1(M1))
      P6=-(-P(M1,J1))/DELT
      F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)/DR(J1)/DR(J1)
    END DO

    F(NC)=(S(L4,J1)-TOT_C*RI*S(L4,J1))/RI/S(L4,J1)

ENDIF

KNDIF

c this section compute the S matrix variables for grid at z=L, the outflow boundary

c compute the molar adsorption
    DO MI=1,NC
      A2=J/(2*D_L(M1)*AINT+1./DELT)
      F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1)))
    END DO

ENDIF IF(J.LEQ.NJ1) THEN

c compute the total amount adsorbed
    RATE_C=0.
    DO MI=1,NC
      RATE_C=RATE_C+K_F(M1)*AINT*(Q(M1,J1)-C(M1+NC,J1))
    END DO

c compute the total heat of adsorption
    RATE_H=RATE_H+HEAT(M1)*K_F(M1)*AINT*(Q(M1,J1)-C(M1+NC,J1))
    END DO

ENDIF IF(J.LEQ.NJ1) THEN

ELSE IF(J.LEQ.NJ1) THEN

c this section compute the s matrix at outflow boundary at the center of bed

    IF(J.LT.EQ.1) THEN
      TOT_C=0.
    END DO

  c compute the component molar density
    DO MI=1,NC-1
      A2=J/(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+4*D_RF(M1)**
      DR(J1)/DR(J1)+1./DELT)
      P1=J/(2*D_L(M1)/DELZ**2+S(M1,J1+1)+BC_1(M1))
      P2=-(S(L4,J1)/DELZ)**(-BC_1(M1))
      P3=-ALF1(J1)**AINT*K_F(M1)**Q(M1,J1)-C(M1+NC,J1))
      P4=J/(2*D_L(M1)/DELZ**2+S(M1,J1+1)+BC_1(M1))
      P5=-(S(L4,J1)/DELZ)**(-BC_1(M1))
      P6=-(-P(M1,J1))/DELT
      F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5)
    END DO

E-17
\[ F(NC) = \frac{(S(L5, J1) - TOT_C*RI*S(L1, J1))}{RI/(S(L1, J1)} - C(NC, J1) \]

c compute the molar adsorption

\[
DO \ M1=1, NC-1 \\
A2=1/(K_F(M1)*AINT+1./DELT) \\
F(M1+NC)=C(M1+NC, J1)+A2*(K_F(M1)*AINT*(Q(M1, J1)))+ \\
P(M1+NC, J1)/DELT \\
END \ DO \\
\]

c this section is for \( r \) at the wall
ELSE IF(J1.EQ.NLR) THEN \\
TOT_C=0. \\
\]

c compute molar density

\[
DO \ M1=1, NC-1 \\
A2=1/(2*D_L(M1)/DELT*2+S(L4, J1)/DELT+2*D_RF(M1) \\
* DR(J1)/DR(J1)+1./DELT) \\
P1=D_L(M1)/DELT*2*(S(M1, J1, J1)) \\
P2=-S(L4, J1)/DELT*(-S(M1, J1, J1)) \\
P3=ALF1(J1)*AINT*K_F(M1)*Q(M1, J1, J1)-C(M1+NC, J1) \\
P4=D_RF(M1)*RP(J1)*(C(M1, J1, J1)-C(M1, J1, J1-1))/(2*DR(J1)) \\
P5=2*D_RF(M1)*C(M1, J1, J1)/DR(J1)/DR(J1) \\
P6=(-P(M1, J1))/DELT \\
F(M1)=C(M1, J1)+A2*(P1=P2+P3+P4+P5+P6) \\
TOT_C=TOT_C+C(M1, J1) \\
END \ DO \\
\]

c compute molar adsorption

\[
DO \ M1=1, NC-1 \\
A2=1/(2*D_L(M1)/DELT*2+S(L4, J1)/DELT+2*D_RF(M1) \\
* DR(J1)/DR(J1)+1./DELT) \\
P1=D_L(M1)/DELT*2*(S(M1, J1, J1)) \\
P2=-S(L4, J1)/DELT*(-S(M1, J1, J1)) \\
P3=ALF1(J1)*AINT*K_F(M1)*Q(M1, J1, J1)-C(M1+NC, J1) \\
P4=D_RF(M1)*RP(J1)*(C(M1, J1, J1)-C(M1, J1, J1-1))/(2*DR(J1)) \\
P5=2*D_RF(M1)*C(M1, J1, J1)/DR(J1)/DR(J1) \\
P6=(-P(M1, J1))/DELT \\
F(M1)=C(M1, J1)+A2*(P1=P2+P3+P4+P5+P6) \\
TOT_C=TOT_C+C(M1, J1) \\
END \ DO \\
\]

c this section computes \( S \) matrix for those grids with constant grid size
ELSE \\
IF(J1.NE.IR)THEN \\
TOT_C=0. \\
\]

c compute molar density

\[
DO \ M1=1, NC-1 \\
A2=1/(2*D_L(M1)/DELT*2+S(L4, J1)/DELT+2*D_RF(M1) \\
* DR(J1)/DR(J1)+1./DELT) \\
P1=D_L(M1)/DELT*2*(S(M1, J1, J1)) \\
P2=-S(L4, J1)/DELT*(-S(M1, J1, J1)) \\
P3=ALF1(J1)*AINT*K_F(M1)*Q(M1, J1, J1)-C(M1+NC, J1) \\
P4=D_RF(M1)*RP(J1)*(C(M1, J1, J1)-C(M1, J1, J1-1))/(2*DR(J1)) \\
P5=2*D_RF(M1)*C(M1, J1, J1)/DR(J1)/DR(J1) \\
P6=(-P(M1, J1))/DELT \\
F(M1)=C(M1, J1)+A2*(P1=P2+P3+P4+P5+P6) \\
TOT_C=TOT_C+C(M1, J1) \\
END \ DO \\
\]

c compute molar adsorption

\[
DO \ M1=1, NC-1 \\
A2=1/(2*D_L(M1)/DELT*2+S(L4, J1)/DELT+2*D_RF(M1) \\
* DR(J1)/DR(J1)+1./DELT) \\
P1=D_L(M1)/DELT*2*(S(M1, J1, J1)) \\
P2=-S(L4, J1)/DELT*(-S(M1, J1, J1)) \\
P3=ALF1(J1)*AINT*K_F(M1)*Q(M1, J1, J1)-C(M1+NC, J1) \\
P4=D_RF(M1)*RP(J1)*(C(M1, J1, J1)-C(M1, J1, J1-1))/(2*DR(J1)) \\
P5=2*D_RF(M1)*C(M1, J1, J1)/DR(J1)/DR(J1) \\
P6=(-P(M1, J1))/DELT \\
F(M1)=C(M1, J1)+A2*(P1=P2+P3+P4+P5+P6) \\
TOT_C=TOT_C+C(M1, J1) \\
END \ DO \\
\]

c this section compute \( S \) for variable grid size
ELSE \\
TOT_C=0. \\
\]

c compute the molar density

\[
DO \ M1=1, NC-1 \\
A2=1/(2*D_L(M1)/DELT*2+S(L4, J1)/DELT+D_RF(M1) \\
* DR(J1)/DR(J1)+1./DELT) \\
P1=D_L(M1)/DELT*2*(S(M1, J1, J1)) \\
P2=-S(L4, J1)/DELT*(-S(M1, J1, J1)) \\
P3=ALF1(J1)*AINT*K_F(M1)*Q(M1, J1, J1)-C(M1+NC, J1) \\
P4=D_RF(M1)*RP(J1)*(C(M1, J1, J1)-C(M1, J1, J1-1))/(2*DR(J1)) \\
P5=2*D_RF(M1)*C(M1, J1, J1)/DR(J1)/DR(J1) \\
P6=(-P(M1, J1))/DELT \\
F(M1)=C(M1, J1)+A2*(P1=P2+P3+P4+P5+P6) \\
TOT_C=TOT_C+C(M1, J1) \\
END \ DO \\
\]
PI=D_L(M1)/DELZ**2*(2*S(M1,J-1,J1))+
P2=S(L4,J1)/DELZ**2*(S(M1,1,J1)+S(M1,J-1,J1))
P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J,J1)-C(M1+NC,J1))
P4=D_RF(M1)*(F21(J1)*C(M1,J+1)+F01(J1)*
C(M1,J-1))
P5=2*D_RF(M1)*(F22(J1)*C(M1,J+1)+F02(J1)*C(M1,J-1))
/DR(J1)/DR(J1)
P6=(-P(M1,J1))/DELT
F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5,J1)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-
C(NC,J1)
c compute molar adsorption
DO M1=1,NC
A2=1/(K_F(M1)*AINT+1./DELT)
F(M1)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J,J1)))+
P(M1+NC,J1)/DELT)
END DO
END IF
ENDIF
C
This section computes the s matrix for grids inside of the column
ELSE
C comp total molar adsorption
RATE_C=0
DO M1=1,NC
RATE_C=RATE_C+K_F(M1)*AINT*(Q(M1,J,J1)-C(M1+NC,J1))
END DO
C compute total heat of adsorption
RATE_C1(J,J1)=RATE_C*(1-EPS(J1))
RATE_H=0
C
HEAT2=-411.93585-57470.2733*C(3,J1)/RO_S+3971259.2258*C*C(3,J1)**2/RO_S/RO_S)*.4
DO M1=1,NC
RATE_H=RATE_H+HEAT(M1)*K_F(M1)*AINT*(Q(M1,J,J1))-
C(M1+NC,J1))
END DO
RATE_H1(J,J1)=RATE_H
C this section copens s for the grids at the center of bed
IF(J1.EQ.1) THEN
TOT_C=0.
C comp molar density
DO M1=1,NC-1
A2=1/(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+4*D_RF(M1)/
DR(J1)/DR(J1)+1./DELT)
P1=D_L(M1)/DELZ**2*(S(M1,1,J1)+S(M1,J-1,J1))
P2=S(L4,J1)/DELZ**2*(S(M1,1,J1)+S(M1,J-1,J1))
P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J,J1)-C(M1+NC,J1))
P4=4*D_RF(M1)*(C(M1,J+1)))/DR(J1)/DR(J1)
P5=(-P(M1,J1))/DELT
F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5)
TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5,J1)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-
C(NC,J1)
c comp molar adsorption
DO M1=1,NC
A2=1/(K_F(M1)*AINT+1./DELT)
F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J,J1)))+
P(M1+NC,J1)/DELT)
END DO

C comp s for the grid at wall
ELSE IF(J1.EQ.NJR) THEN
   TOT_C=0.
C comp molar density
DO M1=1,NC-1
   A2=1./(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+2*D_RF(M1)/DR(J1))
   P1=D_L(M1)/DELZ**2*(S(M1,J-1,J1)+S(M1,J+1,J1))
   P2=-S(L4,J1)/DELZ*(-S(M1,J-1,J1))
   P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J1)-C(M1+NC,J1))
   P4=D_RF(M1)*RP(J1)*(C(M1,J1-1)-C(M1,J1-1))/(2*DR(J1))
   P5=2*D_RF(M1)*(C(M1,J1-1))/DR(J1)/DR(J1)
   P6=-(-P(M1,J1))/DELT
   F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
   TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5,J1)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-
   C(NC,J1)
C comp molar adsorption
DO M1=1,NC
   A2=1./(K_F(M1)*AINT+1./DELT)
   F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1))-
   P(M1+NC,J1)/DELT)
END DO
C this section computes s for variable grid size
ELSE
   IF(J1.NE.JR)THEN
      TOT_C=0.
C comp the molar density
DO M1=1,NC-1
   A2=1./(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+2*D_RF(M1)/DR(J1))
   P1=D_L(M1)/DELZ**2*(S(M1,J-1,J1)+S(M1,J+1,J1))
   P2=-S(L4,J1)/DELZ*(-S(M1,J-1,J1))
   P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J1)-C(M1+NC,J1))
   P4=D_RF(M1)*RP(J1)*(C(M1,J1-1)-C(M1,J1-1))/(2*DR(J1))
   P5=2*D_RF(M1)*(C(M1,J1-1))/DR(J1)/DR(J1)
   P6=-(-P(M1,J1))/DELT
   F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
   TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5,J1)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-
   C(NC,J1)
C comp the molar adsorption
DO M1=1,NC
   A2=1./(K_F(M1)*AINT+1./DELT)
   F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1))-
   P(M1+NC,J1)/DELT)
END DO
C this section computes s for variable grid size
ELSE
   TOT_C=0.
C comp molar density
DO M1=1,NC-1
   A2=1./(2*D_L(M1)/DELZ**2+S(L4,J1)/DELZ+2*D_RF(M1)/DR(J1))
   P1=D_L(M1)/DELZ**2*(S(M1,J-1,J1)+S(M1,J+1,J1))
   P2=-S(L4,J1)/DELZ*(-S(M1,J-1,J1))
   P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J1)-C(M1+NC,J1))
   P4=D_RF(M1)*RP(J1)*(C(M1,J1-1)-C(M1,J1-1))/(2*DR(J1))
   P5=2*D_RF(M1)*(C(M1,J1-1))/DR(J1)/DR(J1)
   P6=-(-P(M1,J1))/DELT
   F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
   TOT_C=TOT_C+C(M1,J1)
END DO

\begin{verbatim}
DR1)/DRU1)\)
P6=-(P(M,1,J1))/DELT
F(M)=-C(M,1,J1)+A2*(P1+P2+P3+P4+P5+P6)
TOT_C=TOT_C+C(M,1,J1)
END DO
F(N)=S(S(L,J,J1))\(S(L,J,J1))/R1/S(L,J,J1)-C(N,J1)

c comp molar adsorption
DO M=1,NC
A2=1/(K\(F(M)\)*AINT+1./DELT)
F(M+NC)=-C(M+NC,J1)+A2*(K\(F(M)\)*AINT*(Q(M,J,J1))+-
P(M+NC,J1)/DELT)
END DO
END IF
ENDIF
ENDIF
ENDIF
C FOR TEMPERATURE
C
ELSE
C
C set the parameters to new variables
H_FW=H_W(J,1,N)
RO_F=S(S(L,J,J1))\(C(J,J1)*R1)
CP_F=CP_P(J,J1)
H_FS=H_FP(J,J1)
CON_L=CON_Z(J,J1)
CON_RF=CON_R(J,J1)
CON_P=CON_S(J,J1)
VISC_F=VISC_P(J,J1)
J=J
KK=0
IF(J.EQ.1)THEN
IF(J.EQ.1)THEN
C
C computation of gas temperature
IF(SOL_FLO.EQ.1)THEN
A2=1/(2*CON_J/DELZ**2+RO_F*CP_F*(S(L,J,J1))/DELZ+
1./DELT)+4*CON_RF/DR(J1)/DR(J1)
P1=CON_L/DELZ**2*(BC_L1+S(L,J,J1))
P2=RO_F*CP_P*(S(L,J,J1))/DELZ*(BC_L1)
P3=-(1-EPS(J1))*EPS(J1)*H_FS*AINT*(C(J,J1)-C(J,J1))
P4=RO_F*CP_F*(S(J,J1))/DELZ
P5=4*CON_RF*(C(J,J1)+S(L,J,J1))/DELZ
F(1)=-C(J,J1)+A2*(P1+P2+P3+P4+P5)
c computation of solid temperature
A2=1./(2*CON_P/DELZ**2+(RO_S*CP_S)/DELZ+
4*CON_P/DR(J1)/DR(J1))
P1=AINT*H_FS*(C(J,J1)-C(J,J1))
P2=-RATE_H1(J,J1)
P3=CON_P*(S(L,J+1,J1)+S(L,J+1,J1))/DELZ
P4=4*CON_P*(C(J,J1))/DELZ
P5=RO_S*CP_S*(-P(J,J1))/DELZ
F(2)=-C(J,J1)+A2*(P1+P2+P3+P4+P5)
c computation of effective temperature
ELSE
A2=1./(EPS(J1)**2*CON_J/DELZ**2+RO_F*CP_P*(S(L,J,J1)/
DELZ)**2+EPS(J1)*RO_F*CP_F*(1-EPS(J1))*RO_S*CP_S)/DELZ+4*
EPS(J1)*CON_RF/DR(J1)/DR(J1))
P1=EPS(J1)*CON_L/DELZ**2*(BC_L1+S(L,J,J1))
P2=EPS(J1)*RO_F*CP_P*S(L,J,J1)/DELZ*(BC_L1)
P3=-(1-EPS(J1))*RATE_H1(J,J1)
P4=EPS(J1)*RO_F*CP_F*(C(J,J1)+S(L,J,J1))
P5=EPS(J1)**4*CON_RF*(C(J,J1)+S(L,J,J1))/DELZ
\end{verbatim}
P6 = -(EPSO1) * RO_F * CP * (1 - EPSO1) * RO_S * CP_S) * (-P(I,J)) / DELT
F(I) = C(1,J) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
F(2) = 0.
ENDIF

c the same computation as above except it is now for the grid at the wall
ELSE IF(J1.EQ.N1) THEN

c comp of gas phase temperature
IF(SOL Flo.EQ.1) THEN
A2 = 1/(2 * CON_L / DELZ * 2 + RO_F * CP_F * S(L4,J,J1) / DELZ +
(RO_F * CP_F) / DELT + 2 * CON_RF / DR(J1) / DR(J1))
P1 = CON_L / DELZ * 2 * (BC_L1 + S(L1,J,J1))
P2 = RO_F * CP_F * S(L4,J,J1) / DELZ * (-BC_L1)
P3 = -(EPS(J1)) * EPS(J1) * H_FW * AINT * (C(1,J) - C(2,J1))
P4 = RO_F * CP_F * C(1,J) * S(L4,J+1,J1)
S(L4,J, J1) / DELZ
P5 = CON_RF * RP(J1) * (2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P6 = CON_RF * (2 * C(J1-1) + 2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P7 = RO_F * CP_F * (-P(I,J)) / DELT
F(I) = -(C(1,J) + A2 * (P1 + P2 + P3 + P4 + P5 + P6 + P7))

ELSE

c compute gas phase temperature
IF(SOL Flo.EQ.1) THEN
A2 = 1/(2 * CON_L / DELZ * 2 + RO_F * CP_F * S(L4,J,J1) / DELZ +
(RO_F * CP_F) / DELT + 2 * CON_RF / DR(J1) / DR(J1))
P1 = CON_L / DELZ * 2 * (BC_L1 + S(L1,J,J1))
P2 = RO_F * CP_F * S(L4,J,J1) / DELZ * (-BC_L1)
P3 = -(EPS(J1)) * EPS(J1) * H_FW * AINT * (C(1,J) - C(2,J1))
P4 = RO_F * CP_F * C(1,J) * S(L4,J+1,J1)
S(L4,J,J1) / DELZ
P5 = CON_RF * RP(J1) * (2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P6 = CON_RF * (2 * C(J1-1) + 2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P7 = -(EPS(J1)) * RO_F * CP_F * (1 - EPS(J1)) * RO_S * CP_S) *
(-P(I,J)) / DELT
F(I) = C(1,J) + A2 * (P1 + P2 + P3 + P4 + P5 + P6 + P7)
F(2) = 0.
ENDIF

ELSE

c comp of gas phase temperature
IF(SOL Flo.EQ.1) THEN
A2 = 1/(2 * CON_L / DELZ * 2 + RO_F * CP_F * S(L4,J,J1) / DELZ +
(RO_F * CP_F) / DELT + 2 * CON_RF / DR(J1) / DR(J1))
P1 = CON_L / DELZ * 2 * (BC_L1 + S(L1,J,J1))
P2 = RO_F * CP_F * S(L4,J,J1) / DELZ * (-BC_L1)
P3 = -(EPS(J1)) * EPS(J1) * H_FW * AINT * (C(1,J) - C(2,J1))
P4 = RO_F * CP_F * C(1,J) * S(L4,J+1,J1)
S(L4,J,J1) / DELZ
P5 = CON_RF * RP(J1) * (2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P6 = CON_RF * (2 * C(J1-1) + 2 * H_FW * DR(J1) / CON_RF * (C(3,J1) -
C(J1)) / DR(J1) / DR(J1))
P7 = -(EPS(J1)) * RO_F * CP_F * (1 - EPS(J1)) * RO_S * CP_S) *
(-P(I,J)) / DELT
F(I) = C(1,J) + A2 * (P1 + P2 + P3 + P4 + P5 + P6 + P7)
F(2) = 0.
ENDIF

ELSE

c the point where the velocity start to change
IF(J1.EQ.N1) THEN

ELSE

c compute gas temperature
IF(SOL Flo.EQ.1) THEN
A2 = 1/(2 * CON_L / DELZ * 2 + RO_F * CP_F * S(L4,J,J1) / DELZ +
(RO_F * CP_F) / DELT + 2 * CON_RF / DR(J1) / DR(J1))
P1 = CON_L / DELZ * 2 * (BC_L1 + S(L1,J,J1))
P2 = RO_F * CP_F * S(L4,J,J1) / DELZ * (-BC_L1)
\[ P_3 = -\left(1 - \text{EPS}(J1)\right)H_F S \cdot \text{AINT} \cdot (C(1,J1) - C(2,J1)) \]
\[ P_4 = -\text{RO}_F \cdot C_P \cdot F \cdot C(1,J1) \cdot \text{S}(L4,J+1,J1) \cdot \text{S}(L4,J,1,J1)/(\text{DELZ}) \]
\[ P_5 = \text{CON}_R_F \cdot \text{RP}(J1) \cdot (C(1,J1+1) - C(1,J1-1))/(2 \cdot \text{DR}(J1)) \]
\[ P_6 = \text{CON}_R_F \cdot (C(1,J1+1) - C(1,J1-1))/\text{DR}(J1)/\text{DR}(J1) \]
\[ P_7 = -\text{RO}_F \cdot C_P \cdot F \cdot \text{P}(J1)/\text{DELZ} \]
\[ \text{F}(1) = C(1,J1) + A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7) \]

c compute solid temperature
\[ A2 = \left(2 \cdot \text{CON}_P / \text{DELZ} \right) + 2 \cdot \text{RO}_S \cdot C_P \cdot S / \text{DELT} + 2 \cdot \text{CON}_P / \text{DR}(J1) \]
\[ P1 = \text{AINT} \cdot H_F S \cdot (C(1,J1) - C(2,J1)) \]
\[ P_2 = \text{RATE}_H(1,J1) \]
\[ P_3 = \text{CON}_P \cdot \text{S}(S(L2,J+1,J1) + S(L2,J+1,J1) - S(L4,J+1,J1))/\text{DELZ}/\text{DELZ} \]
\[ P_4 = \text{CON}_P \cdot \text{RP}(J1) \cdot (C(2,J1+1) - C(2,J1-1))/(2 \cdot \text{DR}(J1)) \]
\[ P_5 = \text{CON}_P \cdot (C(2,J1+1) - C(2,J1-1))/\text{DR}(J1)/\text{DR}(J1) \]
\[ P_6 = -\text{RO}_S \cdot C_P \cdot S \cdot \text{P}(2,J1)/\text{DELZ} \]
\[ \text{F}(2) = C(2,J1) + A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7) \]

c compute effective temperature
\[ \text{ELSE} \]
\[ A2 = 1/(2 \cdot \text{RO}_F \cdot C_P \cdot F \cdot \text{S}(L4,J+1,J1) \cdot \text{S}(L4,J,1,J1))/\text{DELZ} + 2 \cdot \text{CON}_P / \text{DR}(J1) \]
\[ P1 = \text{AINT} \cdot H_F S \cdot (C(1,J1) - C(2,J1)) \]
\[ P_2 = \text{RATE}_H(1,J1) \]
\[ P_3 = \text{CON}_P \cdot \text{S}(S(L2,J+1,J1) + S(L2,J+1,J1) - S(L4,J+1,J1))/\text{DELZ} \]
\[ P_4 = \text{CON}_P \cdot \text{RP}(J1) \cdot (C(2,J1+1) - C(2,J1-1))/(2 \cdot \text{DR}(J1)) \]
\[ P_5 = \text{CON}_P \cdot (C(2,J1+1) - C(2,J1-1))/\text{DR}(J1)/\text{DR}(J1) \]
\[ P_6 = -\text{RO}_S \cdot C_P \cdot S \cdot \text{P}(2,J1)/\text{DELZ} \]
\[ \text{F}(2) = C(2,J1) + A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7) \]

\[ \text{F}(2) = 0. \]

\[ \text{ENDIF} \]

c the same computation as above except it is now for the grids from the point
\[ \text{c where the velocity starts change to the wall} \]
\[ \text{ELSE} \]

c compute the gas temperature
\[ \text{IF}(1 \cdot \text{SOL}_F / \text{EQ} \cdot 1) \text{THEN} \]
\[ A2 = 1/(2 \cdot \text{CON}_P / \text{DELZ} + 2 \cdot \text{RO}_F \cdot C_P \cdot F \cdot \text{S}(L4,J+1,J1) \cdot \text{DELZ} + 2 \cdot \text{CON}_P / \text{DR}(J1)) \]
\[ P1 = \text{AINT} \cdot H_F S \cdot (C(1,J1) - C(2,J1)) \]
\[ P_2 = \text{RATE}_H(1,J1) \]
\[ P_3 = \text{CON}_P \cdot \text{S}(S(L2,J+1,J1) + S(L2,J+1,J1) - S(L4,J+1,J1))/\text{DELZ} \]
\[ P_4 = \text{CON}_P \cdot \text{RP}(J1) \cdot (C(2,J1+1) - C(2,J1-1))/(2 \cdot \text{DR}(J1)) \]
\[ P_5 = \text{CON}_P \cdot (C(2,J1+1) - C(2,J1-1))/\text{DR}(J1)/\text{DR}(J1) \]
\[ P_6 = -\text{RO}_S \cdot C_P \cdot S \cdot \text{P}(2,J1)/\text{DELZ} \]
\[ \text{F}(1) = C(1,J1) + A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7) \]

c compute the solid temperature
\[ A2 = 1/(2 \cdot \text{CON}_P / \text{DELZ} + 2 \cdot \text{RO}_S \cdot C_P \cdot S / \text{DELT} + \text{CON}_P \cdot \text{RP}(J1)) \]
\[ \text{F}(1) = C(1,J1) - 2 \cdot \text{CON}_P / \text{DR}(J1)/\text{DR}(J1) \]
\[ P1 = \text{AINT} \cdot H_F S \cdot (C(1,J1) - C(2,J1)) \]
\[ P_2 = \text{RATE}_H(1,J1) \]
\[ P_3 = \text{CON}_P \cdot \text{S}(S(L2,J+1,J1) + S(L2,J+1,J1))/\text{DELZ} \]
\[ P_4 = \text{CON}_P \cdot \text{RP}(J1) \cdot (C(2,J1+1) - C(2,J1-1) - \text{F}(1)/\text{DR}(J1)) \]
\[ P_5 = \text{CON}_P \cdot (C(2,J1+1) - C(2,J1-1))/\text{DR}(J1)/\text{DR}(J1) \]

E-23
P6 = -RO_S*CP_S*(-P(2,J1))/DELT
F(2) = -C(2,J1)+A2*(P1+P2+P3+P4+P5+P6)
ELSE

c compute the effective temperature
A2 = 1/(EPS(J1))*(2*CON_L/DELT)**2+RO_F*CP_F*S(L4,J1,J1)/
     DELZ+(EPS(J1)*RO_F*CP_F+(1-EPS(J1))*RO_S*CP_S)/DELT+
     EPS(J1)*CON_RF*(RP(J1)*F11(DR(J1)))*2*Fl2(J1)/
     DR(J1)/DR(J1))
P1 = EPS(J1)*CON_L/DELT**2*S(L1,J1,J1)+BC_L1)
P2 = EPS(J1)*RO_F*CP_F*S(L4,J1,J1)/(DELT)*(BC_L1)
P3 = -(1-EPS(J1))*RATE_HI(J1)
P4 = EPS(J1)*RO_F*CP_F*C(RP(J1),F11(DR(J1)))*S(L4,J1,J1)/
     (DELT)
P5 = EPS(J1)*CON_RF*RP(J1)*(F21(DR(J1)))*C(J1,J1+1)-F01(J1)*
     C(J1,J1-1))/(DR(J1))
P6 = EPS(J1)*CON_RF*RP(J1)*(F22(DR(J1)))*C(J1,J1+1)+F02(J1)*
     C(J1,J1-1))/(DR(J1))/DR(J1))
P7 = EPS(J1)*RO_F*CP_F+(1-EPS(J1))*RO_S*CP_S)*
     (P(1,J1))/DELT
F(1) = -C(1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
F(2) = 0.
ENDIF
ENDIF
ENDIF

C
C this section compute the S matrix variables for grid at z=L, the outflow
C boundary
C
c ELSE IF(J.EQ.N1) THEN
IF(J.EQ.1) THEN

c compute the gas temperature
IF(_SOL_FLO_.EQ.1) THEN
A2 = 1/(2*CON_L/DELT)**2+RO_F*CP_F*S(L4,J1,J1)/DELT+
     (RO_F*CP_F)/DELT+(4*CON_RF/DR(J1))/DR(J1))
P1 = CON_L/DELT**2*S(L1,J1,J1))
P2 = RO_F*CP_F*S(L4,J1,J1)/(DELT)*(S(L1,J1,J1))
P3 = -(1-EPS(J1))*(H_FS*AINT*(C(J1,J1)-C(2,J1))
P4 = RO_F*CP_F*C(J1,J1)*S(L4,J1,J1).
P5 = EPS(J1)*CON_RF*(C(J1,J1+1))/DR(J1)/DR(J1)
P6 = RO_F*CP_F*(-P(1,J1))/DELT
F(1) = -C(1,J1)+A2*(P1+P2+P3+P4+P5+P6)
ENDIF
ENDIF
ENDIF

c compute the solid temperature
A2 = 1/(2*CON_P/DELT)**2+RO_S*CP_S/DELT+4*CON_P/
     DR(J1)/DR(J1))
P1 = AINT*(H_FS*(C(J1,J1)-C(2,J1))
P2 = RATE_HI(J1)
P3 = CON_P*(S(L2,J1,J1)+S(L2,J1,J1))/DELT/DELT
P4 = 4*CON_P*C(J1,J1+1)/DR(J1)/DR(J1)
P5 = RO_S*CP_S*(-P(2,J1))/DELT
F(2) = -C(2,J1)+A2*(P1+P2+P3+P4+P5)
ELSE

c compute the effective temperature
A2 = 1/(EPS(J1))*(2*CON_L/DELT)**2+RO_F*CP_F*S(L4,J1,J1)/
     DELZ+(EPS(J1)*RO_F*CP_F+(1-EPS(J1))*RO_S*CP_S)/DELT+
     4*EPS(J1)*CON_RF/DR(J1))/DR(J1))
P1 = EPS(J1)*CON_L/DELT**2*S(L1,J1,J1))
P2 = EPS(J1)*RO_F*CP_F*S(L4,J1,J1)/(DELT)*(S(L1,J1,J1))
P3 = -(1-EPS(J1))*RATE_HI(J1)
P4 = EPS(J1)*RO_F*CP_F*C(RP(J1),F11(DR(J1)))*S(L4,J1,J1)/
     (DELT)
P5 = EPS(J1)*RO_F*CP_F*C(RP(J1),F11(DR(J1)))*S(L4,J1,J1)/
     (DELT)

E-24
P5 = 4 * EPS(J1) * CON_RF * (C(1, J1 + 1)) / DR(J1) / DR(J1)
F(1) = C(1, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
F(2) = 0.
END IF

C this section is for r at the wall
ELSE IF (J1.EQ.NUR) THEN

C compute gas temperature
IF (.NOT. SOL_FLO .EQ. 1) THEN

A2 = 1 / 2 * CON_L / DELZ ** 2 * RO_F * CP_F * S(L4, J1, J1) / DELZ + (RO_F * CP_F / DELT)
P1 = CON_L / DELZ ** 2 * (2 * S(L1, J1, J1))
A2 = RO_F * CP_F * S(L4, J1, J1) / DELZ ** 2 * (S(L1, J1, J1))
P3a = (1 - EPS(J1)) / EPS(J1) * H_FS * AINT * (C(1, J1) - C(2, J1))
P4a = RO_F * CP_F * (C(1, J1) - S(L4, J1, J1)) / DELZ ** 2 * (S(L1, J1, J1))
P5 = CON_RF * RP(J1) * (2 * S(L1, J1, J1))
P6 = CON_RF * (2 * C(1, J1 - 1) + 2 * S(L1, J1, J1)) / DR(J1) / DR(J1)
F(1) = C(1, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6 + P7)
ELSE
C compute solid temperature

A2 = 1 / 2 * CON_P / DELZ ** 2 * RO_S * CP_S / DELT + 2 * CON_P / DR(J1) / DR(J1)

A2 = EPS(J1) * CON_L / DELZ ** 2 * RO_F * CP_F * S(L4, J1, J1) / DELZ + (RO_F * CP_F / DELT)
P1 = EPS(J1) * CON_L / DELZ ** 2 * (2 * S(L1, J1, J1))
P3 = CON_F * S(L2, J1, J1) / DELZ ** 2 * (S(L1, J1, J1))
P4 = CON_F * RP(J1) * (C(2, J1 - 1) - C(2, J1 - 1)) / DR(J1) / DR(J1)
P5 = CON_F * (2 * C(2, J1 - 1)) / DR(J1) / DR(J1)
P6 = RO_S * CP_S * (P(2, J1 - 1) - P(2, J1 - 1) / DELT)
F(2) = C(2, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
ELSE
C compute effective temperature

A2 = 1 / 2 * EPS(J1) * CON_L / DELZ ** 2 * RO_F * CP_F * S(L4, J1, J1) / DELZ + (EPS(J1) * CON_RF / DR(J1) / DR(J1))
P1 = EPS(J1) * CON_L / DELZ ** 2 * (2 * S(L1, J1, J1))
P2a = EPS(J1) * RO_F * CP_F * S(L4, J1, J1) / DELZ ** 2 * (S(L1, J1, J1))
P3a = (1 - EPS(J1)) / EPS(J1) * RATE_HI(J1)
P4a = EPS(J1) * RO_F * CP_F * (C(1, J1) - S(L4, J1, J1)) / DELZ ** 2 * (S(L1, J1, J1))
P5 = EPS(J1) * CON_RF * RP(J1) * (2 * S(L1, J1, J1))
P6 = EPS(J1) * (2 * C(1, J1 - 1) + 2 * S(L1, J1, J1)) / DR(J1) / DR(J1)
P7 = EPS(J1) * RO_F * CP_F * (1 - EPS(J1)) * RO_S * CP_S * (P(1, J1) - P(1, J1) / DELT)
F(1) = C(1, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
F(2) = 0.
END IF

C compute the wall temperature

F(3) = C(3, J1) + DELT / RO_WA / CP_WA * (A_C * H_FW * (C(1, J1) - C(3, J1)) - A_INS * H_OW * (C(3, J1) - TO)) / (P(3, J1))
ELSE
C this section computes S matrix for those grids with constant grid size
IF (J1 .NE. JR) THEN
C compute gas temperature
IF (.NOT. SOL_FLO .EQ. 1) THEN

A2 = 1 / 2 * CON_L / DELZ ** 2 * RO_F * CP_F * S(L4, J1, J1) / DELZ + (RO_F * CP_F / DELT)
F(1) = C(1, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)

F(2) = 0.
END IF

C this section is for r at the wall
ELSE IF (J1.EQ.NUR) THEN

C compute gas temperature
IF (.NOT. SOL_FLO .EQ. 1) THEN

A2 = 1 / 2 * CON_L / DELZ ** 2 * RO_F * CP_F * S(L4, J1, J1) / DELZ + (RO_F * CP_F / DELT)
F(1) = C(1, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)

F(2) = 0.
P1 = CON_L/DELZ**2*(2*S(L1J-J1J))
P2 = RO_F*CP_F*S(L4J-J1J)/(DELZ)*(-S(L1J-J1J))
P3 = -(1-EPS(J1))/EPS(J1)*H_FS*AINT*(C(1J1)-C(2J1))
P4 = RO_F*CP_F*C(1J1)*(S(L4J-J1J))/
    S(L4J-J1J)/(2*DELZ)
P5 = CON_RF*RP(J1)*(C(1J1-1)-C(1J1-1))/(2*DR(J1))
P6 = CON_RF*(C(1J1-1)-C(1J1-1))/(DR(J1))/DR(J1)
P7 = RO_F*CP_F*(-P(J1))/DELT
F(1) = C(1J1)+A2*(P1+P2+P3+P4+P5+P6+P7)

c compute solid temperature
A2 = 1/(2*CON_P/DELZ**2+RO_S*CP_S/DELT+2*CON_P/
     DR(J1)/DR(J1))
P1 = AINT*H_FS*(C(1J1)-C(2J1))
P2 = RATE_H1(J1)
P3 = CON_P*(S(L2J-1J1)-S(L2J-1J1))/DELZ/DELZ
P4 = CON_P*RP(J1)*(C(2J1-1)-C(2J1-1))/(2*DR(J1))
P5 = CON_P*(C(2J1-1)-C(2J1-1))/(DR(J1))/DR(J1)
P6 = RO_S*CP_S*(-P2(J1))/DELT
F(2) = C(2J1)+A2*(P1+P2+P3+P4+P5+P6)
ELSE

c compute effective temperature
A2 = 1/(EPS(J1)**2*CON_L/DELZ**2+RO_F*CP_F*(S(L4J-J1J)/
      DELT)+EPS(J1)*RO_F*CP_F*(1-EPS(J1))*RO_S*CP_S)/DELT+2*
      EPS(J1)*CON_RF/DR(J1)/DR(J1))
P1 = EPS(J1)*CON_L/DELZ**2*(2*S(L1J-J1J))
P2 = EPS(J1)*RO_F*CP_F*S(L4J-J1J)/(DELZ)*(-S(L1J-J1J))
P3 = -(1-EPS(J1))*RATE_H1(J1)
P4 = EPS(J1)*RO_F*CP_F*C(1J1)*S(L4J-J1J)/
     S(L4J-J1J)/(2*DELZ)
P5 = EPS(J1)*CON_RF*RP(J1)*(C(1J1-1)-C(1J1-1))/(2*DR(J1))
P6 = EPS(J1)*CON_RF*(C(1J1-1)-C(1J1-1))/(DR(J1))/DR(J1)
P7 = EPS(J1)*RO_F*CP_F*(-1-EPS(J1))*RO_S*CP_S)*
     (-P(J1))/DELT
F(1) = C(1J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
ELSE

c this section computes for variable grid size
END IF

c compute the gas temperature
IF(SOL_FLO.EQ.1)THEN
A2 = 1/(2*CON_L/DELZ**2+RO_F*CP_F*(S(L4J-J1J)/
     DELT)+1.E-6)
F(1) = C(1J1)-A2*(P1+P2+P3+P4+P5+P6+P7)
ENDIF

c compute the solid temperature
A2 = 1/(2*CON_P/DELZ**2+RO_S*CP_S/DELT+CON_P*RP(J1)*
     F11(J1)/DR(J1)+2*CON_RF*
     F12(J1)/DR(J1))/DR(J1))
P1 = CON_L/DELZ**2*(2*S(L1J-J1J))
P2 = RO_F*CP_F*(S(L4J-J1J)/(DELZ)*(-S(L1J-J1J))
P3 = (1-EPS(J1))*RATE_H1(J1)
P4 = RO_F*CP_F*C(1J1)*(S(L4J-J1J))/S(L4J-J1J)/
     (2*DELZ)
P5 = CON_RF*RP(J1)*(F21(J1)*C(1J1-1)+F01(J1)*C(1J1-1))/
     (DR(J1))
P6 = 2*CON_RF*(F22(J1)*C(1J1-1)+F02(J1)*C(1J1-1))/DR(J1)
P7 = RO_F*CP_F*(-P(J1))/DELT
F(1) = C(1J1)-A2*(P1+P2+P3+P4+P5+P6+P7)
ENDIF

E-26
c compute the effective temperature
A2=1.0*(EPS(J1))*2*CON_L/DELZ**2+RO_F*CP_F*S(L4,J1,J1)/DELZ+EPS(J1)*RO_F*CP_F=(1-EPS(J1)))*RO_S*CP_S)/DELT+
EPS(J1)*CON_RF*(RP(J1)*FL1(J1)/DR(J1)+2*FL2(J1)/DR(J1)
+DR(J1))
P1=EPS(J1)*CON_L/DELZ**2*(S(L1,J1,J1))
P2=EPS(J1)*RO_F*CP_F*S(L4,J1,J1)/DELZ+*S(L1,J1,J1))
P3=(1-EPS(J1))*RATE_HI(J1)
P4=EPS(J1)*RO_F*CP_F*C(1,J1,1)*(S(L4,J1,J1)-
S(L4,J1,J1))/(2*DELZ)
P5=EPS(J1)*CON_RF*RP(J1)*F2(J1,J1)*C(1,J1,J1)-F01(J1)*
C(1,J1,J1)/DR(J1))
P6=2*EPS(J1)*CON_RF*F2(J1,J1)*C(1,J1,J1)-F02(J1)*
C(1,J1,J1)/DR(J1)/DR(J1)
P7=EPS(J1)*RO_F*CP_F=(1-EPS(J1)))*RO_S*CP_S)*
(-P(J1,J1))/DELZ
F(1)=C(1,J1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
ELSE
END IF
ENDIF
ENDIF
ENDIF
C
C
C
C this section computes the s matrix for grids inside of the column
C
ELSE
IF(J1.EQ.1) THEN
C comp gas temperature
IF(I_SOL_FLO.EQ.1) THEN
A2=1.0*(2*CON_L/DELZ**2+RO_F*CP_F*S(L4,J1,J1)/DELZ+
(RO_F*CP_F)/DELT+4*CON_RF/DR(J1)/DR(J1))
P1=CON_L/DELZ**2*(S(L1,J1,J1)+S(L1,J1,J1))
P2=RO_F*CP_F*S(L4,J1,J1)/(DELZ)*(-S(L1,J1,J1))
P3=(1-EPS(J1))*EPS(J1)*CON_L/DELZ**2*(S(L1,J1,J1)+S(L1,J1,J1))
P4=RO_F*CP_F*C(1,J1)*S(L4,J1,J1)-S(L4,J1,J1)/
(2*DELZ)
P5=4*CON_RF*(C(1,J1,J1)+DR(J1)/DR(J1))
P6=RO_F*CP_F*(-P(1,J1))/DELT
F(1)=C(1,J1,J1)+A2*(P1+P2+P3+P4+P5+P6)
ELSE
C comp solid temperature
A2=1.0*(2*CON_P/DELZ**2+RO_F*CP_F*S(L4,J1,J1)/
+RO_S*CP_S/DELZ+4*CON_P/DR(J1)/DR(J1))
P1=AIN**H_FS*(C(1,J1,J1))
P2=RATE_HI(J1)
P3=CON_P*(S(L2,J1,J1)+S(L2,J1,J1))/DELZ/DELZ
P4=4*CON_P*(C(2,J1,J1))/DR(J1)/DR(J1)
P5=RO_S*CP_S*(-P(2,J1,J1))/DELT
F(2)=C(2,J1,J1)+A2*(P1+P2+P3+P4+P5)
ELSE
C comp effective temperature
A2=1.0*(EPS(J1))*2*CON_L/DELZ**2+RO_F*CP_F*S(L4,J1,J1)/
+DELZ+EPS(J1)*RO_F*CP_F=(1-EPS(J1)))*RO_S*CP_S)/DELT+
EPS(J1)*CON_RF*(RP(J1)*FL1(J1)/DR(J1)+2*FL2(J1)/DR(J1)
+DR(J1))
P1=EPS(J1)*CON_L/DELZ**2*(S(L1,J1,J1)+S(L1,J1,J1))
P2=EPS(J1)*RO_F*CP_F*S(L4,J1,J1)/DELZ+*S(L1,J1,J1))
P3=(1-EPS(J1))*RATE_HI(J1)
P4=EPS(J1)*RO_F*CP_F*C(1,J1,J1)*S(L4,J1,J1)-
S(L4,J1,J1)
S(l_j-I \cdot I) / (2 \cdot DELZ)
P_5 = \left( -P_1 \right) \cdot \left( 1 - \text{EPS}(J_1) \right) / \left( \text{CON}_R \cdot \text{F}_P \cdot (\cdot \text{EPS}(J_1) \cdot \text{RO}_S \cdot \text{CP}_S) \right)

\left( -P_1 \right) / \left( \text{DELZ} \right)
F(1)_1 = -C \left( \text{J}_1 \right)_1 + A_2 \left( \text{P} \right)_1 + \text{P}_2 + \text{P}_3 + \text{P}_4 + \text{P}_5 + \text{P}_6

F(2)_1 = 0.
\text{END IF}

\text{c comp s for the grid at wall)
ELSE IF(J_1.EQ.LINE) THEN
\text{c comp gas temperature)
IF(J_1.EQ.LINE) THEN
A_2 = \left( 1 \right)_1 \left( 2 \cdot \text{P} \right)_1 \text{DELZ} + \left( \left( \text{P} \right)_1 \right)_1 \left( 2 \cdot \text{DELZ} \right) + \left( \left( \text{P} \right)_1 \right)_1 \left( \text{CON}_R \cdot \text{F}_P \cdot \text{S}(L_{4J1}) / \text{DELZ} \right)
 \left( \text{P} \right)_1 = \text{DELZ} \left( \left( 1 - \text{EPS}(J_1) \right) \cdot \text{CON}_R \cdot \text{F}_P \cdot \text{S}(L_{4J1}) / \text{DELZ} \right)
 \left( \text{P} \right)_1 = \left( \text{DELZ} \right)_1 \left( \left( \text{DELZ} \right)_1 \right)_1 \left( \left( \text{DELZ} \right)_1 \right)_1 \left( \left( \text{DELZ} \right)_1 \right)_1
\text{F}(2)_1 = -\text{C} \left( \text{J}_1 \right)_1 + A_2 \left( \text{P} \right)_1 + \text{P}_2 + \text{P}_3 + \text{P}_4 + \text{P}_5 + \text{P}_6
\text{ENDIF}

\text{c compute wall temperature)
F(3)_1 = -C \left( \text{J}_1 \right)_1 \cdot \text{DELZ} \cdot \text{RO}_\text{WA} \cdot \text{CP}_\text{WA} \cdot \left( \text{A}_\text{C} \cdot \text{H} \cdot \text{FW} \cdot \text{C} \left( \text{J}_1 \right)_1 \cdot \text{C} \left( \text{J}_1 \right)_1 \cdot \text{A}_\text{INS} \cdot \text{H} \cdot \text{FW} \cdot \text{C} \left( \text{J}_1 \right)_1 \cdot \text{P} \left( \text{J}_1 \right)_1 \right)
\text{c this section compes s for grids of constant size)
ELSE
IF(J_1.NE.LINE) THEN
\text{c comp gas temperature)
IF(J_1.NE.LINE) THEN
A_2 = \left( 1 \right)_1 \left( 2 \cdot \text{P} \right)_1 \text{DELZ} + \left( \left( \text{P} \right)_1 \right)_1 \left( 2 \cdot \text{DELZ} \right) + \left( \left( \text{P} \right)_1 \right)_1 \left( \text{CON}_R \cdot \text{F}_P \cdot \text{S}(L_{4J1}) / \text{DELZ} \right)

E-28
\[(\text{RO}_F \cdot \text{CP}_F)/\text{DELT} + 2 \cdot \text{CON}_R/\text{DR}(J1)/\text{DR}(J1))\]
\[P1 = \text{CON}_L/\text{DELT} \pm 2 \cdot \text{CON}_P/\text{DR}(J1)/\text{DR}(J1)\]
\[P2 = \text{RO}_F \cdot \text{CP}_F \cdot S(L4J1)/\text{DELT} \cdot (-S(L1J1))\]
\[P3 = \text{(1-EPS}(J1)/\text{EPS}(J1) \cdot H_{FS} \cdot \text{AINT} \cdot (C(1J1) - C(2J1))\]
\[P4 = \text{RO}_F \cdot \text{CP}_F \cdot (C(1J1) \cdot S(L4J1+1J1)-\]
\[S(L4J1+1J1))/\text{DELT}\]
\[P5 = \text{CON}_R \cdot \text{CP}_R \cdot (C(1J1+1) - C(1J1-1))/2 \cdot \text{DR}(J1)\]
\[P6 = \text{CON}_P \cdot (C(1J1+1) - C(1J1-1))/\text{DR}(J1)/\text{DR}(J1)\]
\[P7 = \text{-RO}_F \cdot \text{CP}_F \cdot (-P(1J1))/\text{DELT}\]
\[F(1) = C(1J1) \cdot A2 \cdot (P1 \cdot P2 \cdot P3 \cdot P4 \cdot P5 \cdot P6 \cdot P7)\]

\text{c comp solid temperature}\]
\[A2 = L/(2 \cdot \text{CON}_P/\text{DELZ}/\text{DELZ} + 2 \cdot \text{CON}_P/\text{DR}(J1)/\text{DR}(J1)+\]
\[\text{RO}_S/\text{CP}_S/\text{DELZ})\]
\[P1 = \text{AINT} \cdot H_{FS} \cdot (C(J1) - C(2J1))\]
\[P2 = \text{-RATE}_H1(J1)\]
\[P3 = \text{CON}_P \cdot (S(L2J1+1J1) + S(L2J1+1J1))/\text{DELZ}/\text{DELZ}\]
\[P4 = \text{CON}_P \cdot \text{CP}_R \cdot (C(2J1+1) - C(2J1-1))/2 \cdot \text{DR}(J1)\]
\[P5 = \text{CON}_P \cdot (C(2J1+1) - C(2J1-1))/\text{DR}(J1)/\text{DR}(J1)\]
\[P6 = \text{-RO}_S \cdot \text{CP}_S \cdot (C(2J1+1) - C(2J1-1))/\text{DELZ}\]
\[F(2) = C(2J1) \pm A2 \cdot (P1 \cdot P2 \cdot P3 \cdot P4 \cdot P5 \cdot P6 \cdot P7)\]

\text{c comp effective temperature}\]
\[A2 = 1/((\text{EPS}(J1)) \cdot (2 \cdot \text{CON}_L/\text{DELZ} \pm 2 \cdot \text{RO}_F \cdot \text{CP}_F \cdot S(L4J11))/\]
\[\text{DELZ} + (\text{EPS}(J1) \cdot \text{RO}_F \cdot \text{CP}_F \cdot (-1 \cdot \text{EPS}(J1)) \cdot \text{RO}_S \cdot \text{CP}_S)/\text{DELZ} +\]
\[2 \cdot \text{EPS}(J1) \cdot \text{CON}_R/\text{DR}(J1)/\text{DR}(J1)\]
\[P1 = \text{-EPS}(J1) \cdot \text{CON}_L/\text{DELZ} \pm 2 \cdot (S(L1J1-1J1) + S(L1J1-1J1))/\text{DELZ}\]
\[P2 = \text{-EPS}(J1) \cdot \text{RO}_F \cdot \text{CP}_F \cdot S(L4J11)/\text{DELZ} \cdot (-S(L1J1-1J1))\]
\[P3 = (1-\text{EPS}(J1)) \cdot \text{RATE}_H1(J1)\]
\[P4 = \text{EPS}(J1) \cdot \text{RO}_F \cdot \text{CP}_F \cdot (C(1J1) \cdot S(L4J11-1J1)-\]
\[(-S(L1J1-1J1))/\text{DELZ}\]
\[F(1) = C(1J1) \cdot A2 \cdot (P1 \cdot P2 \cdot P3 \cdot P4 \cdot P5 \cdot P6 \cdot P7)\]

\text{ELSE END IF}\]

\text{c this section computes s for variable grid size}\]

\text{ELSE}\]

\text{c compute gas temperature}\]
\[\text{IF SL Flo. Eq. THEN}\]
\[A2 = L/(2 \cdot \text{CON}_L/\text{DELZ} \pm 2 \cdot \text{RO}_F \cdot \text{CP}_F \cdot S(L4J11)/\text{DELZ} +\]
\[1/\text{DELZ} + \text{CON}_R \cdot \text{CP}_R \cdot (F1(J1)/\text{DR}(J1) \pm 2 \cdot \text{CON}_R/\]
\[F12(J1)/\text{DR}(J1)/\text{DR}(J1))\]
\[P1 = \text{CON}_L/\text{DELZ} \pm 2 \cdot (S(L1J1+1J1) + S(L1J1+1J1))/\text{DELZ}\]
\[P2 = \text{RO}_F \cdot \text{CP}_F \cdot S(L4J11)/\text{DELZ} \cdot (-S(L1J1-1J1))\]
\[P3 = (1-\text{EPS}(J1))/\text{EPS}(J1) \cdot \text{H}_{FS} \cdot \text{AINT} \cdot (C(1J1) - C(2J1))\]
\[P4 = \text{RO}_F \cdot \text{CP}_F \cdot (C(1J1) \cdot S(L4J11-1J1)-\]
\[(-S(L1J1-1J1))/\text{DELZ}\]
\[P5 = \text{CON}_R \cdot \text{CP}_R \cdot (F21(J1) - F01(J1))\]
\[C(1J1-1))/\text{DR}(J1))\]
\[P6 = \text{CON}_P \cdot \text{CP}_P \cdot (F22(J1) - F02(J1))/\text{DR}(J1)/\text{DR}(J1)/\]
\[\text{DEL}(F1(J1))/\text{DR}(J1)/\text{DR}(J1))\]
\[P7 = \text{-RO}_F \cdot \text{CP}_F \cdot (-P(1J1))/\text{DELZ}\]
\[F(1) = C(1J1) \cdot A2 \cdot (P1 \cdot P2 \cdot P3 \cdot P4 \cdot P5 \cdot P6 \cdot P7)\]

\text{c compute solid temperature}\]
\[A2 = L/(2 \cdot \text{CON}_P/\text{DELZ} \pm \text{CON}_P \cdot \text{CP}_P \cdot (F1(J1)/\text{DR}(J1) +\]
\[2 \cdot \text{CON}_P \cdot F12(J1)/\text{DR}(J1)/\text{DR}(J1) \pm \text{RO}_S \cdot \text{CP}_S/\text{DELZ})\]
\[P1 = \text{AINT} \cdot H_{FS} \cdot (C(1J1) - C(2J1))\]
\[P2 = \text{-RATE}_H1(J1)\]
\[P3 = \text{CON}_P \cdot \text{CP}_P \cdot (S(L2J1-1J1) + S(L2J1-1J1))/\text{DELZ}\]
\[P4 = \text{CON}_P \cdot \text{CP}_R \cdot (F21(J1) \cdot (C(2J1+1)-\]
\[F01(J1))/\text{DR}(J1))\]

\text{ELSE}\]

\text{ENDIF END IF}\]
PS=2*CON_P*(F22(JJ)*C(2J1+1)+F02(JJ))
*C(2J1-1)/DR(JJ)/DR(JJ)
P6=-RO_S*CP_S*(-P(2J1))/DELT
F(2)=C(2J1)+A2*(P1+P2+P3+P4+P5+P6)
ELSE

C compute effective temperature
A2=1.0*(EPS(JJ)***2+RO_F*CP_F*S(L4JJ11)/
DELZ)**EPS(JJ)*RO_F*CP_F*(-S(L1,J+1,J1)+S(L1,J-1,J1))
P2=-EPS(JJ)*RO_F*CP_F*S(L4JJ11)/DELZ)*(-S(L1,J-1,J1))
P3=-EPS(JJ)*RO_F*CP_F*(-S(L1,J+1,J1)
S(L4JJ11))/DELZ)
P5=-EPS(JJ)*CON_RF*RP(JJ)*/(F21(JJ)*C(1J1+1)-F01(JJ)*
C(1J1-1)/DR(JJ))
P6=2*EPS(JJ)*C(1J1+1)*F01(JJ)
F(1)=C(1JJ)+A2*(P1+P2+P3+P4+P5+P6)

F(2)=0.
ENDIF
ENDIF
ENDIF
ENDIF
RETURN
END

C

C------------------------------------------------------------
C
SUBROUTINE FUNCTIO(JJ)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4),K_FO(4),MOL(4),M_AVE,M_W(4),NU_NP,NU_NW,KGAS,
K_FP(4,201),BC_1(4),D_L(4),Q2(4),MW,A1(14,201),
C1(14,201,101),D_RF(4),U(14,201),EPS(1000),E(30),AKT(30),
C2(14,201,101),F01(101),F11(101),F21(101),F02(101),
F12(101),F22(101),RP(101),DR(101),RR0(101),D_LP_R(4,201,101),
D_LP_Z(4,201,101),U1(101,201),YO(4),SS(4)
COMMON/UG/U GUESS,EPS
COMMON/OLD/AA(14),SUM(14),COLD(14,201,101)
COMMON/BND(A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),G(14),F(14),P(14),(4,201)
COMMON/BND2(A(14,201,101)
COMMON/NEW_GRID/DELX(101),ALF1(101),NKR1,NKR2
COMMON/BND2(NJ2,NJP2,TPRT,JTCNT_NJ1
COMMON/PR_OLD_Z/CON_Z(201,101),CON_R(201,101),CON_S(201,101),
H_W(201,101),CP_P(201,101),H_FP(201,101),Q(4,201,101),
VISC_P(201,101),D_LPP(4,201),RATE_C1(201,101)
COMMON/PROP_WAL/CP_WA,RO_WA,ERROR0,ERROR1
COMMON/PROP_B_Z/REC,VOID,B_D,L_ED,ES_B,ALF,GC,ZM_W
COMMON/PROP_D_Z/DELZ,TIME,DELR1,DELZ,LT,NC,NJR,NP
COMMON/PROP_S_Z/CP_S,RO_S,AINT,R,P,D,P,CON_S1,HEAT(4)
COMMON/INIT_Z/RO_FU,FO_U,F1,CP_FOT,FO,TC,FO(4),K_F,C(4)
COMMON/INDIC/L1L2L3L4L5L6L7L8L9L10L11L12L13L14L15L16L17
COMMON/INDIC/L1/L1/L2/L3/L4/L5/L6/L7/L8/L9/L10/L11/L12/L13/L14/L15/L16/L17
COMMON/RAD/LP
COMMON/GAS/NKRT,NCOMP,MW
COMMON/NCP/N1
COMMON/PRIME/CON2,RA,RAV,EPSEX,ROHS,TAMB,ALPHA:,UN,HWALL LEN

E-30
DATA EMIS.R1,IONCE,IONCE,ICOUNT,ICOND,1/9,555.,.0,0,0,1/
c there is a temperature difference between the gas and solid phases
IF(LL.EQ.ICOM)THEN
  BC_LL=TEMP(1)(TIME)
  ICOM=LL+1
END IF
IF(J1.EQ.1 .AND. IONCE.EQ.0)THEN
  IONCE=1
  NZ.OR.1=1
  LSOL.FLO=0
ENDIF
AN indication number for type of gas to compute the gas conductivity,
c 1=N2, 2=air, 3=co2
IGAS=1
DP=R_1*2.
IF(VEL_1.EQ.1)THEN
  IR=10
ELSE
  IR=5
ENDIF
c calculating the area for heat transfer to the wall or from the wall
  D_T=D_E+D_1
  X_W=D_E-D_1
A_C=2*D_1/(D_1*D_2)*X_W
A_INS=2*D_E/(D_1+D_2)*X_W)*1.4
C heat transfer coefficient outside of the wall
  H_OW=0.1
ENDIF
c call vel_por to compute velocity and porosity profile
IF(J1.EQ.1 .AND. IONCE.EQ.0)THEN
  IONCE=1
ENDIF
c compute the ratio of distance from the center to each grid over the pellet
c diameter
RR=0.
RR0(NJR)=0.
DO 15=NJR-1,1,-1
  RR=RR+DELRO(IS+1)/D_P
  RR0(15)=RR
ENDDO
c this section calculates the coefficients to the discretized PDE's
C
C compute the inverse of distance from the center to each grid
RR=0.
DO 15=1,NJR
IF(15.NE.1)THEN
  RR=RR+DELRO(15)
  RP(15)=1./RR
ELSE
  RP(15)=0.
ENDIF
IF(15.LT.IR) THEN
  DELR=DELRO(1)
  DR(15)=DELR
ELSE IF(15.eq.IR) THEN
  DELR=DELRO(1)
  DR(15)=DELR
ELSE IF(15.eq.IR) THEN
  DELR=DELRO(1)
  DELR2=DELRO(1) +1
  DELR=DELR1
  DR(15)=DELR1
  FR=DELR2/DELR1
C these variables are being computed at the pont where two adjacent grids are
C not the same size
F01(15)=FR/(1+FR)
F11(15)=(1.-FR)/FR
F21(15)=1./(1.+FR)*FR
F02(15)=1./(1.+FR)
F12(15)=1./FR
F22(15)=1./(1.+FR)*FR
ELSE
DELR=DELR0/(R†)
DR(I5)=DELR
ENDIF
END DO
ENDIF
this section calls the proper subroutine to compute the parameters such as
diffusivity, conductivity...
IF(J1.EQ.1 .AND. ICOUNT.LT.J1)THEN
J5=J
ICOUNT=ICOUNT+1
DO I6=1,N/R
DO M1=1,NC
YO(M1)=C(M1,J6)*R1*C(L1,J6)/S(L5,J5,J6)
END DO
TEMP=C(L1,J6)
M_AVE=0
SUM_Y=0.
DO M1=1,NC
M_AVE=M_AVE+YO(M1)*M_W(M1)
SUM_Y=SUM_Y+YO(M1)
END DO
M_AVE=M_AVE+(1.-SUM_Y)/28.
RO_F=S(L5,J5,J6)/(C(L1,J6)*R1)
IF(RO_F.LE.0)RO_F=P_TOT/(C(L1,J6)*R1)
GN2=GN
GN=S(L4,J5,J6)*RO_F/60.*VOID_B
IF(GN.EQ.0)GN=GN2
this computation compute the conductivity of gas and solid in axial and
radial directions
CALL PHI_COND(IGAS,TEMP,CON_S1,EPS(1),PHL,PHLW)
CALL CONDU(MN,JGAS,PHLD_P,CON_S1,RRO(16),U1(1,J6),REY,
TEMP,EPS(1),EPS(1),EFF_CON_R1,CON_R1,EFF_CON_Z1,
CON_Z1,CON_P1,NUR,NGR1,NGR2,J6)
c if there is a temprature difference between the gas and solid
IF(I_SOL_FLO.EQ.1)THEN
CON_Z(J5,J6)=CON_Z1
CON_S(J5,J6)=CON_P1
ELSE
CON_Z(J5,J6)=EFF_CON_Z1
ENDIF
this computation for number of component
DO M1=1,NC
calc the molecular diffusivity of each component in the mixture
DIF=DIFF(M1,TEMP,S(L5,J5,J6),YO)*60
calc schmidt number
SC_N=VISC_P(J5,J6)/DIF/RO_F/M_AVE
calc axial diffusion
CALL AXDIFF_R_Z(MN,JGAS,PHLD_P,DIF,RR0(16),U1(1,J6),
REY,SC_N,TEMP,EPS(1),EPS(1),EFF_DIFF_R,EFF_DIFF_Z,
NJR,NGR1,NGR2,J6)
C D_LP_R(M1,15,16) = EFF_DIFF_R
C D_LP_Z(M1,15,16) = EFF_DIFF_Z
D_LP_Z(M1,15,16) = CON_Z(15,16)/RO_F/CP_P(15,16)
END DO

C calc the heat transfer coefficient between the gas phase and the wall
IF(I6.EQ.NJR) THEN
IF(GN.EQ.0) THEN
REY = RE(GN, TEMP)
CALL HEAT_WALL(J, GAS, PHTW, D_P, CON_S1, RR0(I6), U1(I6),
REY, TEMP, VOID_B, H_W)
H_W(I5, NJR) = H_W1
ENDIF
IF(ICOND1.EQ.1) THEN
VAV = G_F/D_I/D_I/PI*4
GA = G_F/D_I/D_I/PI*4.*RO_F
TAV = S(L1, I, 1, 1)/R1
CP = CP_P(I, 1)
AVIS = VISC_P(I, 1)
AKC = 0.000358895+3.0026706379E-5*S(L1,1,1)/S(L1,1,1,1)*R1
AKC = 5.3528942E-9
S(L1,1,1,1)*SCL1,1,1)
CALL CONDUCI(EMIS, CON_S1, D_P, I, GA, VAV, TAV, RO, CP, AVIS, AKC, NJR, EPSX, EPS(NJR), DELR0, E, AKT)
ICOND1 = 0
ENDIF
CON_R(I5,16) = AKT(I6)
IF(E(I6).LE.0)E(I6) = E(I6-1)
DO M1 = 1, NC
D_LP_R(M1,15,16) = AKT(I6)/RO/CP
D_LP_R(M1,15,16) = E(I6)
END DO
END DO
IF(CON_Z(I5, NJR).EQ.0) THEN
CON_Z(I5, NJR) = CON_Z(I5, NJR-1)
DO M1 = 1, NC
D_LP_Z(M1,15, NJR) = CON_Z(I5, NJR)/RO_F/CP_P(I5, NJR)
END DO
END IF
DO II = 1, NJR
DO M1 = 1, NC
D_RP(M1,11) = D_LP_Z(M1,11,1)
END DO
END DO
END IF

C set the parameters to new variables
J = I
H_FW = H_W(I,1NJR)
RO_F = S(L3, JJ, 1)/C(L1, J1)*R1
CP_F = CP_P(JJ1)
H_FS = H_FP(JJ1)
CON_L = CON_Z(JJ1)
DO M1 = 1, NC
D_L(M1) = D_LP_Z(M1,11,1)
END DO
DO M1 = 1, NC
D_RF(M1) = D_LP_R(M1,11,1)
END DO
CON_RF = CON_R(JJ1)
CON_P = CON_S(JJ1)
KK = 0
D_L_AVE = 0.
DO M1 = 1, NC
IF(D_L(M1).GT.0) THEN
D_L_AVE = D_L_AVE + D_L(M1)
ENDIF
END IF
KK=KK+1
END IF
END DO
D_L_AVE=D_L_AVE/KK
DO J1=1,NC
SS(1)=C(1,J1)
END DO
c call the isotherm to compute the equilibrium concentration
CALL IST_Z(1,C(L2,J1),SS,Q2)
c based the equilibrium per unit volume of pellet
DO J=1,NC
Q(L,J1)=Q2(J)*RO_S
END DO
c this is the boundary, the first grids in axial direction
IF(J.EQ.1)THEN
RATE_C=0
END DO
c compute the total amount is being adsorbed
DO M1=1,NC
RATE_C=RATE_C+K_F(M1)*AINT*(Q(M1,J1)-C(M1+NC,J1))
END DO
RATE_C1=RATE_C*(1-EPS(J1))
RATE_H=0
c compute the total heat of adsorption
C
HEAT(2)=-(411.93585-57470.2733*C(3,J1)/RO_S+3971259.2258*C
C
HEAT(2)**2/RO_S)*44
DO M1=1,NC
RATE_H=RATE_H+HEAT(M1)*K_F(M1)*AINT*(Q(M1,J1)-
C(M1+NC,J1))
END DO
c this "if" calculates the first grid in radial direction, center of the bed
IF(J.EQ.1) THEN
TOT_C=0.0
END DO
c computation of molar density component
DO M1=1,NC-1
A2=1/(2*D_L(M1)/DELZ)**2+S(L4,J1)/DELZ+4*D_RF(M1)/
DR(J1)/DR(J1)**1/DELZ)
P1=D_L(M1)/DELZ**2*(BC_1(M1)+S(M1,J+1,J1))
P2=-S(L4,J1)/(DELZ)**(-BC_1(M1))
P3=ALF1(J1)*AINT*K_F(M1)*(Q(M1,J1)-C(M1+NC,J1))
P4=4*D_RF(M1)*C(M1+NC,J1)/DR(J1)/DR(J1)
P5=-P(M1,J1)/DELZ
F(M1,J1)=A2*(P1+P2+P3+P4+P5)
TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5,J11)-TOT_C*R1*S(L1,J11))/R1/S(L1,J11)-
C(NC,J1)
c computation of molar adsorption for each component
DO M1=1,NC
A2=1/(K_F(M1)*AINT+1./DELZ)
F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J11)+
P(M1+NC,J1))/DELZ)
END DO
c computation of gas temperature
IF(J.EQ.1) THEN
A2=1/(2*CON_L/DELZ)**2+S(L4,J1)/DELZ+4*CON_RF/DR(J1)**1/DELZ)
P1=CON_L/DELZ**2*(BC_L1+S(L1,J+1,J1))
P2=-RO_F*CP_F*S(L4,J1)/DELZ)**(-BC_L1)
P3=(-EPS(J1))/EPS(J1)*H_FS*AINT*(C(L1,J1)-C(L2,J1))
P4=-RO_F*CP_F*C(L1,J1)*S(L4,J+1,J1)-
S(L4,J11)/DELZ)
P5=4*CON_RF*(C(L1,J11))/DR(J1)/DR(J1)
P6=-RO_F*CP_F*(-P(L1,J1))/DELZ
END DO

E-34
\[ F(L_1) = C(L_1, J_1) + A_2^*(P_1 + P_2 + P_3 + P_4 + P_5 + P_6) \]

**c computation of solid temperature**

\[
\begin{align*}
A_2 &= 1/(2*CON_P/DELZ*2 + (RO_S*CP_S)/DELZ + 4*CON_P/(DR(J1)/DR(J1))) \\
P_1 &= \text{INT}^*H_{FS}*(C(L_1, J_1) - C(L_2, J_1)) \\
P_2 &= \text{RATE}_H \\
P_3 &= \text{CON}_P*(S(L_2, J_1 + 1, J_1) + S(L_2, J_1 + 1, J_1))/DELZ/DELZ \\
P_4 &= \text{CON}_P*(C(L_2, J_1 + 1))/DR(J1)/DR(J1) \\
P_5 &= \text{RO}_S*CP_S*(-P(L_2, J_1))/DELZ \\
F(L_2) &= C(L_2, J_1) + A_2^*(P_1 + P_2 + P_3 + P_4 + P_5) \\
\end{align*}
\]

**c computation of effective temperature**

**ELSE**

\[
\begin{align*}
A_2 &= 1/(EPS(J1))*(2*CON_L/DELZ*2 + RO_F*CP_F*S(L_4, J_1))/DELZ + (EPS(J1)*RO_F*CP_F*(1 - EPS(J1))*RO_S*CP_S)/DELZ + 4*EPS(J1)*CON_RF/DR(J1)/DR(J1)) \\
P_1 &= EPS(J1)*CON_L/DELZ*2*(BC_L + S(L_1, J_1 + 1, J_1)) \\
P_2 &= EPS(J1)*RO_F*CP_F*S(L_4, J_1)/DELZ)*(-BC_L, J_1) \\
P_3 &= -(EPS(J1))*RATE_H \\
P_4 &= EPS(J1)*RO_F*CP_F*(C(L_1, J_1)*S(L_4, J_1 + 1, J_1) - S(L_4, J_1))/DELZ \\
P_5 &= 4*EPS(J1)*CON_RF*(C(L_1, J_1 + 1))/DR(J1)/DR(J1) \\
P_6 &= EPS(J1)*RO_F*CP_F*(1 - EPS(J1))*RO_S*CP_S) \\
F(L_1) &= C(L_1, J_1) + A_2^*(P_1 + P_2 + P_3 + P_4 + P_5 + P_6) \\
\end{align*}
\]

**TOT_C = 0**

**c comp of molar density of component**

**DO** M_1 = 1, NC - 1

\[
\begin{align*}
A_2 &= 1/(2*D_L(M_1)/DELZ*2 + S(L_4, J_1, J_1))/DELZ + 2*D_RF(M_1)/DR(J1)/DR(J1) + 1/DELZ) \\
P_1 &= D_L(M_1)/DELZ*2*(BC_1(M_1)*S(M_1, J_1 + 1, J_1)) \\
P_2 &= -(S(L_4, J_1, J_1))/DELZ*(BC_1(M_1)) \\
P_3 &= -ALF_1*INT*K_F(M_1)*(Q(M_1, J_1, J_1) - C(M_1, J_1 + NC, J_1)) \\
P_4 &= D_RF(M_1)*RO_F*(C(M_1, J_1 - 1, J_1) - C(M_1, J_1 + 1, J_1))/2*DR(J1)) \\
P_5 &= 2*D_RF(M_1)*C(M_1, J_1 - 1)/DR(J1)/DR(J1) \\
P_6 &= P(M_1, J_1)/DELZ \\
F(M_1) &= C(M_1, J_1) + A_2^*(P_1 + P_2 + P_3 + P_4 + P_5 + P_6) \\
TOT_C &= TOT_C + C(M_1, J_1) \\
END DO \\
F(NC) &= S(L_5, J_1, J_1) - TOT_C*R_1*S(L_1, J_1, J_1)) / R_1/S(L_1, J_1, J_1) - C(NC, J_1)) \\
\]

**c comp the molar adsorption**

**DO** M_1 = 1, NC

\[
\begin{align*}
A_2 &= 1/(K_F(M_1)*AI_N + 1)/DELZ) \\
F(M_1 + NC) &= C(M_1, NC, J_1) + A_2^*(K_F(M_1)*AI_N*(Q(M_1, J_1, J_1)) \\
P(M_1 + NC, J_1)/DELZ \\
END DO \\
\]

**c comp of gas phase temperature**

**IF SOL, FLO, EQL THEN**

\[
\begin{align*}
A_2 &= 1/(2*CON_L/DELZ*2 + RO_F*CP_F*S(L_4, J_1, J_1)/DELZ + (RO_F*CP_F)/DELZ*2 + CON_RF/DR(J1)/DR(J1)) \\
P_1 &= CON_L/DELZ*2*(BC_L + S(L_1, J_1 + 1, J_1)) \\
P_2 &= RO_F*CP_F*S(L_4, J_1, J_1)/DELZ*(-BC_L) \\
P_3 &= -(EPS(J1))*RO_F*CP_F*(C(L_1, J_1)*S(L_4, J_1, J_1)) \\
P_4 &= RO_F*CP_F*(C(L_1, J_1))*S(L_4, J_1, J_1))/DELZ \\
P_5 &= CON_RF*RO_F*(2*H_FW*DR(J1))/CON_RF*(C(L_3, J_1) - C(L_1, J_1))/2*DR(J1)) \\
P_6 &= CON_RF*(2*C(L_1, J_1, J_1) + 2*H_FW*DR(J1))/CON_RF*(C(L_3, J_1) - C(L_1, J_1))/DR(J1)/DR(J1) \\
\end{align*}
\]
P7=RO_F*CP_F*(-P(L1,J1))/DELT
F(L1)=C(L1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)

c comp of solid phase temperature
A2=1/(2*CON_P/DELT**2+(RO_S*CP_S)/DELT+
2*CON_P/(DR(J1)/DR(J1))
P1=AINT*H_FS*(C(L1,J1)-C(L2,J1))
P2=-RATE_H
P3=CON_P*(S(L2,J1+1,J1)+S(L2,J1-1,J1))/DELT/DELT
P4=CON_P*RP(J1)*(C(L2,J1-1)-C(L2,J1-1))/DELT/DELT
P5=CON_P*(2*C(L2,J1-1)/DR(J1)/DR(J1))
P6=RO_S*CP_S*(-P(L2,J1))/DELT
F(L2)=C(L2,J1)+A2*(P1+P2+P3+P4+P5+P6)

ELSE
A2=1/(2*EPS(J1)*CON_L/DELT**2+RO_F*CP_F*S(L4,J1)+
DELZ*EPS(J1)*RO_F*CP_F*(1-EPS(J1))/EPS(J1)*RO_F*CP_F+
1-EPS(J1))*RO_S*CP_S)/DELT+(EPS(J1)*RO_F*CP_F+S(L4,J1)/
DELZ+1.0/(2*DR(J1)/DR(J1))
P1=EPS(J1)*CON_L/DELT**2*(BC_L1+S(L1,J1,J1))
P2=-EPS(J1)*RO_F*CP_F*S(L4,J1)/DELT*(BC_L1)
P3=-(1-EPS(J1))*RATE_H
P4=-EPS(J1)*RO_F*CP_F*C(L1,J1)*(S(L4,J1,J1-1)+C(S(L1,J1,J1)))/
DELZ
P5=EPS(J1)*CON_RF*RP(J1)*(2.*H_FW*DR(J1)/CON_RF*
(C(L3,J1)-C(L1,J1)))/DELT/DELT
P6=EPS(J1)*CON_RF*RP(J1)*(2*(C(L1,J1-1)+S(L1,J1,J1)))/
CON_RF*(C(L3,J1)-C(L1,J1))/DELT/DELT
P7=-(EPS(J1)*RO_F*CP_F*P1+1-EPS(J1))/EPS(J1)*RO_F*CP_F+
(P(L1,J1))/DELT
F(L1)=C(L1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
F(L2)=C(L2,J1)-BC_L1
ENDIF

ELSE
A2=1/(2*D_L(M1)/DELT**2+S(L4,J1,J1)+2*D_RF(M1)/
/DR(J1)/DR(J1))
P1=D_L(M1)/DELT**2*(BC_I(M1)+S(M1,J1,J1))
P2=-S(L4,J1,J1)/DELT*(BC_I(M1))
P3=-ALF1(J1)*AINT*K_F(M1)*Q(M1,J1,J1)+C(M1,J1+1)
P4=-D_RF(M1)*RP(J1)*(C(M1,J1,J1)-C(M1,J1,J1-1))/
(2*DR(J1))
P5=-D_RF(M1)*(C(M1,J1,J1)+C(M1,J1,J1-1))/
DR(J1)/DR(J1)
P6=-(-P(M1,J1))/DELT
F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
TOT_C=TOT_C+C(M1,J1)
ENDIF

DO M1=1,NC-1
A2=1/(2*D_L(M1)/DELT**2+S(L4,J1,J1)+2*D_RF(M1)/
/DR(J1))/DELT)
P1=D_L(M1)/DELT**2*(BC_1(M1)+S(M1,J1,J1))
P2=-S(L4,J1,J1)/DELT*(BC_1(M1))
P3=-ALF1(J1)*AINT*K_F(M1)*Q(M1,J1,J1)+C(M1,J1+1)
P4=-D_RF(M1)*RP(J1)*(C(M1,J1,J1)-C(M1,J1,J1-1))/
(2*DR(J1))
P5=-D_RF(M1)*(C(M1,J1,J1)+C(M1,J1,J1-1))/
DR(J1)/DR(J1)
P6=-(-P(M1,J1))/DELT
F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=S(L5,J1,J1)-TOT_C*R1*S(L1,J1,J1)/R1/S(L1,J1,J1)-
C(NC,J1)

ELSE
IF(I_SOL_FLO.EQ.1)THEN
A2=1/(2*CON_L/DELT**2+RO_F*CP_F*S(L4,J1,J1)/DELT+

ENDIF
\[(RO_F^*CP_F^*/DELT+2*CON_RF/DR(J1))/DR(J1))\]
\[P1=CON_L/DELT**2*(BC_L1+S(L1J1+1))\]
\[P2=RO_F^*CP_F^*S(L4,J1)/DELT^2*(BC_L1)\]
\[P3=-(1-EPS(J1))*EPS(J1)^*H^*_FS^*AINT^*(C(L1,J1)-C(L2,J1))\]
\[P4=RO_F^*CP_F^*(C(L1,J1))*S(L4,J1+1)-\]
\[S(L4,J1+1)/DELT\]
\[P5=CON_RF^*RP(J1)*S(C(L1,J1+1)-C(L1,J1-1))/(2*DR(J1))\]
\[P6=CON_RF^*(C(L1,J1+1)+C(L1,J1-1))/DR(J1)/DR(J1)\]

\(F(L1)=C(L1,J1)+A2^*(P1+P2+P3+P4+P5+P6+P7)\)

**c compute solid temperature**

**ELSE**

\[A2=1/(2*CON_P/DELZ**2+2*(RO_S^*CP_S)/DELT+\]
\[2*CON_P/DR(J1)/DR(J1))\]

\[P1=AINT^*H^*_FS^*(C(L1,J1)+C(L2,J1))\]

\[P2=-RATE_H^*\]

\[P3=CON_P^*(S(L2,J1+1)+S(L2,J1+1))/DELT/DELZ\]

\[P4=CON_P^*RP(J1)*S(C(L2,J1+1)-C(L2,J1-1))/(2*DR(J1))\]

\[P5=CON_P^*(C(L2,J1+1)+C(L2,J1-1))/DR(J1)/DR(J1)\]

\[P6=RO_S^*CP_S^*(-P(L2,J1))/DELT\]

\(F(L2)=C(L2,J1)-BC_L1\)

**ENDIF**

**c the same computation as above except it is now for the grids from the point**

**c where the velocity starts to change to the wall**

**ELSE**

\[TOT_C=0\]

**DO** \(MI=I,NC-1\)

\[A2=1/(2*D_L(M1)/DELZ**2+S(I,A,J,J1)/DELT+\]
\[F1(J1)*D_RF(M1)*RP(J1)/DR(J1)+2*D_RF(M1)*F12(J1)/DR(J1)/DR(J1)-1./DELT)\]

\[P1=D_L(M1)/DELZ**2*(S(M1,J1+1)+BC_1(M1))\]

\[P2=S(L4,J1+1)/DELZ^2*(BC_1(M1))\]

\[P3=-ALF1(J1)*AINT*K^*_F(M1)*Q(M1,J1)+C(M1+NC,J1))\]

\[P4=D_RF(M1)*RP(J1)*F21(J1)*C(M1,J1+1)+F01(J1)*\]

\[C(M1,J1-1))/DR(J1))\]

\[P5=2*D_RF(M1)*(F22(J1)*C(M1,J1+1)+F02(J1)*C(M1,J1+1-1))/\]

\[DR(J1)/DR(J1)\]

\[P6=-(P(M1,J1))/DELZ\]

\[F(M1)=C(M1,J1)+A2^*(P1+P2+P3+P4+P5+P6)\]

\[TOT_C=TOT_C+C(M1,J1)\]

**END DO**

\[F(NC)=(S(L5,J1+1)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-\]

\[C(NC,J1)\]

**c compute molar adsorption**

**DO** \(M1=1,NC\)

\[A2=1/(K_F(M1)+AINT+1./DELZ)\]

\[F(M1+NC)=C(M1+NC,J1)+A2^*(K_F(M1)+AINT*(Q(M1,J1))+\]

\[C(NC,J1)\]

**E-37**
P(M1+NCJ1)/DELT)
END DO

c compute the gas temperature
IF(SOL_FLO.EQ.1)THEN
A2=1/(2*CON_L/DELT)**2+RO_F*CP_F*(S(L4J1J1)/DELT+
1/DELT)+CON_RF*RP(J1)*F11(J1)/DR(J1)+2*CON_RF*F12(J1)/
(DR(J1)/DR(J1))
P1=CON_L/DELT**2*(S(L1J,J+1J1)+BC_L1)
P2=RO_F*CP_F*(S(L4J1J1)/DELT)*(-BC_L1)
P3=(-1*EPS(J1)/EPS(J1)*H_FS*AINT*(C(L1J1J1-C(L2J1J1))
P4=RO_F*CP_F*C(L1J1J1)*S(L4J1J1)/DELT)
P5=CON_RF*RP(J1)*F21(J1)*C(L1J1J1-1)/
(DELZ)*DR(J1))
P6=2*CON_RF*(F22(J1)*C(L1J1J1-1)+F02(J1)*C(L1J1J1-1))/
(DR(J1)/DR(J1))
P7=RO_F*CP_F*(-P(L1J1J1))/DELZ
F(L1)=C(L1J1J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
ENDIF
ENDIF

C
C this section compute the S matrix variables for grid at z=L, the outflow
C boundary
ELSE IF(J.EQ.NJ1)THEN

C compute the total amount adsorbed
RATE_C=0
DO M1=1,NC
F(L1)=C(L1J1J1)-BC_L1
END IF
END IF
\[ \text{RATE}_C = \text{RATE}_C + K_F(M) \cdot A/N'F \]
\[ = (Q(M) - C(M) + NCJ) \]
\[ \text{END DO} \]
\[ \text{compute the adsorption heat} \]
\[ \text{RATE}_C1(J) = \text{RATE}_C \cdot (1 - \text{EPS}(J)) \]
\[ \text{RATE_H} = 0 \]
\[ \text{HEAT}(2) = -(411.93585 - 57470.2733 \cdot C(3j1) / RO_S + 3971259.2258) \cdot \frac{c\ w_3}{2/RO_S/RO_S} \cdot \alpha_4 \]
\[ \text{DO MI=I,NC} \]
\[ \text{RATE_H} = \text{RATE_H} + \text{HEAT}(M) \cdot K_F(M) \cdot A/N'F \]
\[ \text{END DO} \]
\[ \text{compute the molar density} \]
\[ \text{DO MI=I,NC-1} \]
\[ A_2 = \frac{J(2*CON_L/DELZ**2 + S(L4JJ1)/DELZ + 4*D_RF(M)/DR(J1)^2 + I/DELZ)}{\text{DELZ} + 2*S(M1,J-1,J1)} \]
\[ P_1 = 2*S(M1,J)/DELZ \]
\[ P_2 = 2*S(M1,J)/DELZ \]
\[ P_3 = -P(M1,J) \]
\[ F(M1) = -C(M1,J) + A_2 \cdot P_1 + P_2 + P_3 + P_4 + P_5 \]
\[ \text{TOT}_C = \text{TOT}_C + C(M1,J) \]
\[ \text{END DO} \]
\[ \text{compute the molar adsorption} \]
\[ \text{DO MI=I,NC} \]
\[ A_2 = \frac{J(K_F(M) \cdot A/N'F + 1/DELZ)}{\text{DELZ} + 2*S(M1,J-1,J1)} \]
\[ F(M1+NC) = -C(M1+NC,J) + A_2 \cdot (K_F(M) \cdot A/N'F + (Q(M1,J+1) - C(M1+NC,J))) \]
\[ \text{END DO} \]
\[ \text{compute the gas temperature} \]
\[ \text{IF(I_SOL_FLO.EQ.1) THEN} \]
\[ A_2 = 1/(2*CON_L/DELZ**2 + (2*S(S1JJ1)/DELZ + 4*D_RF(DR(J1)/DR(J1)))) \]
\[ P_1 = 2*S(S1JJ1)/DELZ \]
\[ P_2 = 2*S(S1JJ1)/DELZ \]
\[ P_3 = -P(S1JJ1) \]
\[ F(S1JJ1) = -C(S1JJ1) + A_2 \cdot P_1 + P_2 + P_3 + P_4 + P_5 \]
\[ \text{ELSE} \]
\[ \text{compute the solid temperature} \]
\[ A_2 = 1/(2*CON_P/DELZ**2 + (2*S(S1JJ1)/DELZ + 4*D_RF(DR(J1)/DR(J1)))) \]
\[ P_1 = 2*S(S1JJ1)/DELZ \]
\[ P_2 = 2*S(S1JJ1)/DELZ \]
\[ P_3 = -P(S1JJ1) \]
\[ F(S1JJ1) = -C(S1JJ1) + A_2 \cdot P_1 + P_2 + P_3 + P_4 + P_5 \]
\[ \text{ELSE} \]
\[ \text{compute the effective temperature} \]
\[ A_2 = 1/(2*CON_L/DELZ**2 + (2*S(S1JJ1)/DELZ + 4*D_RF(DR(J1)/DR(J1)))) \]
\[ P_1 = 2*S(S1JJ1)/DELZ \]
\[ P_2 = 2*S(S1JJ1)/DELZ \]
\[ P_3 = -P(S1JJ1) \]
\[ F(S1JJ1) = -C(S1JJ1) + A_2 \cdot P_1 + P_2 + P_3 + P_4 + P_5 \]
\[ \text{END ELSE} \]
c this section is for r at the wall.
ELSE IF(1.EQ.N.) THEN
TOT_C=0.
c compute molar density
DO M1=1,NC-1
   A2=1./((2*D_L(M1))/DELZ)**2+S(L4J-J1)/DELZ+2*D_RF(M1)/
   DR(J1)/DR(J1)+1./DELT)
   P1=S(L4J-J1)/DELZ**2*(-S(M1,J1-J1))
   P2=S(L4J-J1)/DELZ*(-S(M1,J1-J1))
   P3=-A2*H_FS*AINT*(K_F(M1)*Q(M1,J1)-C(M1+NC,J1))
   P4=D_RF(M1)*Rp(J1)*C(M1,J1-1,J1))
   P5=2*D_RF(M1)*C(M1,J1-1)/DR(J1)/DR(J1)
   P6=-(P(M1))/DELT
   F(M1)=C(M1,J1)+A2*(P1+P2+P3+P4+P5+P6)
   TOT_C=TOT_C+C(M1,J1)
END DO
F(NC)=(S(L5J,J1)-TOT*C*R1*S(L1,J1))/R1/S(L1,J1)-
   C(NC,J1)
c compute molar adhesion
DO M1=1,NC
   A2=1./((K_F(M1)*AINT+1.)/DELZ)
   F(M1+NC)=C(M1+NC,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1))+
   P(M1+NC,J1))/DELT)
END DO
c compute gas temperature
IF(I_SOL_H.O) THEN
   A2=1./((2*CON_L)/DELZ)**2+RO_F*CP_P*S(L4,J1)/DELZ+
   (RO_F*CP_P)/DELT+2*CON_RF/DR(J1)/DR(J1)
   P1=CON_L/DELZ**2*(2*S(L4,J1-J1))
   P2=-RO_F*CP_P*S(L4,J1-J1)
   P3=-eps(J1)*H_FS*AINT*(C(L1,J1)-C(L2,J1))
   P4=-RO_F*CP_P*C(L1,J1)*S(L4,J1-J1)
   P5=CON_RF*Rp(J1)*S(L4,J1-J1)/(2*DR(J1))
   P6=CON_RF*Rp(J1)*S(L4,J1-J1)/(2*DR(J1))
   P7=-RO_F*CP_P*(-P(L1,J1))/DELT
   F(L1)=C(L1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
c compute solid temperature
A2=1./((2*CON_P)/DELZ)**2+(RO_S*CP_S)/DELZ+
   2*CON_P/DR(J1)/DR(J1))
   P1=AINT*H_FS*(C(L1,J1)-C(L2,J1))
   P2=-RATE_H
   P3=CON_P*(S(L2,J1-J1)+S(L2,J1-J1))/DELZ/DELZ
   P4=CON_P*Rp(J1)*(C(L2,J1-1,J1)-C(L2,J1-1,J1))
   P5=CON_P*Rp(J1)*(C(L2,J1-1,J1)-C(L2,J1-1,J1))
   P6=RO_S*CP_S*(-P(L1,J1))/DELT
   F(L2)=C(L2,J1)+A2*(P1+P2+P3+P4+P5+P6)
ELSE
   c compute effective temperature
   A2=1./((2*CON_L)/DELZ)**2+RO_F*CP_P*S(L4,J1)/
   DELZ+(EPS(J1))*RO_F*CP_P*(1-EPS(J1))*RO_S*CP_S/DELZ+
   2*EPS(J1)*CON_RF/DR(J1)/DR(J1)
   P1=EPS(J1)*CON_L/DELZ**2*(2*S(L1,J1,J1))
   P2=-EPS(J1)*RO_F*CP_P*S(L4,J1)/DELZ*(-S(L1,J1,J1))
EOF
\[ \begin{align*}
P_3 &= -(1 - \text{EPS}(J1)) \cdot \text{RATE}_H \\
P_4 &= -\text{EPS}(J1) \cdot \text{RF} \cdot \text{CP}_F \cdot \text{C}(L1,J1) \cdot (S(L4,J1) - S(L4,J1-1)) / (2 \cdot \text{DELZ}) \\
P_5 &= \text{EPS}(J1) \cdot \text{CON}_RF \cdot \text{RF}(J1) \cdot (2 \cdot \text{H_FW} \cdot \text{DR}(J1) / \text{CON}_RF) \cdot (C(L3,J1) - C(L1,J1)) / (2 \cdot \text{DR}(J1)) \\
P_6 &= \text{EPS}(J1) \cdot \text{CON}_RF \cdot (2 \cdot \text{C}(L1,J1-1) \cdot \text{H_FW} \cdot \text{DR}(J1)) / \text{CON}_RF \cdot (C(L3,J1) - C(L1,J1)) / (\text{DR}(J1) / \text{DR}(J1)) \\
P_7 &= -(\text{EPS}(J1) \cdot \text{RF} \cdot \text{CP}_F \cdot (1 - \text{EPS}(J1)) \cdot \text{RF} \cdot \text{CP}_S) \\
&= (-P(L1,J1)) / \text{DEL} \\
F(L1) &= -(C(L1,J1) + A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7)) \\
F(L2) &= C(L2,J1) - B.C.L_1 \\
\text{END IF} \\
\text{c compute the wall temperature} \\
F(L3) &= -(C(L3,J1) + \text{DEL} / \text{RO} \cdot \text{WA} / \text{CP}_W \cdot \text{A}(A \cdot \text{C} \cdot \text{H_FW} \cdot (C(L1,J1) - C(L3,J1))) - \text{A} \cdot \text{INS} \cdot \text{H_OW} \cdot (C(L3,J1) - TO) - (-P(L3,J1)) \\
\text{ELSE} \\
\text{c this section computes S matrix for those grids with constant grid size} \\
\text{IF}(J1 \neq \text{IR}) \text{THEN} \\
\text{TOT}_C &= 0. \\
\text{c compute molar density} \\
\text{DO} M1 = 1, \text{NC} - 1 \\
A2 &= 1. / (2 \cdot \text{D}_L(M1) / \text{DELZ} + 2 \cdot S(L4,J1) / \text{DELZ} + 2 \cdot \text{D}_R(F(M1) / \text{DR}(J1) / \text{DR}(J1))) \\
P1 &= \text{D}_L(M1) / \text{DELZ} + 2 \cdot (2 \cdot \text{S}(M1,J1-1)) \\
P2 &= -\text{S}(L4,J1) / \text{DELZ} \cdot (-S(M1,J1-1)) \\
P3 &= -\text{ALF} \cdot \text{AINT} \cdot \text{F}(M1) \cdot \text{C}(M1,J1) / (\text{Q}(M1,J1)) \\
P4 &= -\text{RF}(M1) \cdot \text{RF}(J1) / \text{DR}(J1) / \text{DR}(J1) \\
P5 &= \text{RF}(M1) / \text{DR}(J1) / \text{DR}(J1) \\
P6 &= -(P(M1,J1)) / \text{DEL} \\
F(M1) &= -(C(M1,J1) \cdot A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6)) \\
\text{TOT}_C &= \text{TOT}_C + C(M1,J1) \\
\text{END DO} \\
F(NC) &= (S(L5,J1) - TOT_C \cdot \text{R1} \cdot S(L1,J1)) / (R1 / S(L1,J1)) - C(NC,J) \\
\text{c compute molar adsorption} \\
\text{DO} M1 = 1, \text{NC} - 1 \\
A2 &= 1. \cdot (K \cdot F(M1) \cdot AINT + 1) / \text{DEL} \\
F(M1,J1) &= -C(M1,J1) + A2 \cdot (K \cdot F(M1) \cdot AINT \cdot (Q(M1,J1))) + (P(M1,J1) / \text{DEL}) \\
\text{END DO} \\
\text{c compute gas temperature} \\
\text{IF}(L \cdot \text{SOL} \cdot \text{FLO} \cdot \text{EQ} \cdot 1) \text{THEN} \\
A2 &= 1. / (2 \cdot \text{CON}_L / \text{DELZ} + 2 \cdot \text{RO}_F \cdot \text{CP}_F \cdot S(L4,J1) / \text{DELZ} + 2 \cdot \text{RO}_F \cdot \text{CP}_F \cdot \text{S}(L4,J1) / \text{DELZ} + 2 \cdot \text{F}(J1) / \text{DR}(J1)) \\
P1 &= \text{CON}_L / \text{DELZ} + 2 \cdot (2 \cdot \text{S}(M1,J1-1)) \\
P2 &= -\text{S}(L4,J1) / \text{DELZ} \cdot (-S(M1,J1-1)) \\
P3 &= -\text{RF}(M1) \cdot \text{RF}(J1) / \text{DR}(J1) / \text{DR}(J1) \\
P4 &= -\text{RF}(M1) \cdot \text{RF}(J1) / \text{DR}(J1) / \text{DR}(J1) \\
P5 &= \text{RF}(M1) / \text{DR}(J1) / \text{DR}(J1) \\
P6 &= -(P(M1,J1)) / \text{DEL} \\
F(M1) &= -(C(M1,J1) \cdot A2 \cdot (P1 + P2 + P3 + P4 + P5 + P6 + P7)) \\
\text{c compute solid temperature} \\
A2 &= 1. / (2 \cdot \text{CON}_P / \text{DELZ} + 2 \cdot \text{RO}_S \cdot \text{CP}_S / \text{DELZ} + 2 \cdot \text{RO}_S \cdot \text{CP}_S / \text{DELZ} + 2 \cdot \text{CON}_P / \text{DR}(J1) / \text{DR}(J1)) \\
P1 &= \text{CON}_P / \text{DELZ} \cdot (C(L1,J1) - C(L2,J1)) \\
P2 &= \text{RATE}_H \\
P3 &= \text{CON}_P \cdot S(L2,J1-1) \cdot S(L2,J1-1) / \text{DELZ} / \text{DELZ} \\
P4 &= \text{CON}_P \cdot \text{RF}(J1) \cdot (C(L2,J1-1) - C(L2,J1-1) / (2 \cdot \text{DR}(J1)) \\
P5 &= \text{CON}_P \cdot (C(L2,J1-1) - C(L2,J1-1) / \text{DR}(J1) / \text{DR}(J1)) \\
P6 &= \text{RO}_S \cdot \text{CP}_S \cdot (-P(L2,J1)) / \text{DEL} \\
\end{align*} \]
**c compute effective temperature**

\[ A_2 = \frac{1}{(2^2 + \text{CON}_L/\text{DELZ}^2) + \text{DELZ}^2 + 2 + \text{RO}_F^2 \cdot \text{CP}_F \cdot \text{S}(L4, JJ1, J1) / \text{DELT} + 2} \]

\[ \text{EPS}(JJ1)^{\text{CON}_R / \text{DR}(JJ1)} \]

\[ P_1 = \frac{\text{EPS}(JJ1)^{\text{CON}_L/\text{DELZ}^2} + \text{DELZ}^2 + 2 (S(L1, J1, J1))} {\text{RO}_F^2 \cdot \text{CP}_F \cdot \text{S}(L4, JJ1, J1) / \text{DELT} + 2} \]

\[ P_2 = \text{EPS}(JJ1)^{\text{RO}_F^2 \cdot \text{CP}_F \cdot \text{S}(L4, JJ1, J1) / \text{DELT}} \]

\[ P_3 = (1 - \text{EPS}(JJ1)) \cdot \text{RATE} \_H \]

\[ P_4 = \text{EPS}(JJ1)^{\text{RO}_F^2 \cdot \text{CP}_F \cdot \text{C}(L1, JJ1) \cdot \text{S}(L4, JJ1, J1)} \]

\[ P_5 = \text{EPS}(JJ1)^{\text{CON}_R / \text{DR}(JJ1)} - \text{RO}_F^2 \cdot \text{CP}_F \cdot \text{C}(L1, JJ1) \cdot \text{S}(L4, JJ1, J1) / (2 \cdot \text{DELZ}) \]

\[ P_6 = \text{EPS}(JJ1)^{\text{CON}_R / \text{DR}(JJ1)} \cdot \text{C}(L1, JJ1, J1) \cdot \text{C}(L1, JJ1, J1) / (2 \cdot \text{DELZ}) \]

\[ F(L2) = -C(L2, JJ1) \cdot A_2 \cdot (P_1 + P_2 + P_3 + P_4 + P_5 + P_6) \]

**ELSE**

**c this section computes \( \text{S} \) for variable grid size**

**ELSE**

**TOT_C = 0.**

**c compute the molar density**

**DO M1=1,NC-1**

\[ A_2 = \frac{1}{(2^2 + \text{CON}_L / \text{DELZ}^2) + \text{DELZ}^2 + 2 + \text{S}(L4, JJ1, J1) / \text{DELZ} + \text{F11}(JJ1)^{\text{DF}(M1)^2} \cdot \text{DF}(M1) / \text{DELT}} \]

\[ \text{RP}(JJ1)^{\text{DR}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) + 1 / \text{DELZ}} \]

\[ P_1 = 1 / (2^2 + \text{CON}_L / \text{DELZ}^2) + \text{DELZ}^2 + 2 + \text{S}(M1, JJ1, J1) / \text{DELZ} + \text{F11}(JJ1)^{\text{DR}(JJ1)} / \text{DELT} \]

\[ P_2 = \text{S}(L4, JJ1, J1)^{\text{DELZ}^2} / (S(M1, JJ1, J1)) \]

\[ P_3 = \text{ALF}(JJ1)^{\text{K}_F^2} \cdot \text{AINT}^2 \cdot (Q(M1, JJ1, J1) - \text{S}(M1, JJ1, J1)) \]

\[ P_4 = \text{CON}_R / \text{DR}(JJ1) \cdot \text{DR}(JJ1) \]

\[ P_5 = 2 \cdot \text{RO}_F^2 \cdot \text{CP}_F \cdot \text{C}(M1, JJ1, J1) \cdot \text{C}(M1, JJ1, J1) / \text{DELZ} \]

**END DO**

\[ F(NC) = (S(L5, JJ1, J1) - \text{TOT}_C \cdot \text{R}^2 \cdot \text{S}(L1, JJ1, J1)) / \text{R}^2 \cdot \text{S}(L1, JJ1, J1) / \text{C}(NC, JJ1) \]

**c compute molar adsorption**

**DO M1=1,NC**

\[ A_2 = \frac{1}{(K_F^2(M1)^2) / \text{DELZ}^2} \]

\[ \text{F}(M1, NC) = -C(M1, JJ1, J1) \cdot \text{AINT}^2 \cdot (C(M1, JJ1, J1)) \]

**END DO**

**c compute the gas temperature**

**IF(SOL_FLO.EQ.1) THEN**

\[ A_2 = \frac{1}{(2^2 + \text{CON}_L / \text{DELZ}^2) + \text{DELZ}^2 + 2 + \text{RO}_P^2 \cdot \text{CP}_P \cdot \text{S}(L4, JJ1, J1) / \text{DELZ} + 1 / \text{DELZ}) + \text{CON}_R \cdot \text{DR}(JJ1) + \text{DF}(JJ1) + 2 \cdot \text{CON}_R \cdot \text{DR}(JJ1) \]

\[ \text{F12}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) / \text{DR}(JJ1) \]

\[ P_1 = 1 \cdot \text{CON}_L / \text{DELZ}^2 + 1 \cdot \text{S}(L1, JJ1, J1) / \text{DELZ} + 1 \cdot \text{DELZ}^2 \]

\[ P_2 = \text{RO}_P^2 \cdot \text{CP}_P \cdot \text{S}(L4, JJ1, J1) / \text{DELZ} / (S(L1, JJ1, J1)) \]

\[ P_3 = (1 - \text{EPS}(JJ1)) / \text{EPS}(JJ1) \cdot \text{DELZ} / (\text{S}(L1, JJ1, J1)) \]

\[ P_4 = -\text{F22}(JJ1) / \text{C}(L1, JJ1, J1) \cdot \text{C}(L1, JJ1, J1) \cdot \text{C}(L1, JJ1, J1) / \text{DELZ} \]

**END IF**

**c compute the solid temperature**

\[ A_2 = \frac{1}{(2^2 + \text{CON}_P / \text{DELZ}^2 + 2 \cdot \text{CON}_R / \text{DELZ} + \text{RO}_S^2 \cdot \text{CP}_S \cdot \text{DELZ} + \text{DELZ} + 2 \cdot \text{DELZ} + 2} \]

\[ \text{F(L1)} = -C(L1, JJ1) \cdot \text{AINT}^2 \cdot (P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7) \]

\[ \text{F(L2)} = -C(L2, JJ1) \cdot A_2 \cdot (P_1 + P_2 + P_3 + P_4 + P_5 + P_6) \]

\[ \text{F(L1)} = -C(L1, JJ1) \cdot A_2 \cdot (P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7) \]
E-43
\[ p_4 = 4 \times D_{RF}(M_1) \times (C(M_1, J_1 + 1)) / (DR(J_1) / DR(J_1 + 1)) \]
\[ p_5 = -(P(M_1, J_1)) / \text{DELT} \]
\[ F(M_1) = C(M_1, J_1) + A_2 \times (P_1 + P_2 + P_3 + P_4 + P_5) \]
\[ \text{TOT}_C = \text{TOT}_C + C(M_1, J_1) \]
\[ \text{END DO} \]
\[ F(NC) = (S(L_5, J_1 + 1) - \text{TOT}_C \times R_1 \times S(L_1, J_1 + 1)) / (R_1 / S(L_1, J_1 + 1)) \]
\[ C(NC, J_1) \]

\[ c \text{ comp molar adsorption} \]
\[ \text{DO } M_1 = 1, \text{NC} \]
\[ A_2 = 1 \times (K_F(M_1) \times A\text{INT}^1 / \text{DELT}) \]
\[ F(M_1 + NC) = C(M_1 + NC, J_1) + A_2 \times (K_F(M_1) \times A\text{INT} \times (Q(M_1, J_1)) + P(M_1 + NC, J_1)) / \text{DELT} \]
\[ \text{END DO} \]

\[ c \text{ comp gas temperature} \]
\[ \text{IF}(\text{SOL}_1 \_\text{FLG}, \text{EQ} = 1) \text{THEN} \]
\[ A_2 = 1 \times (2 \times \text{CON}\_L / \text{DELZ} + 2 \times \text{RO\_F} \times \text{CP}\_S \times S(L_4, J_1) / \text{DELZ} + \text{RO\_F} \times \text{CP}\_F \times \text{DELZ} + 4 \times \text{CON}\_RF / (\text{DR}(J_1) / \text{DR}(J_1))) \]
\[ P_1 = \text{CON}\_L / \text{DELZ} + 2 \times S(L_1, J_1 + 1) / (S(L_1, J_1 + 1)) \]
\[ P_2 = 2 \times \text{EPS}(J_1) / (\text{DELZ}) \]
\[ P_3 = -S(L_1, J_1) / (\text{DELZ}) \]
\[ P_4 = 2 \times \text{EPS}(J_1) / (\text{DELZ}) \]
\[ P_5 = 2 \times \text{EPS}(J_1) / (\text{DELZ}) \]
\[ \text{ELSE IF}(J_1 = \text{NJR}) \text{THEN} \]
\[ \text{TOT}_C = 0 \]

\[ c \text{ comp molar density} \]
\[ \text{DO } M_1 = 1, \text{NC} - 1 \]
\[ A_2 = 1 \times (2 \times \text{D}_L(M_1) / \text{DELZ} + 2 \times S(L_4, J_1) / (\text{DELZ} + 2) \times D_{RF}(M_1) / (\text{DR}(J_1) / \text{DR}(J_1 + 1))) \]
\[ P_1 = \text{D}_L(M_1) / (\text{DELZ} + 2) \times S(M_1, J_1 - 1, J_1) / (S(M_1, J_1 - 1, J_1)) \]
\[ P_2 = 2 \times S(L_4, J_1) / (\text{DELZ} + 2) \]
\[ P_3 = -A\text{INT}^1 \times K_F(M_1) \times (Q(M_1, J_1) - C(M_1 + NC, J_1)) \]
\[ P_4 = D_{RF}(M_1) \times C(M_1, J_1 - 1) - C(M_1, J_1 - 1) / (2 \times \text{DR}(J_1)) \]
\[ P_5 = 2 \times D_{RF}(M_1) \times C(M_1, J_1 - 1) / (\text{DR}(J_1) / \text{DR}(J_1)) \]
\[ P_6 = -(P(M_1, J_1)) / \text{DELT} \]

E-44
F(M1) = -C0*vl 1,1*A2
F(NC) = (S(I._dj1) - TOT_C*RI*S(L1JJ1))/RI/S(L1JJ1) - C(NC,J)

DO MI = 1, NC
A2 = I./(K_F0*Vl 1)'AIN'T*DELT)
F(MI+NC) = -C(M1+NC,J,A2*(K_F(M1)*AIN'T)*(Q(M1,J,JI) - P(MI+NC,J))
END DO

F(L1) = -C(L1,J1) + A2*(P1 + P2 + P3 + P4 + P5 + P6)
F(L2) = C(I2,J1) - BC_L1
ENDIF

F(L3) = -(C(L3,J1)+DELT/RO_WA/CP_WA*(A_C*H_FW*(C(L1,J1)-C(L3,J1)) - A_INS*H_OW*(C(L3,J1)-TO)) - (-P(L3,J1))

ELSE
ENDIF

c compute effective temperature
A2 = 1./(2*CON_P/DELZ**2+RO_F*CP_F*S(L4,J1))/DELZ+
. (RO_F*CP_F)/(DELZ+2*CON_RF/(DR(J1)/DR(J1))
P1 = CON_L/DELZ**2*(S(L1,J1,J1)+S(L1,J1,1,1))
P2 = -RO_F*CP_F*S(L4,J1,J1)/(DELZ+(-S(L4,J1,J1)))
P3 = -(EPS(J1)*EPS(J1)*H_FS*AIN'T*(C(L1,J1)+C(L2,J1))
P4 = -RO_F*CP_F*C(L1,J1)*S(L4,J1,J1)-
. S(L4,J1,J1)/DELZ)
P5 = CON_RF*RP(J1)*(2.*H_FW*(DR(J1)))/CON_RF*(C(L3,J1)+
. C(L1,J1)/2*DR(J1))
P6 = -RO_S*CP_S*(-P(L1,J1))/DELZ
F(L1) = -C(L1,J1) + A2*(P1 + P2 + P3 + P4 + P5 + P6 + P7)

ELSE
IF(J1.NE.IR) THEN
ELSE
DO MI = 1, NC - 1
  A2 = 1 / (2 * D_L(MI) / DELZ**2 + S(L4J, J1) / DELZ + 2 * D_RF(MI) / DR(J1) / DR(J1) + DELT)
  P1 = D_L(MI) / DELZ**2 * (S(L1, J1 + 1) + S(L1, J1 + J1))
  P2 = S(L4J, J1) / DELZ**2 * (S(L1, J1 - 1) - S(L1, J1 - J1))
  P3 = -ALF(J1) * AINT * K_F(MI) * (Q(MI, J1) - C(MI, J1) + NC, J1 - 1)
  P4 = D_RF(MI) * R_P(J1) * (C(MI, J1) - C(MI, J1 - 1) - C(MI, J1 - J1 + J1)) / (2 * DR(J1))
  P5 = D_RF(MI) * C(MI, J1 + 1) - C(MI, J1 - 1) / DR(J1) / DR(J1)
  P6 = -(P(MI, J1) / DELT)
  F(MI) = -C(MI, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
  TOT_C = TOT_C + C(MI, J1)
ENDDO
F(NC) = (S(L5, J1) - TOT_C * R1 * S(L1, J1)) / R1 / S(L1, J1 - J1) - C(NC, J1)

C comp the molar adsorption
DO MI = 1, NC
  A2 = 1 / (K_F(MI) * AINT + 1 / DELT)
  F(MI + NC) = C(MI + NC, J1) + A2 * (K_F(MI) * AINT * (Q(MI, J1) + P(MI + NC, J1) / DELT)
ENDDO

C comp gas temperature
IF (L_SOL_FLO.EQ.1) THEN
  A2 = 1 / (2 * CON_L / DELZ**2 + RO_F*CP_F*S(L4J, J1) / DELZ + (RO_F*CP_F)/DELT + 2 * CON_RF / DR(J1) / DR(J1))
  P1 = CON_L / DELZ**2 * (S(L1, J1 - 1) + S(L1, J1 + J1))
  P2 = -RO_F*CP_F*S(L4J, J1) / DELZ**2 * (S(L1, J1 - 1) - S(L1, J1 + J1))
  P3 = -EPS(J1) / EPS(J1)**H_F*S*INT*C(L1, J1) - C(L2, J1))
  P4 = RO_F*CP_F*C(L1, J1)**S(L4J, J1 - J1)) - S(L4J, J1 - J1)) / 2 * DELZ)
  P5 = CON_RF*RP(J1)**C(L1, J1 - 1) - C(L1, J1 - J1 + J1)) / 2 * DR(J1))
  P6 = RO_F*CP_F*(-P(L1, J1)) / DELT)
  F(L1) = -(C(L1, J1)) + A2 * (P1 + P2 + P3 + P4 + P5 + P6)
ENDIF

C comp solid temperature
A2 = 1 / (2 * CON_P / DELZ**2 + 2 * CON_P / DR(J1) / DR(J1) + RO_S*CP_S / DELT)
  P1 = AINT**H_F*S*(C(L1, J1) - C(L2, J1))
  P2 = RATE_H
  P3 = CON_F*(S(L2, J1 - 1) + S(L2, J1 + J1)) / DELZ / DELZ
  P4 = CON_F*RP(J1)**C(L2, J1 - 1) - C(L2, J1 - J1 + J1) / 2 * DR(J1))
  P5 = CON_F**C(L2, J1 - 1) - C(L2, J1 - J1 - J1)) / DR(J1) / DR(J1)
  P6 = RO_S*CP_S*(-P(L2, J1)) / DELT)
  F(L2) = -(C(L2, J1) + A2 * (P1 + P2 + P3 + P4 + P5 + P6) + ELSE

C compute effective temperature
A2 = 1 / (EPS(J1)**2 * CON_L / DELZ**2 + RO_F*CP_F*S(L4J, J1) / DELZ + (EPS(J1)**RO_F*CP_F*EPS(J1)**RO_S*CP_S) / DELT + 2 * EPS(J1)**CON_RF / DR(J1) / DR(J1))
  P1 = EPS(J1) / CON_L / DELZ**2 * (S(L1, J1 - 1) + S(L1, J1 + J1))
  P2 = EPS(J1)**RO_F*CP_F*S(L4J, J1) / DELZ**2 * (S(L1, J1 - 1) - S(L1, J1 + J1))
  P3 = -(1 - EPS(J1)) / EPS(J1)**H_F*S*INT*C(L1, J1) - C(L2, J1))
  P4 = EPS(J1)**RO_F*CP_F*C(L1, J1)**S(L4J, J1 - J1)) - S(L4J, J1 - J1)) / 2 * DELZ)
  P5 = EPS(J1)**CON_RF*RP(J1)**C(L1, J1 - 1) - C(L1, J1 - J1 + J1)) / 2 * DR(J1))
  P6 = EPS(J1)**CON_RF*(-P(L1, J1)) / DELT)
  F(L1) = -(EPS(J1)**RO_F*CP_F*(1 - EPS(J1)**RO_S*CP_S)**EPS(J1)**RO_F*CP_F*(-P(L1, J1)) / DELT)
  F(L2) = C(L2, J1) - BC_L1
END IF

ELSE
C this section computes s for variable grid size
ELSE
TOT_C=0.

c comp molar density
DO M=1,NC
  A2=1.0*D_L(M1)*DELZ**2+S(L4,J1)*DELZ=F11(J1)*D_RF(M1)*
    RP(11)*DR(11)+2*D_RF(M1)*F12(J1)/DR(11)+1./DELZ
  P1=D_L(M1)*DELZ**2*(S(M1,J+1,J1)+S(M1,J-1,J1))
  P2=S(L4,J1)*(DELZ*-(S(M1,J-1,J1))
  P3=ALF1(J)*AINT*K_F(M1)*(Q(M1,J1))+(M1+NC,J1))
  P4=D_RF(M1)*RP(11)*F21(J1)*C(M1,J1+1)-F01(J1)*
    C(M1,J1-1)/(DR(J1))
  P5=-2*D_RF(M1)*F22(J1)*C(M1,J1+1)+F02(J1)*C(M1,J1-1))
  A2=1.0*(K_F(M1)*AINT+1./DELZ)
  F(M1)=C(M1,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1)))+
    P(M1+NC,J1)/DELZ)
END DO

F(NC)=(S(L5,J11)-TOT_C*R1*S(L1,J1))/R1/S(L1,J1)-
    C(NC,J1)

c comp molar adsorption
DO M=1,NC
  A2=1.0*(K_F(M1)*AINT+1./DELZ)
  F(M1)=C(M1,J1)+A2*(K_F(M1)*AINT*(Q(M1,J1)))+
    P(M1+NC,J1)/DELZ)
END DO

c compute gas temperature
IF(I_SOL,FLO.EQ.1)THEN
  A2=1.0*D_L(M1)/DELZ**2+S(L4,J1)/DELZ=F11(J1)*D_RF(M1)*
    RP(11)*DR(11)+2*D_RF(M1)*F12(J1)/DR(11)+1./DELZ
  P1=D_L(M1)/DELZ**2*(S(M1,J+1,J1)+S(M1,J-1,J1))
  P2=S(L4,J1)*(DELZ*-(S(M1,J-1,J1))
  P3=(1-EPS(J1))*EPS(J1)*H_F*S*AINT*(C(L1,J1)-C(L2,J1))
  P4=RO_F*CP_F*C(L1,J1)*(S(L4,J+1,J1))
  S(L4,J1))/2*DELZ)
  P5=CON_RF*RP(11)*F21(J1)*C(L1,J1+1)-F01(J1)*
    C(L1,J1-1)/(DR(J1))
  P6=-2*CON_RF*(F22(J1)*C(L1,J1+1)+F02(J1)*C(L1,J1-1))/
    DR(J1)
  P7=-RO_F*CP_F*(-P(L1,J1))/DELZ
  F(L1)=C(L1,J1)+A2*(P1+P2+P3+P4+P5+P6+P7)
ELSE
  c compute solid temperature
  A2=1.0*D_L(M1)/DELZ**2+S(L4,J1)/DELZ=F11(J1)*D_RF(M1)*
    RP(11)*DR(11)+2*D_RF(M1)*F12(J1)/DR(11)+1./DELZ
  P1=AINT*H_F*S*(C(L1,J1)-C(L2,J1))
  P2=RATE_H
  P3=CON_P/DELZ/S*(S(L2,J-1,J1)+S(L2,J+1,J1))
  P4=CON_P*RP(J1)*F21(J1)*C(L2,J1+1)-
    F01(J1)*C(L2,J1-1)/(DR(J1))
  P5=2*CON_P*(F22(J1)*C(L2,J1+1)+F02(J1)*
    C(L2,J1-1))/DR(J1)
  P6=-RO_S*CP_S*(-P(L2,J1))/DELZ
  F(L2)=C(L2,J1)+A2*(P1+P2+P3+P4+P5+P6)
END IF
\[ P_6 = 2 \times \text{EPS}(J_1) \times \text{CON_RF} \times (F_2(J_1) \times C_{g,1} J_1 + I) + F_02(J_1) \times \frac{C(L_1 J_1 - 1))}{\text{DRU}_1} \]

\[ \text{FT} = -\left( \text{EPS}_U \right) \times \text{RO_F} \times \text{CP_F} + (1 - \text{EPS}_U) \times \text{RO_S} \times \text{CP_S} \times \frac{-P(L_1 J_1)}{\Delta L} \]

\[ F(L_1) = -C(L_1 J_1) \times A_2 \times (P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7) \]

\[ F(L_2) = \text{C(I..2d J_1)} - \text{BC_L} \]

```
c this subroutine compute the amount of adsorbed gas in equilibrium with gas
molar density. for single component uses Langmuir-fredrich isotherm. the
compution of equilibrium for multi component uses the Ideal Solution Theory
(IST). since the equations are non linear and implicit a numerical method
was used to compute the adsorbed equilibrium amount. the method is by Forysthe.
Computer Methods for Mathematical Computation. it is an bisection method with
quadratic convergence.

c B,V,PO arrays are single equilibrium constant:
```

```
SUBROUTINE IST_ZI(METHOD,T,SS,Q1)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4),PI(4),XI(4),X1 (4),Y1 (4)
COMMON/INDIC1/IND(4)
COMMON/NCY/NC1
REAL*8 Q1(4),SS(4)
EXTERNAL FCN1
DATA XTOLFTOL.LNLIM/1.0E.-5,1.0E.5,0,50/
DATA R555/
T_G=T
NC=NC1
c the partial pressure
DO II=1,NC
Y1(II)=SS(II)
END DO
do I=1,NC
PP(I)=Y1(I)*T_G*R
END DO
c no mole fraction return
Z=1.0E-32
DO I=1,NC
Q1(I)=0.
END DO
RETURN
END IF
N1=1
c set the constant as a function of temperature
IF(IND(1).EQ.1)THEN
C
V(N1)=81.2983138-.21118560043*T+1.587732293D-4*T*T)/44/100
V(N1)=17.044/100
C
B(N1)=686.9000131*EXP(-.019625791466*T)
B(N1)=5.323235056e-6*T**(-.5)*EXP(13948.544244/1.987/T)
PO(N1)=-8
N1=N1+1
END IF
```
```
IF(IND(2).EQ.1)THEN
  V(N1)=1.69305
  B(N1)=1.8879094E-4*EXP(5467.4817024/T)
  IF(T.LT.560.) THEN
    B(N1)=4.5597278759E-7*EXP(9628.9655743/T)
  ELSE
    B(N1)=5.8089066684E-7*EXP(9115.734593/T)
  END IF
  N1=N1+1
  PO(N1)=1.0
END IF
IF(IND(3).EQ.1)THEN
  V(N1)=1.637879912E-5*T+.00961297026
  IF(T.LE.532)THEN
    B(N1)=3.2694515539E-7*T+4.59988799E-4
  ELSE
    B(N1)=7.90864008E-5*T-4.1400420E-2
  END IF
  PO(N1)=1.0
  N1=N1+1
END IF
IF(IND(4).EQ.1)THEN
  V(N1)=1.637879912E-5*T+.00961297026
  IF(T.LE.532)THEN
    B(N1)=3.2694515539E-7*T+4.59988799E-4
  ELSE
    B(N1)=7.90864008E-5*T-4.1400420E-2
  END IF
  PO(N1)=1.0
END IF
!
!
calculate the equilibrium isotherm by Langmuir method
!
IF(NC.EQ.1)THEN
  Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
  RETURN
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0)THEN
  Q1(2)=V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
  Q1(1)=0
  RETURN
ELSE IF(NC.EQ.2 .AND. PP(2).EQ.0)THEN
  Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
  Q1(2)=0
  RETURN
END IF
!
TERM1=0.
DO I=1,NC
  TERM1=B(I)*PP(I)**PO(I)+TERM1
END IF
!
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0.) THEN
    TERM1=B(I)*PP(I)**PO(I)+TERM1
  END IF
END DO
!
IF(METHOD.EQ.1)THEN
  RETURN
END IF
!
c if the Langmuir method is asked for then returned
IF(METH..EQ.1)THEN
  RETURN
END IF
!
c if not, take the result as the first guess for IST theory
DO := 1, NC
E-49
X1(I)=Q1(I)/SUM
IF(X1(I).GT.0) THEN
  P1(I)=PP(I)/X1(I)
ELSE
  P1(I)=0.
ENDIF
END DO

c calculate the spread pressure
DO I=1,NC
  IF(PP(I).LE.0.) THEN
    X1(I)=0
  ELSE
    X1(I)=V(I)/PO(I)*LOG(1+B(I)*PI(I)**PO(I))
    IF(I==1) THEN
    END IF
END DO
ENDDO

X=X1(IF)
DO I=1,NC
  IF(X1(I).LT.X AND X1(I).GT.0)THEN
    X=X1(I)
  END IF
END DO
AX=X
DELX=AX
BX=AX

c call Zeroin subroutine to find the rout to the IST equation
DO I=1,100
  BX=BX+DELX
  FUN=FCN1(BX)
  IF(FUN.LT.0)GO TO 113
END DO
113 X=ZEROIN(FCN1,AX,BX,TOL)
c rout was found
DO I=1,NC
  IF(PP(I).LE.0) THEN
    PP(I)=1.0E-32
  END IF
END IF

c calculate the fraction in the solid phase
PART1=PO(I)*X/V(I)
IF(PART1.GT.73) PART1 =73
PI(I)=(EXP(PART1)-1)/B(I)
X1(I)=PP(I)*PI(I)
END DO
TOT_Q=0

c calculate the total amount adsorbed
DO I=1,NC
  Q1(I)=V(I)*B(I)*PI(I)**PO(I)/(1+B(I)*PI(I)**PO(I))
  TOT_Q=TOT_Q+X1(I)*Q1(I)
END DO

c calculate the amount adsorbed for each component
DO I=1,NC
  Q1(I)=1./TOT_Q*X1(I)
END DO
80 RETURN
END

c IST function
REAL FUNCTION FCN1(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NCY/NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
PARTI = PO(I) * X / V(I)
IF (PARTI .GT. 73) PARTI = 73
SUM = SUM + PP(I) / ((EXP(PARTI) - 1) / B(I)) ** (1 / PO(I))
END IF
C IF (PP(I) .LE. 0.0) PP(I) = 1.0E-32
C PARTI = PO(I) * X / V(I)
C IF (PARTI .GT. 73) PARTI = 73
C SUM = SUM + PP(I) / ((EXP(PARTI) - 1) / B(I)) ** (1 / PO(I))
END DO
FCN = SUM - 1
RETURN
END

C subroutine to find the root of equation by bisect method

REAL FUNCTION ZEROIN(FCN, AX, BX, TOL)
IMPLICIT REAL*8 (A-H, O-Z)
REAL*8 AX, BX, FCN, TOL
REAL*8 A, B, C, D, EPS, FA, FB, FC, TOL, XM, P, Q, R, S
EPS = 1.0
10 EPS = EPS / 2.
TOL = 1.0 + EPS
IF (TOL .GT. 1.0) GO TO 10
A = AX
B = BX
FA = FCN(A)
FB = FCN(B)
C begin step
20 C = A
FC = FA
D = B - A
E = D
30 IF (ABS(FC) .GE. ABS(FB)) GO TO 40
A = B
B = C
C = A
FA = FB
FB = FC
FC = FA
C convergence test
40 TOL = 2.0 * EPS * ABS(B) + 5.0 * TOL
XM = 0.5 * (C - B)
IF (ABS(XM) .LE. TOL) GO TO 90
IF (FB .EQ. 0.0) GO TO 90
C is bisection necessary
IF (ABS(FC) .LE. TOL) GO TO 70
IF (ABS(FA) .LE. ABS(FB)) GO TO 70
C is quadratic interpolation possible
IF (A .NE. C) GO TO 50
C linear interpolation
S = FB / FA
P = 2.0 * XM * S
Q = .5 - S
GO TO 60
C inverse quadratic interpolation
50 Q = FC / FA
R = FB / FC
S = FB / FA
P = S * (2.0 * XM * Q * (Q - R) - (B - A) * (R - 1.0))
Q = (Q - 1.0) * (R - 1.0) * (S - 1.0)
c adjust signs
60 IF(P.GT.0.0)Q=-Q
P=ABS(P)
c is interpolation acceptable
IF((2.0*P).GE.(3.*XM*Q-ABS(TOL1*Q))) GO TO 70
IF(P.GE.ABS(.5*E*Q)) GO TO 70
E=D
D=P/Q
GO TO 80
c bisection
70 D=XM
E=D
c complete step
80 A=B
FA=FB
IF(ABS(D).LT.TOL1)B=B+D
FB=FCN(B)
IF((FB*FCN(B)).LT.0.) GO TO 20
GO TO 30
c done
90 ZEROIN=B
RETURN
END
C
C
C
C
C the second method, this method is faster but the initial guess must be near
C the root of the equation.
C
c this subroutine compute the amount of adsorbed gas in equilibrium with gas
C mole density, for single component uses Langmuir isotherm the
C computation of equilibrium for multi component uses the Ideal Solution Theory
C (IST), since the equations are none linear and implicit, a numerical method
C was used to compute the adsorbed equilbirium amount, the method is Newton,
C
C B,V,PO arrays are single equilibrium constant
SUBROUTINE IST_Z0VfETHOD,T,SS,Q1)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4),PI(4),XI(4),X1(4),Y1(4)
COMMON/NCY/NC1
COMMON/INDIC1/IND(4)
REAL*8 Q1(4),SS(4)
INTEGER LLIM
EXTERNAL FCN,FDER
DATA XTOL,FTOL,LNLIB/1.0E-5,1.0E-5,0.50/
DATA R,555.0/
T_G=T
NC=NC1
DO 11=1,NC
Y1(I1)=SS(I1)
11 END DO
DO 1=1,NC
PP(I)=Y1(I)*T_G*R
1 END DO
C no mole fraction return
Z=1.0E-32
IF((PP(1)).LT.Z) THEN
DO 1=1,NC
Q(I)=0.
1 END DO
RETURN
END
N1=1

c set the constant as a function of temperature
IF(IND(1).EQ.1) THEN

c 13x by l, grace

n:=(m'D(t).EQ. )

\[ c_{set} \]

\[ \text{if}(pp(n1).lt.1.) \text{then} \]

\[ V(N1)\text{=}1.5671.205874+9.00256903 \times 1.0172347 \times t+1.100806e-5 \times t^3 \]

\[ \text{if}(pp(n1).gt.1.) \text{then} \]

\[ V(N1)\text{=}01.2883158-21113560043 \times T+1.587732293D-4 \times T^4/100 \]

\[ B(N1)\text{=}6864.9000131 \times \text{EXP}(-0.19625791466 \times T) \]

\[ \text{po}(n1)\text{=}1.0 \]

\[ \text{else} \]

\[ V(n1)\text{=}23.32228/44/100 \]

\[ B(n1)\text{=}4.9639763e-4 \times T^3(-5)\times \text{EXP}(9233.33778/1.987/T) \]

\[ \text{po}(n1)\text{=}2.9138991288+0.17181761178 \times T-2.8549083257 \times 5 \times T^5+ \]

\[ 1.622511757e-8 \times T^9 \]

\[ \text{end if} \]

\[ \text{if from Firm data 5A} \]

\[ \text{if}(pp(n1).lt.1.\text{ then}) \]

\[ B(N1)\text{=}2.37022397e-6 \times T^3(-5)\times \text{EXP}(14907.65351/1.987/T) \]

\[ V(N1)\text{=}16.6/44/100 \]

\[ \text{po}(n1)\text{=}0.8 \]

\[ \text{else} \]

\[ V(n1)\text{=}25.97135008-6.084518e-3 \times T-2.179516646e-5 \times T^5 \times T^4/100 \]

\[ B(n1)\text{=}1.88863393e-5 \times T^3(-5)\times \text{EXP}(12170.875335/1.987/T) \]

\[ \text{po}(n1)\text{=}1. \]

\[ \text{end if} \]

C 5A BY GRACE, BY L_F

\[ V(N1)\text{=}17.0/44/100 \]

\[ B(N1)\text{=}2.3414777e-4 \times T^5(-5)\times \text{EXP}(10427.166145/1.987/T) \]

\[ \text{po}(n1)\text{=}3.830450111e-4 \times T^5(1.188379956) \]

C 5A BY GRACE, BY L

\[ V(N1)\text{=}4.2786889+.087218022 \times T-9.1010715804 \times 5 \times T^5 \times T^4/100 \]

\[ B(N1)\text{=}9.253309123E-5 \times T^5(-5)\times \text{EXP}(10719.0/1.987/T) \]

\[ \text{po}(n1)\text{=}1. \]

C 5A BY GRACE; BY L_F BETWEEN 0-75 C

\[ V(N1)\text{=}0399.3942+1.93842896e+3 \times T^3 \times T- \]

\[ 1.8226211899e-6 \times T^5 \times T^4/100 \]

\[ B(N1)\text{=}35.358072159-17016733 \times T+2.7458762e-4 \times T^5 \times T- \]

\[ 1.484116035 \times T^5(-3) \]

\[ \text{po}(n1)\text{=}29.3861079+.1538898497 \times T-2.61225877e-4 \times T^5+ \]

\[ 1.78184694E-7 \times T^5 \]

\[ \text{linde 5a} \]

\[ V(n1)\text{=}0.005 \]

\[ B(n1)\text{=}1.129015193-5 \times \text{EXP}(5055.015089/t) \]

\[ \text{po}(n1)\text{=}0.6 \]

\[ N1=N1+1 \]

END IF

h2o on 5a by grace li
IF(IN(2).EQ.1) THEN

C IND(1).EQ.1 FOR CO2+H2O+N2; IND(1).EQ.0 FOR H2O+N2

C IF(IN(1).EQ.1) THEN

\[ \text{if}(pp(n1).lt.4.) \text{then} \]

\[ V(n1)\text{=}39.914452-8.87103e-2 \times t+6.839502987e-5 \times t^3 \times t^4/100 \]

\[ \text{else} \]

\[ V(n1)\text{=}873.44464-3.867384937 \times t+5.80375049e-3 \times t- \]

\[ 2.9346685e-6 \times t^3\times t^4/100 \]

\[ \text{end if} \]

\[ B(n1)\text{=}29690.66923-137.837129 \times T+2.14456126 \times t \]

\[ \text{po}(n1)\text{=}1. \]

\[ \text{else} \]

\[ B(n1)\text{=}48.566639771-2.2620239975e-1 \times t+3.9101703168e-4 \times t^3- \]

\[ 2.379098497e-7 \times t^5 \]

E-53
```plaintext
v(n1)=(95.093824733-.21725775358*t÷1.4628603e-4*r*t)/100/18
po(nlp)=

C ELSE
CC  
C b(n1)=24.573259-5.8385278e-2*t+3.473682438e-5 *t*t
C
C v(n1)=(66.62520167-.12299345*t÷7.1897316221e-5*Pt)/100/18
C
C if(_le.600)_en
C po(nl)=.8219916486-3.3519986e-3* t+4.679276479e-6*t*t
C else
C po(nl)=-6.0926707634+2.043004e-2*t-2.924858439e-5*t*t+
C . 1.1746734108e-8*t*t*t
C end if
C END IF
C
C b(n1)=.2247292664*t** (-.5)*expC7858.45996/1.987/t)
C v(n1)=
C
C IF(T.LE.532)THEN
B(N1)=3.2694515539E-7*T+4.59988799E-4
C ELSE
B(N1)=7.90864008E-5*T-4.14400420E-2
C END IF
PO(N1)=L0
END IF

n=(N(4).EQ.DTtmN
V(N1)-- 1.637879912E-5*T+.00961297026
IF(T.LE.532)THEN
B(N1)=3.2694515539E-7*T+4.59988799E-4
ELSE
B(N1)=7.90864008E-5*T-4.14400420E-2
ENDIF
PO(N1)=L0
ENDIF
_(NC.EQ.1)THEN
Q1(1)=V(1)*B(I)**PP(1)**PO(1)/(1+B(I)*PP(1)**PO(1))
RETURN
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0)THEN
Q1(2)=V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
Q1(1)=0
RETURN
ELSE IF(NC.EQ.2 .AND. PP(2).EQ.0)THEN
Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
Q1(2)=0
RETURN
ELSE IF(NC.EQ.3)THEN
if(pp(1).le.0 .and. pp(2).le.0)then
Q1(3)=V(3)*B(3)*PP(3)**PO(3)/(1+B(3)*PP(3)**PO(3))
Q1(1)=0
Q1(2)=0
return
else if(pp(1).le.0 .and. pp(3).le.0)then
Q1(2)=V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
Q1(1)=0
Q1(3)=0
return
else if(pp(2).le.0 .and. pp(3).le.0)then
Q1(1)=V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
Q1(2)=0
RETURN
```

E-54
Q1(3)=0

END IF
TERM1=0.

c calculate the equilibrium by Langmuir isotherm
DO I=1,NC
IF(PP(I).GT.0) THEN
TERM1=B(I)*PP(I)**PO(I)+TERM1
ENDIF
ENDDO

SUM=0.
DO I=1,NC
IF(PP(I).LE.0.) THEN
Q1(I)=0.
ELSE
Q1(I)=V(I)*B(I)*PP(I)**PO(I)/(1+TERM1)
SUM=SUM+Q1(I)
ENDIF
ENDDO

c if the Langmuir method is asked for, then return. If not use it as first guess

c for IST theory
IF(METHOD.EQ.1) THEN
RETURN
ENDIF
DO I=1,NC
X1(I)=Q1(I)/SUM
IF(X1(I).GT.0)
ELSE
PI(I)=PP(I)/X1(I)
ENDIF
END IF

c set the initial guess for the spreading pressure
DO I=1,NC
IF(PP(I).LE.0.) THEN
X1(I)=0
ELSE
X1(I)=V(I)/PO(I)*LOG(1+B(I)*PI(I)**PO(I))
ENDIF
END DO
X=X1(IF)
DO I=2,NC
IF(X1(I).LT.X. AND. X1(I).GT.0) THEN
X=X1(I)
ENDIF
END DO

c call newton method to the rout to IST equation
IF(X .LE. 1.0E-17) GO TO 80
CALL NEWTN(FCN,FDER,X,XTOL,FTOL,NLIM,1)

c rout was found, calculate the fraction in the solid phase
DO I=1,NC
IF(PP(I).LE.0) THEN
X1(I)=0.
ELSE
PART1=PO(I)*X/V(I)
IF(PART1.GT.73)PART1=73
PI(I)=(EXP(PART1)-1)/B(I)
X1(I)=PP(I)/PI(I)
ENDIF
END DO

c calculate the total amount in the solid phase
TOT_Q=0
DO I=1,NC
IF(PP(I).LE.0) THEN
  Q1(I)=0.
ELSE
  Q1(I)=(V(I)**B(I)**PI(I)**PO(I)/(1+B(I)**PI(I)**PO(I)))
  TOT_Q=TOT_Q*X1(I)/Q1(I)
ENDIF
END DO

c calculate the amount in equilibrium with the gas phase for each component
DO I=1,NC
  Q1(I)=1/TOT_Q*X1(I)
END DO
80 RETURN
END

C
C IST final equation
C
REAL FUNCTION FCN(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART1=PO(I)*X/V(I)
    IF(PART1.GT.73) PART1=73
    SUM=SUM+PP(I)/(EXP(PART1)-1)/B(I)**(1/PO(I))
  END IF
END DO
FCN=SUM-1
RETURN
END

C
C IST final derivative
C
REAL FUNCTION FDER(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART3=PO(I)**X/V(I)
    IF(PART3.LT.25) THEN
      PART1=-PP(I)/B(I)/V(I)*EXP(PART3)
      PART2=EXP(PART3)/(EXP(PART3)-1)*B(I)**(1/PO(I))
      SUM=SUM+PART1/PART2
    ELSE IF(PART3.LT.73) THEN
      SUM=SUM-B(I)**((1+PO(I))/PO(I))*PP(I)/B(I)/V(I)*
        EXP(-PART3/PO(I))
    ELSE
      PART3=73
      SUM=SUM-B(I)**((1+PO(I))/PO(I))*PP(I)/B(I)/V(I)*
        EXP(-PART3)
    END IF
  END IF
END DO
FDER=SUM
RETURN
END
SUBROUTINE NEWT(FCN, FDER, X, XTOL, FTO, NLIM, I)
IMPLICIT REAL*8(A-H,O-Z)
INTEGER NLIM, I
FX=FCN(X)
X1=X
DO J=1,NLIM
DELX=FX/FDER(X)
X=X-DELX
FX=FCN(X)
IF (ABS(X-X1)/X.LE.XTOL) THEN
RETURN
ENDIF
END IF
FX=FX1
IF (ABS(FX-FX1)/FX.LE.FTO) THEN
RETURN
ENDIF
X1=X
FX1=FX
END DO
I=-1
PRINT 200, NLIM, X, FX
200 FORMAT(/'TOLERANCE NOT MET ',/4,' ITERATIONS X= ',Q.E12.5)
RETURN
END

FUNCTION CPGAS(TEM, Y)
C THIS FUNCTION CALCULATES THE HEAT CAPACITIES OF CMRIER GAS IN BTU/#MOLE/K
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 A(4), B(4), C(4), D(4), Y(4)
COMMON/GAS_INERT, NCOMP
COMMON/NCT/NC1
COMMON/INDIC1/IND(4)
C CO2
DATA A/36.11, 33.46, 29.19, 29.19/
C H2O
DATA B/4.233E-2, 4.688E-2, 2.199E-2, 2.158E-2/
C N2
DATA C/-2.597E-5, 7.604E-5, 5.723E-5, 6.076E-5/
C O2
DATA D/-7.464E-9, -3.593E-9, -2.87E-9, 1.311E-9/
NC=NC1
T=TEM/1.8-273.15
IF (INERT.EQ.1) THEN
CPGAS=0.
YO=0.
N1=1
DO I=1,4
IF (IND1.EQ.1) THEN
CP=A(I)+B(I)*T+C(I)*T*T+D(I)*T*T*T
CPGAS=CP*Y(N1)*4.18669+CPGAS
YO=Y(N1)+YO
N1=N1+1
ENDIF
END DO
CPGAS=CPGAS+(A(3)+B(3)*T+C(3)*T*T+D(3)*T*T*T*T)*(1-YO)/4.18669
ELSE
CPGAS=4.97
ENDIF
FUNCTION CPS(TEMP)
IMPLICIT REAL*8(A-H.O-Z)
C THIS FUNCTION CALCULATES THE HEAT CAPACITY
C BTU/LB/°R.
CPS=1.0
RETURN
END

REAL FUNCTION KGAS (TEMP)
C THIS FUNCTION CALCULATES THE THERMAL CONDUCTIVITY OF CARRIER.
C BTU/MIN/FT/°R
IMPLICIT REAL*8(A-H.O-Z)
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
KGAS=3.88E-7*TEMP+0.4052E-4
ELSE
KGAS=1.667E-6*TEMP+6.1E-4
ENDIF
RETURN
END

FUNCTION RE (G,TEMP)
C THIS FUNCTION CALCULATES THE PARTICLE REYNOLDS NUMBER ASSUMING THAT
C THE MOLECULAR WEIGHT OF THE GAS IS EQUAL TO THAT OF CARRIER GAS.
IMPLICIT REAL*8(A-H.O-Z)
REAL*8 LEN
COMMON/GAS/INERT,NCOMP
DATA IFLAG/O/
IF (IFLAG.EQ.0) THEN
IFLAG=1
ENDIF
RE=CONST*MW*ABS(G)/VIS(TEMP)
RETURN
END

FUNCTION VIS(TEMP)
IMPLICIT REAL*8(A-H.O-Z)
C THIS FUNCTION CALCULATES THE VISCOSITY OF CARRIER GAS AS A FUNCTION
C OF TEMPERATURE (LB/MIN/FT).
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
VIS=1.0E-6*TEMP+1.65E-4
VIS=-0.00707182+5.38463937E-5*TEMP-8.7973727E-8*TEMP*TEMP+
2 4.811387495E-11*TEMP*TEMP*TEMP
ELSE
VIS=0.9444E-6*TEMP+2.863E-4
ENDIF
RETURN
END

FUNCTION RHOG(TEMP)
IMPLICIT REAL*8(A-H.O-Z)
REAL*8 LEN
C THIS FUNCTION CALCULATES THE MOLAR DENSITY OF AN IDEAL GAS IN
C LBMOLES/CV FS.
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UNS,HWALL,LEN
DATA R555./
RHOG=P/R/TR
RETURN
END

FUNCTION EFFD(ICOMP,G,TEMP,RHO,PT,YO)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL DIFFUSIVITIES IN A PACED BED
C USING THE EDWARDS AND RICHARDSON CORRELATION. (FT^2/FT/MIN)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LAMBDA1,LAMBDA2,LEN,YO(4)
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UNS,HWALL,LEN
DATA IFLAG/0/,LAMBDA1/0.73/
IF(IFLAG.EQ.0)THEN
  CONST=2.*RA/EPSEX
  IFLAG=1
ENDIF
DIF=DIFF(ICOMP,TEMP,PT,YO)
EFFD=LAMBDA1*DIF+CONST*ABS(G)*LAMBDA2(G,DIF,RHO)/RHO
RETURN
END

FUNCTION EFFK(G,T,CP,RHO,P,YO)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL THERMAL CONDUCTIVITY OF A
C PACED BED IN BTU/FT/FT/MIN/F.
COMMON/NCY/NC1
REAL*8 YO(a)
NC=NC1
EFFK=0.
KK=0
DO II=1,NC
  SUM=CP*RHO*EFFD(II,G,T,RHO,P,YO)
  IF(SUM.GT.0)KK=KK+1
  EFFK=SUM+EFFK
END DO
EFFK=EFFK/KK
RETURN
END

REAL FUNCTION LAMBDA2(G,DIF,RHO)
C THIS FUNCTION CALCULATES THE DIMENSIONLESS PARAMETER OF THE EDWARDS AND
C RICHARDS CORRELATION MODIFIED FOR SMALL DIAMETER PARTICLES.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
DATA IFLAG/0/
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UNS,HWALL,LEN
IF(IFLAG.EQ.0)THEN
  IF(RA.GT.0.00492)THEN
    PE=2.
  ELSE
    PE=406.4*RA
  ENDIF
  CONST=2.*RA/EPSEX
  IFLAG=1
ENDIF
LAMBDA2=1./PE/(1.495*DIF/CONST/ABS(G)*RHO)
RETURN
END

FUNCTION DIFF(ICOMP,TEMP,PT,YO)
C THIS FUNCTION CALCULATES THE MOLECULAR DIFFUSION COEFFICIENTS BY CORRECTING
C FOR PRESSURE AND TEMPERATURE (FT^2/FT/MIN).
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN,YO(4),V(4),MW1(4),V(4),MW(4),DIF(4)
COMMON/GAS/INERT,NCOMP
COMMON/NCY/NC1
COMMON/INDIC/IND(4)
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UINS,HWALL,LEN
DATA V1/26.9,12.7,17.9,16.6/
DATA MW1/44.01,18.01,6.28,0.91,31.999/
NC=NC1
K=ICOMP
P=P1/760.
T=TEM/I.8
N1=1
DO II=1,4
   IF (IND(II).EQ.1) THEN
      MW(N1)=MW1(II)
      V(N1)=V1(II)
      N1=N1+1
   END IF
   END DO
DO I=1,NC
   IF (NC.EQ.1) THEN
      MW(I)=MW(K)
      V(I)=V(K)
   END IF
   PART1=(MW(K)+MW(I))/MW(K)*MW(I)**.5
   PART2=(V(K)**(1./3)-V(I)**(1./3))**2
   DIF(I)=PART1/PART2*T**1.75/P*1.0E-3
   END DO
IF (NC.EQ.1) THEN
   DIFF=DIF(1)*3.8745
   RETURN
ENDIF
IF (NC.EQ.2) THEN
   IF (K.EQ.1) DIFF=DIF(2)*3.8745
   IF (K.EQ.2) DIFF=DIF(1)*3.8745
   RETURN
ENDIF
DO I=1,NC
   IF (I.NE.K) THEN
      SUM=SUM+YO(I)/DIF(I)
   END IF
   END DO
END IF
if (sum.ne.0) then
   DIFF=(1-YO(K))/SUM*3.8745
else
   DIFF=1
endif
RETURN
END

FUNCTION HFILM(MW,TEMP,REY,CP)
C THIS FUNCTION CALCULATES THE FLUID FILM HEAT TRANSFER COEFFICIENT
C IN BTU/ SQ FT/MIN/R USING THE CORRELATION OF PETROY AND THODOS.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 ID,KGAS,KG,LEN,MW
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UINS,HWALL,LEN
COMMON/KGAS/MW,TEMP
KG=KGAS(TEMP)
PR=CP/MW*VIS(TEMP)/KG
HFILM=0.357/EPSEX*REY**0.64*PR**0.33*KG**0.5/R
RETURN
END
FUNCTION DHADS(IUNIT,T)
C THIS FUNCTION CALCULATES THE ISOTERIC HEAT OF ADSORPTION (BTU/#MOLE)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
COMMON/PRIME/GN2,RA,RAV,EPSEX,RHOS,TAMB,ALPHA1,UNINS,HWALL,LEN
IF(IUNIT.EQ.2) THEN
   DHADS=20400.0
ELSE
   DHADS=20000.0
ENDIF
RETURN
END

C THIS FUNCTION CALCULATES THE CONDUCTIVITY OF FLUID IN AXIAL AND RADIAL DIRECTION.

SUBROUTINE CONDUC1(EMIS,AKS,D_P,D_LGA,VAV,TAV,RO,CP,AVIS,1
AKC,NJR,DELAV,DELTA1,DELTA2,DELRO,EAKT)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION V(30),VS(30),AK(30),AKST(30),DELTA(30),1
E(30),ES(30),DER(30),DKR(30),W(30),AKT(30),DELRO(30)
DELTA(1)=DELTA1
DELTA(NJR)=DELTA1
DELTA(1)=DELTA1
DELTA(NJR)=DELTA2
RP(1)=0.
RP(NJR)=1.
DO K=2,NJR
   RP(K)=2*DELRO(K)/D_LGA/RP(K-1)
ENDIF
C VELOCITY CALCULATION
C
NJ=NJR
RMS=1.2*D_P/D_LGA
BO=.16*(D_P/D_LGA)**(-3./2.)
AO=1./(BO+2.)-RMS/(BO+1.)
A2=RMS/(BO+1.)
A3=1./(BO+2.)
D=AO/2.+A2/(BO+3.)-A3/(BO+4.)
DO I=1,NJR
   VS(I)=(AO+A2*(RP(I)**(BO+1.))-A3*(RP(I)**(BO+2.)))/(2.*D)
ENDDO
DO I=1,NJR
   V(I)=VS(I)*VAV
ENDDO
DPDT=D_P/(D_LGA)
RW=1.-DPDT
VW=(AO+A2*(RW**2*(BO+1.))-A3*(RW**2*(BO+2.')))/(4.*D)
C CALC OF EAV, EO, AND EW
C
R1=1.-4.*DPDT
EO=VS(1.)*(1.+19.4*DPDT**2)**9./8.
EAV=D_P*VAV/(9.*(1.+19.4*DPDT**2))
CCC=(1.+R1+0.1*R1**2.)/6.
EM=(.5-1.5*EO*R1**2)/CCC
EW=EM*(1.-RW)/(1.-R1)/2.
C CALC OF AKAV, OK, WK
C
ANPR=CP*AVIS/AKC
E(1)=EO*EAV
E(NJR)=EW*EAV
V(NJR)= VW*VAV
DO J=1,3
IF(J.EQ.3)THEN
  I=3
  V(3)=VAV
  DELTA(3)=DELAV
  E(3)=EAV
ELSE IF(J.EQ.1)THEN
  I=1
ELSE IF(J.EQ.2)THEN
  I=NI
END IF
ANRE=D_P*RO*V(T)/AVIS
IF((ANRE-350).LE.0)THEN
  AH=1.95*ANRE**(-.51)
ELSE
  AH=1.06*ANRE**(-.41)
END IF
HC=AH*CP*RO*V(T)*(ANPR**(-2.3))
AKR=4.*EMI*D_P*1.173*(TAV**1.8)**3.*V((100.*EMI)**2.*EMIS))
AKP=EXP((-1.76+.0129*AKS/DELTA(T))/434)
H=HC+300.
DO K=1,50
  HR=AKR*(2.*AKS+H*D_P)/(D_P*AKS)
  HP=AKP*(2.*AKS+H*D_P)/(D_P*AKS)
  HI=HC+HR+HP
  IF((ABS(H(1)-H/I).LE.0.01) GO TO 60
H=HI
ENDDO
60
AK(1)=DELTA(T)*(AKC+CI*RO*E(T)/DELTA(T)+AKR)+
  (I.-DELTA(T))*OI*AK$/(2.*AKS+H*D_P)
END DO
AKAV=AK(3)
OK=AK(1)/AKO)
WK=AK(NIR)/AKO)
C CALC OF ES, AKST, DER, D KR
C
AKM=(.5-.15*OK**2-WK'(RI**3-2.*R1+I.)/(6.*I-R1))*/CCC
DO I=1,NIJ
IF(RP(1).GE.RI)THEN
  ES(I)=EI*(I.-RP(1))I(I.-R1)
  AKST(I)=AKM-(AKM-WK)*(RP(1)-R1)/(I-R1)
  DER(I)=-EM/(I.-RI)
  DKR(I)=6.*(AKM-OK)*RP(1)*RI**2-6.*(OK-AKM)*RP(1)**2/R1**3
ELSE
  ES(I)=EO+3.*(EM-EO)*(RP(I)/RI)**2+(EO-EM)*2.*(RP(I)/RI)**2
  AKST(I)=OK+3.*(AKM-OK)*(RP(I)/RI)**2+(OK-AKM)*2.*(RP(I)/RI)**2
  DER(I)=6.*(EM-EO)*RP(1)/(RI)**2-6.*(EO-EM)*RP(1)**2/R1**3
END IF
END DO
DO I=1,NIJ
E(I)=ES(I)*EAV
AKT(I)=AKST(I)*AKAV
END DO
RETURN
END

SUBROUTINE CONDU(ITEST,IGAS,PHLD_P,CON_P,RR,U0,RE_N,TEM,EPS,
  EPS_INF,EFF_CON,R,CON_R,EFF_CON,Z,CON_Z,CON_S,NI,NGR,NGR1,NGR2,NN)
IMPLICIT REAL*8(A-H,O-Z)
DATA ALF_BET1,ALF_BET2,PE_N,EPS_W,CO/13.,8.9.,7.,15/
C NITROGEN
C
IF(GAS.EQ.1)THEN
  CON_F=.000358895+3.0026706379E-5*TEM-.52528942E-9*TEM*TEM
  PR_N=.8485-.0003845398*TEM+.27374798E-7*TEM*TEM-
  5.6289861E-11*TEM*TEM*TEM
C AIR
C ELSE IF(GAS.EQ.2)THEN
  CON_F=.0002153778+3.006679595E-5*TEM-.4.8615223803E-9*TEM*TEM-
  PR_N=.822301567-.000315649*TEM+.2.155594425E-7*TEM*TEM-
  4.22896146E-11*TEM*TEM*TEM
C CO2
C ELSE
  CON_F=.00146886721+1.652016966E-5*TEM+.7.3392609982E-9*TEM*TEM-
  PR_N=1.033870689-.000842560218*TEM+.8.33846183E-7*TEM*TEM-
  3.45364137E-10*TEM*TEM*TEM
ENDIF

C IF(TEST.EQ.1) THEN
  CON_0=EPS*(1-EPS)/(PHI+2.*CON_F/CON_P/3.)
  CON_1=ALF_BET1*PR_N*RE_N/eps
  EFF_CON_1=CON_0+CON_1
  EFF_CON_R=EFF_CON_1*CON_F
  CON_R=EFF_CON_R-CON_F*CON_0
  EFF_CON_Z=CON_F*(CON_0+CON_01*ALF_BET2/ALF_BET1)
  CON_S=CON_F*CON_0
ELSE
  EFF_CON_1=EFF_CON_1*(1-EPS_INF)/(PHI+2.*CON_F/CON_P/3.)
  CONST=1./CON_0-1.
  TEXP=EXP(-5.*RR)
  IF(NN.GT.NGR1) THEN
    CON_0=RR*ALF_BET1*PR_N*RE_N/eps
    CON_02=CON_0*(1+CONST*TEXP)
  ELSE
    CON_0=ALF_BET1*PR_N*RE_N/eps
    CON_02=CON_0
  ENDIF
  EFF_CON_1=CON_02*CON_03
  EFF_CON_R=EFF_CON_1*CON_F
  CON_R=EFF_CON_R-CON_F*CON_02
  EFF_CON_Z=CON_F*(CON_02+CON_03*ALF_BET2/ALF_BET1)
  CON_S=CON_F*CON_02
ENDIF

C RETURN

END

C THIS SUBROUTINE COMPUTE THE DIFFUSIVITY IN AXIAL AND RADIAL DIRECTION FOR
C TWO DIM
C
C THIS SUBROUTINE COMPUTE THE DIFFUSIVITY IN AXIAL AND RADIAL DIRECTION FOR
C TWO DIM
C
SUBROUTINE AXIDIFF_R_ZIT(IGAS.PHID_P.DIFF_F.RR.U0.RE_N,SC_N,
  TEM, EPS, EPS_INF, EFF_DIFF_R, EFF_DIFF_Z, ngr1, ngr2, ngr2, ngr2, ngr2)
IMPLICIT REAL*(A-H,O-Z)
DATA ALF_BET1, ALF_BET2, PE_N, EPS_W, CO/1.1.0.10.,7.,15/
C NITROGEN
C
IF(TEST.EQ.1) THEN
  DIFF_0=1-(1.-EPS)**.5
  DIFF_01=ALF_BET1*SC_N*RE_N/EPS
  EFF_DIFF_1=DIFF_0+DIFF_01
  EFF_DIFF_R=EFF_DIFF_1*DIFF_F
  EFF_DIFF_Z=DIFF_F*(DIFF_01+DIFF_F*ALF_BET2/ALF_BET1)
ELSE
  DIFF_0=1-(1.-EPS_INF)**.5
  CONST=1./DIFF_0-1.
  TEXP=EXP(-8.*RR)
IF(NN.GT.NFLR) THEN
  DIFF_02=DIFF_0*(1.+CONST*TEXP)
  DIFF_03=ALF_BET1*SC_N*RE_N
  DIFF_02=DIFF_0*(1.+CONST*TEXP)
ELSE
  DIFF_0=ALF_BET1*SC_N*RE_N
  DIFF_02=DIFF_0
END IF
EFF_DIFF_1=DIFF_01+DIFF_F
EFF_DIFF_Z=DIFF_F*(DIFF_02+DIFF_F*ALF_BET2/ALF_BET1)
END IF
RETURN
C
END
C
C THIS SUBROUTINE COMPUTE THE HEAT TRANSFER COEFFICIENT FOR THE GAS AND WALL
C
SUBROUTINE HEAT_WALL(IGAS,PHIW,D_P,CON_P,RILU0,RE_D,TEM,EPS_W)
IMPLICIT REAL*8(A-I,LO-Z)
DATA ALF_BET1,ALF_BET2,PE N,EPS_W,CO/.13,.8.9...7..15/
C NITROGEN
C
IF(IGAS.EQ.1) THEN
  CON_F=.000358895+3.0036706379E-5*TEM-5.3528942E-9*TEM*TEM
  PR_N=,8485-.0003845398*TEM+2.75374798E-7*TEM*TEM-
  5.62898861E-11*TEM*TEM
C
  ELSE IF(IGAS.EQ.2) THEN
    CON_F=.0002153778+3.0066679595E-5*TEM-4.8615223803E-9*TEM*TEM
    PR_N=.822301567-.000315649*TEM+2.155594425E-7*TEM-
    4.22896146E-11*TEM*TEM
    C
  ELSE
    CON_F=-.001 a6886721
    ÷1.652016966E-5 *TEM+73392509982E-9*TEM*TEM
    PR_N= 1.038870689-.000842560218*TEM+8.3386183E-7*TEM*TEM-
    3.453641637E-10*TEM*TEM
    END IF
C
END IF(IGAS.EQ.2) THEN
  CON_F=.0002153778+3.0066679595E-5*TEM-4.8615223803E-9*TEM*TEM
  PR_N=822301567-.000315649*TEM+2.155594425E-7*TEM*TEM-
  4.22896146E-11*TEM*TEM
C
END IF(IGAS.EQ.2) THEN
  CON_F=.0002153778+3.0066679595E-5*TEM-4.8615223803E-9*TEM*TEM
  PR_N=822301567-.000315649*TEM+2.155594425E-7*TEM*TEM-
  4.22896146E-11*TEM*TEM
C
ELSE
  CON_F=-.001 a6886721
    ÷1.652016966E-5 *TEM+73392509982E-9*TEM*TEM
    PR_N= 1.038870689-.000842560218*TEM+8.3386183E-7*TEM*TEM-
    3.453641637E-10*TEM*TEM
END IF
CON_0=EPS+(1.-EPS)/(PHIW+2.*CON_F/CON_P/3.)
CON_01=ALF_BET1*PR_N*RE_D
EFF_CON_1=CON_0+CON_01
CON_W1=EPS+W+(1.-EPS_W)/(PHIW+2.*CON_F/CON_P/3.)
H_W0=CO*PR_N**1.5*RE_D**(3./4)*CON_F/D_P
CON_W2=CON_W1+1/(1.2*PR_N*RE_D)+1./(H_W0*PR_N*D_P/2./CON_F))
H_W1=1./CON_W2-1/EFF_CON_1
H_W=1./CON_F/D_P/2./H_W1
RETURN

E-64
This subroutine computes a constant for calculation of thermal conductivity

SUBROUTINE PHI_COND(IGAS, TEM, CON_P, EPS, PHI, PHI_W)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 XI(I_I), YI(I_I), Z(I_I), YZ(I_I), XINT
DATA XI/20000., 4000., 1000., 200., 80., 6., 2., 0.7, 0.01/
DATA YI/0.04, 0.05, 0.06, 0.08, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0/
DATA XI/20000., 400., 200., 40., 80., 2., 0.8, 0.4, 0.2, 0.1/
DATA YI/0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 0.12/
DATA XI/10000., 20000., 4000., 2000., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.0/
DATA YI/0.06, 0.08, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0/
C NITROGEN
IF(IGAS.EQ.1) THEN
CON_F=.000358895+3.0026706379E-5*TEM-5.3528942E-9*TEM**2
C AIR
ELSE IF(IGAS.EQ.2) THEN
CON_F=.0002153778+3.0066679595E-5*TEM-4.8615223803E-9*TEM**2
C CO2
ELSE
CON_F=.0014688672+1.652016966E-5*TEM+7.3392609982E-9*TEM**2
END IF
N=I_I
XMAX1=CON_P/CON_F
ITEST1=0
ITEST2=0
ITEST3=0
DO I=I,N
IF(XI(I).LT.XMAX1 .AND. ITEST1.EQ.0) THEN
SLOPE=(YI(I-1)-YI(I))/(XI(I-1)-XI(I))
PHI1=SLOPE*(XMAX1-XI(I-1))+YI(I-1)
ITEST1=1
END IF
IF(XI(I).LT.XMAX1 .AND. ITEST2.EQ.0) THEN
SLOPE=(YI(I-1)-YI(I))/(XI(I-1)-XI(I))
PHI2=SLOPE*(XMAX1-XI(I-1))+YI(I-1)
ITEST2=1
END IF
IF(XI(I).LT.XMAX1 .AND. ITEST3.EQ.0) THEN
SLOPE=(YI(I-1)-YI(I))/(XI(I-1)-XI(I))
PHI3=SLOPE*(XMAX1-XI(I-1))+YI(I-1)
ITEST3=1
END IF
IF(ITEST1.EQ.1 .AND. ITEST2.EQ.1 .AND. ITEST3.EQ.1) GO TO 20
END DO
20 IF(EPS.LT.0.26) THEN
PHI=PHI2
ELSE IF(EPS.GT.0.476) THEN
PHI=PHI1
ELSE
PHI=PHI2+(PHI1-PHI2)*(EPS-.26)/.216
END IF
RETURN
END
SUBROUTINE TO CALCULATE THE POROSITY VARIATION

SUBROUTINE COEF2(Y1,VOID_B,D_P,C1,POR)
IMPLICIT REAL*8(A-H,O-Z)
C2=6.0
POR=VOID_B*(1+C1*EXP(-C2*Y1/D_P))
RETURN
END

SUBROUTINE COEF1(E,EPL,Y,C)
IMPLICIT REAL*8(A-H,O-Z)
CB=2
C$1=-.16329931237*Y*EPL/(1-EPL)
CB=3
C$1=-.244048968*Y*EPL/(1-EPL)
CB=4
C$1=-.326598632*Y*EPL/(1-EPL)
CB=5
C$1=-.4082482808*Y*EPL/(1-EPL)
CB=6
C$1=-.48987937*Y*EPL/(1-EPL)
CB=8
C$1=-.653197264*Y*EPL/(1-EPL)
E=EPL*(1.+1.4*EXP(S1))
E=EPL*(1.+C*EXP(S1))
RETURN
END

THE SUBROUTINE IS BEING CALLED BY DIFFEQ1 WHICH IS ALSO BEING CALLED BY
SUBROUTINE FUNCT TO COMPUTE THE VELOCITY AND THE PRESSURE DROP IN THE BED.
THE EQUATIONS ARE BEING SOLVED BY NEWMAN'S METHOD.

SUBROUTINE FUNCT2(I)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 D_L(2),M_AVE
COMMON/OLD/AA(14),SUM(14),COLD(14,201)
COMMON/BND/AA(14),B(14,201),C(14,201),D(14,29),X(14,14),
Y(14,14),G(14),P(14,201)
COMMON/BND2/N,N2,NJ,TPRT,JTCNT
COMMON/PR_OLD_Z/CON_Z(201,101),CON_R(201,101),CON_S(201,101),
H_W(201,101),CP_P(201,101),H_FP(201,101),Q(4,201,101),
VISC_P(201,101),D_LPP(4,201),RATE_C1(201,101),
COMMON/PR_OLD_Z/CP_S,RO_S,INT,R_P,D_P,CON_S
COMMON/PROP_S,Z/CP_S,RO_S,INT,R_P,D_P,CON_S
COMMON/PROP_D_Z/DELZ,DEL,TIME,DEL1,DELZ,INT,NC,NJR,NP
DATA L1,L4,L5,L6,R1,CONV/4.1,1.2,3.555,0.51.714752314/
DATA FAC,GC,M_AVE/2.78450526316,416975040.0,28.0/

THE FIRST ROW

ALFE=(1-ESEXY/ESEX
RATE_C=RATE_C1(J,1)
VISC_F=VISC_P(J,1)
DO M1=1,NC
D_L(M1)=D_LPP(M1,J)
END DO
KK=0
D_L_AVE=0
DO M1=1,NC
IF(D_L(M1).GT.0.0 THEN

E-66
D_L_AVE=D_L_AVE+D_L(M1)
Kx=KK+1
ENDIF
END DO
RO_F=(C(L5,J)/(C(L1,J)*R1))
IF(J.EQ.1)THEN
  c equation for velocity
  F(L4)=FAC*(C(L5,J)-BC_L5*CONV)/DELZ+1./GC*(RO_F*M_AVE*C(L4,J)*
  .(C(L4,J)-(C(L4,J-1))/DELZ+150*(1-EPSEX)**2*VISC_F*C(L4,J)/
  .D_P/D_P*EPSEX/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
  .D_P*EPSEX-RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELT)
  c equation for pressure not considering the pressure drop due to temperature
  c change, dynamic pressure
  F(L5)=(C(L5,J)-P(L5,J))/DELZ-D_L_AVE/DELZ**2*(BC_L5*CONV-
  .2*C(L5,J)-(C(L5,J)+1))/DELZ+(C(L4,J)-BC_L5*CONV)/DELZ+
  .C(L5,J)/(C(L4,J)-BC_L4)/DELZ+R1*C(L1,J)*ALF*RATE_C
  c total pressure
  F(L6)=(C(L6,J)-P(L6,J))/DELZ-D_L_AVE/DELZ**2*(C(L5,J-1)-
  .2*C(L6,J)+(C(L6,J)-1))/DELZ+(C(L4,J)-(C(L6,J)-1))/DELZ+
  .C(L5,J)-(C(L6,J)-C(L4,J-1))/DELZ+R1*C(L1,J)*ALF*RATE_C
  c equation for velocity
  ELSE IF(J.EQ.NJ)THEN
  F(L4)=FAC*(C(L5,J)-(C(L5,J-1))/DELZ+1./GC*(RO_F*M_AVE*C(L4,J)*
  .(C(L4,J)-(C(L4,J-1))/DELZ+150*(1-EPSEX)**2*VISC_F*C(L4,J)/
  .D_P/D_P*EPSEX/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
  .D_P*EPSEX-RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELT)
  c equation for pressure not considering the pressure drop due to temperature
  c change, dynamic pressure
  F(L5)=(C(L5,J)-P(L5,J))/DELZ-D_L_AVE/DELZ**2*(C(L5,J-1)-
  .2*C(L5,J)-(C(L5,J)+1))/DELZ+(C(L4,J)-(C(L5,J)-1))/DELZ+
  .C(L5,J)/(C(L4,J)-C(L5,J-1))/DELZ+R1*C(L1,J)*ALF*RATE_C
  c total pressure
  F(L6)=(C(L6,J)-P(L6,J))/DELZ-D_L_AVE/DELZ**2*(C(L5,J-1)-
  .2*C(L6,J)-(C(L6,J)-1))/DELZ+(C(L4,J)-(C(L6,J)-1))/DELZ+
  .C(L5,J)-(C(L6,J)-C(L4,J-1))/DELZ+R1*C(L1,J)*ALF*RATE_C
  c the last grid
  C
  C---------------------------------------------------------------------------
  C the last grid
  C
  C---------------------------------------------------------------------------
  C
  C equation for velocity
  c grids inside the column
  ELSE
  F(L4)=FAC*(C(L5,J)-(C(L5,J-1))/DELZ+1./GC*(RO_F*M_AVE*C(L4,J)*
  .(C(L4,J)-(C(L4,J-1))/DELZ+150*(1-EPSEX)**2*VISC_F*C(L4,J)/
  .D_P/D_P*EPSEX/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
  .D_P*EPSEX+RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELT)
  c equation for pressure not considering the pressure drop due to temperature
  c change, dynamic pressure
  F(L5)=(C(L5,J)-P(L5,J))/DELZ-D_L_AVE/DELZ**2*(C(L5,J-1)-
  .2*C(L5,J)-(C(L5,J)+1))/DELZ+(C(L4,J)-(C(L5,J)-1))/DELZ+
  .C(L5,J)/(C(L4,J)-C(L5,J-1))/DELZ+R1*C(L1,J)*ALF*RATE_C
  c total pressure
  F(L6)=(C(L6,J)-P(L6,J))/DELZ-D_L_AVE/DELZ**2*(C(L5,J-1)-
  .2*C(L6,J)-(C(L6,J)-1))/DELZ+(C(L4,J)-(C(L6,J)-1))/DELZ+
  .C(L5,J)-(C(L6,J)-C(L4,J-1))/DELZ+R1*C(L1,J)*ALF*RATE_C
  c total pressure
C(L4,J)'(C(L4,J)-C(L4,J-1))/(2*DELZ))+R I*C(L4,J)*ALF'*RATE_C
ENDIF
210 RETURN
END
C
C
C this subroutine is being called by diffeq1 which is also being called by
C funct subroutine. it compute the velocity profile in the radial direction
C it uses the Newman method.
SUBROUTINE FUNCT3(J)
IMPLICIT REAL*8(A-H,O-Z)
RKAL'8
DR(200kEPS(200)_C_K1(200)_C_K2(200)
COMMON/U/G/U_GUESS,EPS
COMMON/OLD/AA(14),SUM(14),COLD(14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),G(14),F(14),P(14,201)
COMMON/BND2/N,NJ2,NJ/TPRT,ITCNT
COMMON/PROP_Z/ZCP_S,RO_.AINT,R_P,D_P,CON_S1
COMMON/PROP_B_Z/REC VOID B_D_I
COMMON/PROP_D_Z/DDEL,TIME,DEL,T1,DEL12,EL,NC,NJR,NP
C
IF(J.EQ.1 .AND. M1.EQ.0) THEN
c radial fraction of constant velocity
FRACI=.93
FRAC2=.07
C
K1=21
K2=99
C
dimensionless constant
FAC=(1-VOID_B)/VOID_B*12.247449
C
dimensionless radial size
DELR11=FRAC1*D_12/D_P*FAC/(K1-1)
DELR22=FRAC2*D_12/D_P*FAC/(K2)
EC=1./VOID_B-1.
EC=1.4
C
c compute the porosity variation
DO I=1,NP-1
R=(DELR22*(K2)+DELR11*(K1-I))
IF(I.LT. K1) THEN
R=DELR22*(NP-I)
ENDIF
CALL COEFI(POR, VOID_B, R, F,C)
C_K1(I)=D_P*D_P*EPS(I)*EPS(I)/150./(1-EPS(I))
C_K2(I)=1.75*(1-EPS(I))/D_P/EPS(I)/EPS(I)
END DO
C
c calculate the constant coefficient in PDE's
C_K1(I)=C_K1(I)
C_K22=C_K2(I)
BETA=C_K11/D_P/D_P
EPS(NP)=EPS(I)*(1+1.4)
DELR11=DELR11/FAC
DELR22=DELR22/FAC
FR=DELR22/DELR11
F01=FR/(1+FR)
P11=(1-FR)/FR
P21=1./((1-+FR)*FR)
F02=1./F01
F12=1./FR
C
F22 = I/((1 + FR)^*FR)
M1 = 1
END IF

c computed the radius from the center to the grid
IF(J.LE.K1 .AND. J.NE.1) THEN
  DELR = DELR11
  RP = (J-1)*DELR
  RP = 1/RP
ELSE IF(J.GT.K1) THEN
  DELR = DELR22
  RP = (K1-1)*DELR11+(J-K1)*DELR22
  RP = 1/RP
END IF

c computed the velocity equation for the center grid
IF(J.EQ.1) THEN
  F(1) = U_GUESS - C(1,J)
ELSE IF(J.EQ.NJ) THEN
  F(1) = 0 - C(1,J)
ELSE
  c computed the velocity for grids in radial directions
  IF(J.NE.K1) THEN
    P1 = 1 - C_K1/C_K1(J)*C(1,J)
    P2 = C_K2(J)/C_K22*REC*C(1,J)*C(1,J)
    P3 = RP*(C(1,J+1)-C(1,J-1))/(2*DELR)
    P4 = (C(1,J+1)-2*C(1,J)+C(1,J-1))/DELR/DELR
    F(1) = P1 + P2 + BETA/EPS(J)*(P3 + P4)
  ELSE
    P1 = 1 - C_K1/C_K1(J)*C(1,J)
    P2 = C_K2(J)/C_K22*REC*C(1,J)*C(1,J)
    P3 = RP*(P2*(C(1,J+1)-F11*C(1,J)-F01*C(1,J-1))/DELR)
    P4 = 2*(P22*C(1,J+1)-F12*C(1,J)+F02*C(1,J-1))/DELR/DELR
    F(1) = P1 + P2 + BETA/EPS(J)*(P3 + P4)
  END IF
END IF
210 RETURN
END

This subroutine is the main routine for Newman method for solution of PDEs.

C Generalized calling program for Band(j) to solve differential equations taking partial derivatives numerically

C Called by: Main calling program

C Subroutines called:
  WRITOUT (for data output)
  BAND (to solve banded tridiagonal coefficient matrix)
  FUNCT (to obtain value for function for a given value for a variable)

C List of important variables:
A coefficient described in Newman, Appendix C

AA first, AA is F(WORKC*CU). Later AA is the
value of the derivative df/dc used in Newton's
method

B coefficient described in Newman, Appendix C

C variables to be solved for

CD multiplication factor used in obtaining
numerical derivatives

COLD value of C from previous iteration

CU 2.0 - CD

D D coefficient described in Newman, Appendix C

ERR convergence criterion

F value of function f(C), calculated in FUNCT

G residual of f(C) calculated with updated C value

I index used for equation number

ITCNT index for iteration number

ITPRT flag used for determining whether intermediate
calculations are output; for ITPRT=0, only
converged results are output; for
ITPRT=1, results of each iteration are printed.

J index for node number

K index for equation number

M index used in working through nodes used to
calculate numerical derivatives

MM used to determine starting node (in relation to
J) for estimation of numerical derivatives

N number of equations (no. of variables)

NJ number of node points

SAVEC saved value of C

SUM intermediate value used in calculating G

TINIER criterion used to avoid working with small numbers

TINY criterion used to avoid working with small numbers

TNIEST criterion used to avoid working with small numbers

WORKC saved value of C; modified when C less than Tinier

X X value described in Newman, Appendix C

Y Y value described in Newman, Appendix C

------------------------------------------------------------------------

DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT, AND CHANGE THE SECOND
DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
WHATEVER YOU WANT TO.

SUBROUTINE DIFFEQ1(C1,P1,N1,NP2,IND,ITPRT)

IMPLICIT REAL*8(A-H,O-Z)

REAL*8 C1(14,201),P1(14,201)

COMMON/OLD/AA(14),SUM(14),COLD(14,201)

COMMON/OLD2/N,NJ2,JNJ,ITPRT,ITCNT

DATA TINY,TINIER,TNIEST,ERR/1.0D-10,1.0D-15,1.0D-15,1.0D-4/

DATA CU,CD/1.0001,.9999/

ITCNT INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT

IF ITPRT=1.

ITPRT=0

L1=N

L2=NJ

L3=NJ2

NJ2=NP2

N=N1
NJ=NP2
IF (ITPRT.GT.0) CALL WRTOUT2
IF(INR.EQ.1) THEN
  DO I1=1,N1
  DO I2=1,NP2
    CI1(I2) = CI1(I1,I2)
    Pi1(I2) = Pi1(I1,I2)
  END DO
  END DO
ELSE IF(INR.EQ.2) THEN
  DO I1=1,N1+1
  DO I2=1,NP2
    CI1(I2) = CI1(I1,I2)
  END DO
ELSE IF(INR.EQ.3) THEN
  DO I1=1,N1
  DO I2=1,NP2
    CI1(I2) = CI1(I1,I2)
    Pi1(I2) = Pi1(I1,I2)
  END DO
ENDIF

C LOOP BEGUN FOR ITERATIONS
C
DO ITCNT=I,ITRAT
C
C COLD ARRAY SET UP
DO K=1,N
  DO J=1,NJ
    COLD(K,J) = C(K,J)
  END DO
END DO
C
C LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
C PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F(I).
C
DO J=1,NJ
  IF(INR.EQ.1) THEN
    CALL FUNCT0(I)
  ELSE IF (IND.EQ.2) THEN
    CALL FUNCT1(I)
  ELSE IF (IND.EQ.3) THEN
    CALL FUNCT2(I)
  END IF
  DO I=1,N
    SUM(D,I) = 0.0
    G(I) = -F(I)
  END DO
C
C THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
C TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
C (IN RELATION TO J).
C
C IF (J.EQ.1) THEN
  MM = 0
ELSE IF (J.LT.NJ) THEN
  MM = 1
ELSE
  MM = 2
ENDIF
DO M=MM,MM+2
DO K=1,N
    SAVEC=C(K,J+M)
    WORKC=SAVEC

DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)

    IF (ABS(WORKC).LT.TINY) THEN
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        DO I=1,N
            AA(I)=-F(I)
        END DO
        C(K,J+M)=1.1*WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        DO I=1,N
            AA(I)=AA(I)+4.0*F(I)
        END DO
        C(K,J+M)=WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        DO I=1,N
            AA(I)=AA(I)+4.0*F(I)
        END DO
        C(K,J+M)=1.2*WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        END IF
        DO I=1,N
            AA(I)=AA(I)+4.0*F(I)
        END DO
    END IF
    ELSE
        C(K,J+M)=WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        END IF
        DO I=1,N
            AA(I)=AA(I)+4.0*F(I)
        END DO
    END IF

DERIVATIVES CALCULATED FOR LARGER VALUES OF C (GREATER THAN TINY)

    ELSE
        C(K,J+M)=WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        END IF
        DO I=1,N
            AA(I)=F(I)
        END DO
        C(K,J+M)=WORKC
        IF(IND.EQ.1)THEN
            CALL FUNCT1(J)
        ELSE IF(IND.EQ.2)THEN
            CALL FUNCT2(J)
        ELSE IF(IND.EQ.3)THEN
            CALL FUNCT3(J)
        END IF
        END IF
        DO I=1,N
            AA(I)=F(I)
        END DO
    END IF

E-72
ELSE IF (IND.EQ.3) THEN
    CALL FUNCT3(J)
ENDIF
DO I=1,N
    AA(I)=(AA(I)-F(I))/((CU-CD)*WORKC)
END DO
ENDIF
C
VALUES FOR A,B,D,X AND Y GIVEN. SUM IS ALSO INCREMENTED
C
DO I=1,N
    SUM(I)=SUM(I)+AA(I)*C(KJ+M)
    IF (M.EQ.-2) Y(ILK)=AA(I)
    IF (M.EQ.-1) A(ILK)=AA(I)
    IF (M.EQ.0) B(ILK)=AA(I)
    IF (M.EQ.1) D(ILK)=AA(I)
    IF (M.EQ.2) X(ILK)=AA(I)
END DO
END DO
END DO
DO I=1,N
    GO=OO>,SUMO)
END DO
C
BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(J)
END DO
C
CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO K=1,N
    DO J=1,NJ
        IF (DABS(C(KJ)).GT.TNIEST) THEN
            IF (DABS((C(KJ)-COLD(KJ))/C(KJ)).GT.ERR) GO TO 70
        ENDIF
    END DO
END DO
GO TO 80
70 IF (ITPRG .GT. 1) CALL WRTOUT2
END DO
80 CONTINUE
DO I1=1,N
    DO I2=1,NJ
        C1(I1,I2)=C(I1,I2)
    END DO
END DO
N=L1
NJ=L2
NJ2=L3
RETURN
END

C
This subroutine is the main routine for Newman method for solution of PDE's.
C
******************************************************************************
C GENERALIZED CALLING PROGRAM FOR BAND(J) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY
C
C
E-73
CALLED BY: MAIN CALLING PROGRAM

SUBROUTINES CALLED:
  WRTOUT (FOR DATA OUTPUT)
  BAND (TO SOLVE BANDED TRIDIAGONAL COEFFICIENT MATRIX)
  FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
         FOR A VARIABLE)

LIST OF IMPORTANT VARIABLES:

A  A coefficient described in Newman, Appendix C
AA first, AA is F(WORKC*CU). Later AA is the
    value of the derivative d/dc used in Newton’s
    method
B  B coefficient described in Newman, Appendix C
C  variables to be solved for
CD multiplication factor used in obtaining
    numerical derivatives
COLD value of C from previous iteration
CU 2.0 - CD
D  D coefficient described in Newman, Appendix C
ERR convergence criterion
F value of function f(C), calculated in FUNCT
G residual of f(C) calculated with updated C value
I  index used for equation number
ITCNT index for iteration number
ITPRT flag used for determining whether intermediate
    calculations are output; for ITPRT=0, only
    converged results are output; for
    ITPRT=1, results of each iteration are printed.
J  index for node number
K  index for equation number
M  index used in working through nodes used to
    calculate numerical derivatives
MM used to determine starting node (in relation to
    J) for estimation of numerical derivatives
N  number of equations (no. of variables)
NJ number of node points
SAVEC saved value of C
SUM intermediate value used in calculating G
TINIER criterion used to avoid working with small numbers
TINY criterion used to avoid working with small numbers
TNIES criterion used to avoid working with small numbers
WORKC saved value of C; modified when C less than Tinier
X  X value described in Newman, Appendix C
Y  Y value described in Newman, Appendix C

DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT, AND CHANGE THE SECOND
DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
WHATEVER YOU WANT TO.

SUBROUTINE DIFFEQ2(C1,P1,N1MP2,INDXI'CNT0)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 C1(14,201),P1(14,201)
COMMON/OLD/AA(14),SUM(14),COLD(14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
      .Y(14,14),G(14),F(14),P(14,201)

E-74
COMMON/BND2/N,J1,J2,ITPRT,ITCNT
COMMON/NCy/NC1
DATA TINY,TINIER,TINIEST,ERR/1.0D-10,1.0D-15,1.0D-15,1.0D-4/
DATA CU,CD/1.0001..9999/

ITCNT INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT
IF ITPRT=1.

ITPRT=0
ITCNT=0
L1=N
L2=NJ
L3=NTJ
NJ2=NP2
N=N1
NJ=NP2
IF (ITPRT.GT.0) CALL WRTOUT2
IF(IND.EQ.1) THEN
  DO II=1,N1+3
  DO 12=1,NP2
     C(II,12)=C1(II,12)
     P(II,12)=P1(II,12)
  END DO
  END DO
ELSE IF(IND.EQ.2) THEN
  DO II=1,N1
  DO 12=1,NP2
     C(II,12)=C1(II,12)
     P(II,12)=P1(II,12)
  END DO
  END DO
ENDIF

LOOP BEGUN FOR ITERATIONS
DO ITCNT=1,ITCNT0
COLD ARRAY SET UP
DO K=1,N
  DO J=1,NJ
     COLD(K,J)=C(K,J)
  END DO
END DO

LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F(I).
DO J=1,NJ
CALL FUNCT4(J)
DO I=1,N
  SUM(I)=0.0
  GI=-F(I)
END DO

THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
(IN RELATION TO J).
IF (J.EQ.1) THEN
  MM=0
ELSE IF (J.LT.NJ) THEN
  MM=-1
ELSE
MM=-2
ENDIF
DO M=MM,MM+2
C
C ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC
C
DO K=1,N
SAVEC=C(K,J+M)
WORKC=SAVEC
C
C DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)
C
IF (ABS(WORKC).LT.TINY) THEN
  IF(ABS(WORKC).LT.TINY) WORKC=SIGN(TINY,WORKC)
  C(K,J+M)=1.2*WORKC
  CALL FUNCT4(I)
  DO I=1,N
    AA(I)=-F(I)
  END DO
  C(K,J+M)=1.1*WORKC
  CALL FUNCT4(I)
  DO I=1,N
    AA(I)=AA(I)+4.*F(I)
  END DO
  C(K,J+M)=WORKC
  CALL FUNCT4(I)
  DO I=1,N
    AA(I)=(AA(I)-3.*F(I))/(0.2*WORKC)
  END DO
C
C DERIVATIVES CALCULATED FOR LARGER VALUES OF C (GREATER THAN TINY)
C
ELSE
  C(K,J+M)=WORKC*C
  CALL FUNCT4(I)
  DO I=1,N
    AA(I)=-F(I)
  END DO
  C(K,J+M)=WORKC*C
  CALL FUNCT4(I)
  DO I=1,N
    AA(I)=(AA(I)-F(I))/((C0-C)*WORKC)
  END DO
ENDIF
C
C VALUES FOR A,B,D,X AND Y GIVEN. SUM IS ALSO INCREMENTS
C
DO I=1,N
  SUM(I)=SUM(I)+AA(I)*C(K,J+M)
  IF (M.EQ.-2) Y(LK)=AA(I)
  IF (M.EQ.-1) A(LK)=AA(I)
  IF (M.EQ.0) B(LK)=AA(I)
  IF (M.EQ.1) D(LK)=AA(I)
  IF (M.EQ.2) X(LK)=AA(I)
END DO
END DO
END DO
DO I=1,N
  G(I)=G(I)+SUM(I)
END DO
C
C BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(J)
END DO

C
C CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO K=1,N
DO I=1,NJ
IF(DABS(C(KJ)).GT.TNIEST) THEN
IF(DABS((C(KJ)-COLD(KJ))/C(KJ)).GT.ERR) GO TO 70
ENDIF
END DO
END DO
GO TO 80
70 IF(ITPRT.GT.0) CALL WRTOUT2
END DO
80 CONTINUE
DO I=1,N
DO I2=1,PJ
C1(I1,I2)=C(I1,I2)
END DO
END DO
N=1L
NJ2=1L
RETURN
END

SUBROUTINE WRTOUT2

IMPLICIT REAL*8(A-H.O-Z)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
.Y(14,14),G(14),F(14),P(14,201)
COMMON/BND2/N,NJ2,NJ,ITPRT,ITCNT
IF (ITCNT.NE.0) WRITE (*,99)ITCNT
WRITE (*,100)
DO K=1,NJ2
WRITE(*,101)K,C(LK),L=1,N)
ENDDO
99 FORMAT(' ITCNT=',J2)
100 FORMAT( ' J ',' C1 C2 C3 '
& ' C4 C5 C6'/)
101 FORMAT(1X,J3,6(1PE16.8))
RETURN
END

C BLOCK TRIDIAGONAL MATRIX SUBROUTINE
SUBROUTINE BAND2(J)
IMPLICIT REAL*8(A-H.O-Z)
DIMENSION E(14,14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
.Y(14,14),G(14),F(14),P(14,201)
COMMON/BND2/N,NJ2,NJ,ITPRT,ITCNT
101 FORMAT(0DEI'ERM=.0 AT J=',J4)
IF (DEI'.ERM.EQ.0) WRITE (*,99)
CALL MATINV2(N,2*N+1,DETERM)
C IF(DETERM.EQ.0) WRITE (2,101) J

E-77
DO K=I,N
E(K,NP1,1)=D(K,2*N+1)
DO L=I,N
E(K,L,1)=D(K,L)
X(K,L)=D(K,L+N)
END DO
END DO
RETURN
ELSE IF(J.EQ.2)THEN
DO I=1,N
DO K=1,N
DO L=1,N
D(LK)=D(LK)+A(LL)*X(L,K)
END DO
END DO
ELSE IF(J.EQ.NJ2) THEN
DO I=1,N
DO L=1,N
G(I)=G(I)-Y(LL)*E(L,NP1,J-2)
DO M=1,N
A(LL)=A(LL)-Y(L,M)*E(M,L,J-2)
END DO
END DO
ENDIF
DO I=1,N
D(LNP1)=G(I)
DO L=1,N
D(LNP1)=D(LNP1)+A(LL)*E(L,NP1,J-1)
DO K=1,N
B(LK)=B(LK)+A(LL)*E(L,K,J-1)
END DO
END DO
CALL MATINV2(N,NP1,DETERM)
C IF(DETERM.EQ.0) WRITE(2,101) J
DO K=1,N
DO M=1,NP1
E(K,M,J)=D(K,M)
END DO
END DO
IF(J.EQ.NJ2)THEN
DO K=1,N
C(K,J)=E(K,NP1,J)
END DO
DO M=NJ2-1,-1,-1
DO K=1,N
C(K,M)=E(K,NP1,M)
DO L=1,N
C(K,M)=C(K,M)+E(K,L,M)*C(L,M+1)
END DO
END DO
END DO
DO L=1,N
DO K=1,N
C(K,1)=C(K,1)+X(K,L)*C(L,3)
END DO
ENDIF
RETURN
END

C MATRIX INVERSION SUBROUTINE

E-78
SUBROUTINE MATINV2(N,M,DETERM)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION ID(14)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29)
DETERM=1.0
DO I=1,N
ID(I)=0
END DO
DO NN=1,N
BMAX=0.0
DO I=1,N
IF(ID(I).EQ.0)THEN
DO J=1,N
IF(ID(J).EQ.0)THEN
IF(DABS(B(I,J)).GT.BMAX) THEN
BMAX=DABS(B(I,J))
IROW=I
JCOL=J
ENDIF
ENDIF
END DO
IF(BMAX.EQ.0.0)THEN
DETERM=0.0
RETURN
ENDIF
ID(JCOL)=1
IF(JCOL.NE.IROW) THEN
DO J=1,N
SAVE=B(IROW,J)
B(IROW,J)=B(JCOL,J)
B(JCOL,J)=SAVE
ENDDO
DO K=1,M
SAVE=D(IROW,K)
D(IROW,K)=D(JCOL,K)
D(JCOL,K)=SAVE
ENDDO
END DO
END DO
DO K=1,M
SAVE=D(IROW,K)
D(IROW,K)=SAVE
END DO
FF = 1.0/B(JCOL,JCOL)
DO J=1,N
B(JCOL,J)=B(JCOL,J)*FF
END DO
DO K=1,M
D(JCOL,K)=D(JCOL,K)*FF
END DO
DO J=1,N
IF(JCOL.NE.JCOL) THEN
IF = B(JCOL)
DO J=1,N
B(LJ) = B(LJ) -FF*B(JCOL,J)
END DO
DO K=1,M
D(LK) = D(LK) -FF*D(JCOL,K)
END DO
ENDIF
END DO
END DO
RETURN
END
SUBROUTINE CUBSPL(X,Y,N,IEND,SUM1)
IMPLICIT REAL*8(A-H-O-Z)
C
C THIS SUBROUTINE COMPUTE THE MATRIX FOR FINDING THE COEFFICIENTS OF A
C CUBIC SPLINE THROUGH A SET OF DATA. THE SYSTEM THEN IS SOLVED THE
C SECOND DERIVITIVE VALUE.
C
C
C X,Y ARRAY OF X AND Y VALUES TO BE FITTED
C S ARRAY OF SECOND DERIVITIVE VALUES AT THE POINTS
C N NUMBER OF POINTS
C IEND TYPE OF END CONDITION TO BE USED
C IEND=1, LINEAR ENDS, S(1)=S(N)=0.
C IEND=2, PARABOLIC ENDS, S(1)=S(2)= S(N)=S(N-1)
C IEND=3, CUBIC ENDS, S(1),S(N) ARE EXTRAPOLATED
C F AUGMENTED MATRIX OF COEFFI AND R.H.S FOR FINDING S
C
C
REAL*4 SUM1
REAL*8 X(N),Y(N),S(101),F(101,4)A(100),B(100),C(100),D(100),
1 DX1, DY1, DX2, DY2, DXN1, DXN2
INTEGER N,IEND,NM1,NM2,NM2,I

C
C COMPUTE FOR THE N-2 ROWES
C
NM2=N-2
NM1=N-1
DX1=X(2)-X(1)
DY1=(Y(2)-Y(1))/DX1*6.0
DO I=1,NM2
DX2=X(I+2)-X(I+1)
DY2=(Y(I+2)-Y(I+1))/DX2*6.0
F(I,1)=DX1
F(I,2)=2.0*(DX1+DX2)
F(I,3)=DX2
F(I,4)=DY2-DY1
DX1=DX2
DY1=DY2
END DO

C
C ADJUST FIRST AND LAST ROWES APPROPRIATE TO END CONDITION.
C
GO TO (20,50,80), IEND
C
C FOR IEND=1, NO CHANGE IS NEEDED
C 20 GO TO 100
C
C FOR IEND=2
C 50 F(1,2)=F(1,2)+X(2)-X(1)
F(NM2,2)=F(NM2,2)+X(N)-X(NM1)
GO TO 100
C
C FOR IEND=3
C 80 DX1=X(2)-X(1)
DX2=X(3)-X(2)

E-80
\[ F(1.2) = \frac{(DX1+DX2)(DX1+2*DX2)}{DX2} \]
\[ F(1.3) = \frac{(DX2*DX2-DX1*DX1)}{DX2} \]
\[ DXN2 = X(N(N1)-X(NM2) \]
\[ DXN1 = X(N)-X(NM1) \]
\[ F(NM2.1) = \frac{(DXN2*DXN2-DXN1*DXN1)}{DXN2} \]
\[ F(NM2.2) = \frac{(DXN1+DXN2)(DXN1+2*DXN2)}{DXN2} \]

GO TO 100

C

100 DO I=2,NM2
   \[ F(1.2) = \frac{F(L2)-F(L1)}{F(1.2)-F(I-1.2)} \]
   \[ F(I.4) = \frac{F(I.4)-F(L1)}{F(I-1.2)-F(I-1.4)} \]
   END DO

BACK SUBSTITUTION

\[ F(NM2.4) = \frac{F(NM2.4)}{F(NM2.2)} \]
DO I=2,NM2
   \[ J = NM1-I \]
   \[ F(I.4) = \frac{F(J.4)-F(J.3)}{F(J.4)-F(J.2)} \]
   END DO

C

NOW PUT THE VALUES INTO THE S VECTORS
DO I=1,NM2
   \[ S(I+1) = F(I,4) \]
   END DO

C

GET S(1) AND S(N)

GO TO (150,160,170),END

C

150 \[ S(1) = 0. \]
   \[ S(N) = 0. \]
   GO TO 200

C

160 \[ S(1) = S(2) \]
   \[ S(N) = S(N-1) \]
   GO TO 200

C

170 \[ S(1) = \frac{(DX1+DX2)*(S(2)-DX1*S(3))}{DX2} \]
   \[ S(N) = \frac{(DXN2+DXN1)*(S(NM1)-DXN1*S(NM2))}{DXN2} \]

C

FIND THE INTEGRATION
C

FIND THE COEFFICIENTS
C

200 CONTINUE
DO I=1,N-1
   \[ A(I) = \frac{(S(I+1)-S(I))}{(6*(X(I+1)-X(I)))} \]
   \[ B(I) = S(I)/2 \]
   \[ C(I) = \frac{(Y(I+1)-Y(I))}{(X(I+1)-X(I))} \]

E-81
\[ \frac{2(X(I+1)-X(I))S(I)+(X(I+1)-X(I))S(I+1))}{6} \]

\[ D(I)=Y(I) \]

\[
\begin{align*}
\text{SUM} &= 0. \\
\text{DO } I=1,N-1 \\
\text{PART1} &= \frac{A(I)}{4}(X(I+1)-X(I))^4 \\
\text{PART2} &= \frac{B(I)}{3}(X(I+1)-X(I))^3 \\
\text{PART3} &= \frac{C(I)}{2}(X(I+1)-X(I))^2 \\
\text{PART4} &= \frac{D(I)}{6}X(I+1)-X(I) \\
\text{SUM} &= \text{SUM} + \text{PART1} + \text{PART2} + \text{PART3} + \text{PART4} \\
\text{ENDDO} \\
\text{SUM1} &= \text{SUM} \\
\text{RETURN} \\
\text{END} \\
\end{align*}
\]

C INTEGRATION BY CUBIC SPLINE

C SUBROUTINE SIMPS(F,N,H,RESULT)

IMPLICIT REAL*8(A-H,O-Z)

C SUBROUTINE SIMPS:

C THIS SUBROUTINE PERFORMS SIMPSON'S RULE INTEGRATION

C OF A FUNCTION DEFINED BY A TABLE OF EQUISPAECED VALUES.

PARAMETERS ARE:

F - ARRAY OF VALUES OF THE FUNCTION

N - NUMBER OF POINTS

H - THE UNIFORM SPACING BETWEEN X VALUES

RESULT - ESTIMATE OF THE INTEGRAL

REAL*8 F(N),H,RESULT

INTEGER N,NPANEL,NHALF,NBEGIN,NEND

CHECK TO SEE IF NUMBER OF PANELS IS EVEN. NUMBER OF PANELS IS N-1.

NPANEL=N-1
NHALF=NPANEL/2.
NBEGIN=1
RESULT=0.
IF(NPANEL.1*NPANEL) .NE. 0) THEN

NUMBER OF PANEL IS ODD. USE 3/8 RULE ON FIRST THREE, 1/3 RULE ON REST.

RESULT=3.0*H/8.*(F(1)+3.*F(2)+3.*F(3)+F(4))
NBEGIN=4
IF(N.EQ.4)RETURN
END IF

APPLY 1/3 RULE- ADD IN FIRST, SECOND AND LAST VALUES.

RESULT=RESULT+H/3.0*(F(NBEGIN)+4.0*F(NBEGIN+1)+F(N))
NBEGIN=NBEGIN+2
IF(NBEGIN.EQ.N)RETURN

THE PATTERN AFTER NBEGIN+2 IS REPEETTIVE. GET NEND, THE PLACE TO STOP

C
REAL*8 FUNCTION TEMPIN(TIME)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES CURRENT INLET TEMPERATURE
C BASED ON THE TIME FOR A TEMPERATURE CHARACTERIZATION
C COMPARISON RUN
IF(TIME.LT.0.2) THEN
    T0 = 74.713
    T1 = 33.11
    T2 = -775.68
    T3 = 5027.2
    T4 = 0.0
    T5 = 0.0
ELSE
    T0 = 25.789
    T1 = 396.87
    T2 = -403.93
    T3 = 251.85
    T4 = -85.612
    T5 = 11.979
ENDIF
X = TIME
TEMPIN = T0+T1*X+T2*X**2.+T3*X**3.+T4*X**4.+T5*X**5.
TEMPIN = TEMPIN+.460.
RETURN
END
APPENDIX F
VACMOL FORTRAN CODE

C RELAXATION METHOD
C
C PROGRAM COND
C DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 201 NODE POINTS; IF
C IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
C IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT, AND CHANGE THE SECOND
C DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
C NODE POINTS ARE DESIRED, CHANGE THE 201 IN THE DIMENSION STATEMENTS TO
C WHATEVER YOU WANT.
C
IMPLICIT REAL*8(A-H,O-Z)
REAL*4 PL(11,201),QP(14,201),PL_TIME,T_TIME
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),Q(14),X,NU,TPRT,ITCNT,F(14),P(14,201),Z,U_Fi
COMMON/PROP_D/D,DELZ1,DELT1,DELZ,NC,II,LL,ITEST1,K_F
COMMON/INDIC/L1,L2,L3,L4,L5,L6
COMMON/PR_OLD,Z/VISC_P(201),RO_P(201),CP_P(201),CON_FPP(201),
CON_LPP(201),D_LPP(4,201),H_FP(201),H_TTP(201),H_IIP(201),
H_OWPP(201),H_FWPP(201),Q(4,201),RATE_C1(201),AMOL_W(201)
COMMON/Q_SOURCE/DELH
COMMON/BC_PRE/BC_L55,TIM
DATA DELH0/270.0/
OPEN (50,FILE='ASCII.DAT',STATUS='NEW',RECL=32766)
OPEN (66,FILE='CON_CO2.DAT',STATUS='NEW')
OPEN (88,FILE='CON_H20.DAT',STATUS='NEW')
OPEN (99,FILE='RE.M.DAT',STATUS='NEW')
C WRITE HEADER DATA TO ASCII FILE
WRITE(50,42)
C
CALL INITIAL_Z
ICOT=1
T_TIME=0
DO 301 LL=1,20000
IF(CLL.LT.(400.+460.))THEN
DELH=DELH0
ELSE
DELH=0.
ENDIF
CALL DIFEQ
ITEST1=0
T,time=T_TIME+DEL*Z/U_F1*60.
TIME=T_TIME
IF(LL.EQ.200)THEN
DELT=DELT1*2
DEL=DEL*T2
ENDIF
IF(LL.EQ.400)THEN
DELT=DELT1*2
DEL=DEL*T2
ENDIF
IF(LL.EQ.600)THEN
DELT=DELT1*2
DEL=DEL*T2
ENDIF
IF(LL.EQ.800)THEN
DELT=DELT1*2
DEL=DEL*T2
ENDIF
END IF
IF(LL.EQ.1000)THEN
  DELT=.0001
  DELT=U_F1*DELT1/Z
END IF
DO 74 M2=1,NJ
  QP(1,M2)=C(1,M2)*C(L5,M2)
  QP(2,M2)=C(2,M2)*C(L5,M2)
  QP(3,M2)=C(L1,M2)-460.
  QP(4,M2)=C(L2,M2)-460.
  QP(5,M2)=C(L3,M2)-460.
  QP(6,M2)=C(L4,M2)
  QP(7,M2)=C(L5,M2)
  QP(8,M2)=C(3,M2)
  QP(9,M2)=C(4,M2)
CONTINUE
WRITE(*,*)LL,LL,LL,TIME
WRITE(*,*)QP(1,1),QP(1,2),QP(1,3),QP(1,4),QP(1,126),QP(1,168)
WRITE(*,*)QP(2,1),QP(2,2),QP(2,3),QP(2,4),QP(2,126),QP(2,168)
WRITE(*,*)QP(3,1),QP(3,2),QP(3,3),QP(3,4),QP(3,126),QP(3,168)
WRITE(*,*)QP(4,1),QP(4,2),QP(4,3),QP(4,4),QP(4,126),QP(4,168)
WRITE(*,*)QP(5,1),QP(5,2),QP(5,3),QP(5,4),QP(5,126),QP(5,168)
WRITE(*,*)QP(6,1),QP(6,2),QP(6,3),QP(6,4),QP(6,126),QP(6,168)
WRITE(*,*)QP(7,1),QP(7,2),QP(7,3),QP(7,4),QP(7,126),QP(7,168)
WRITE(*,*)QP(8,1),QP(8,2),QP(8,3),QP(8,4),QP(8,126),QP(8,168)
WRITE(*,*)QP(9,1),QP(9,2),QP(9,3),QP(9,4),QP(9,126),QP(9,168)
DO 520 I=1,151
  PL(1,J)=QP(1,J)
  PL(2,J)=QP(2,J)
  PL(3,J)=QP(3,J)
  PL(4,J)=QP(4,J)
  PL(5,J)=QP(5,J)
  PL(6,J)=QP(6,J)
520
PL(5,1)=QP(7,1)
PL_TIME=T
print*, pl_time
IF((LL/ISAMP)*ISAMP.EQ.LL) THEN
WRITE(50,43)PL_TIME,PL(1,1),PL(1,2),PL(1,3),PL(1,4),PL(1,126),PL(1,168)
& PL(2,1),PL(2,2),PL(2,3),PL(2,4),PL(2,126),PL(2,168)
& PL(3,1),PL(3,2),PL(3,3),PL(3,4),PL(3,126),PL(3,168)
& PL(4,1),PL(4,2),PL(4,3),PL(4,4),PL(4,126),PL(4,168)
& PL(5,1),PL(5,2),PL(5,3),PL(5,4),PL(5,126),PL(5,168)
ENDIF
DO 78 I1=1,N
  DO 78 I2=1,NJ
    P(I1,I2)=C(I1,I2)
78
CONTINUE
200
CONTINUE
301
FORMAT(1X,TIME,ppCO2@1,ppCO2@2,ppCO2@3,ppCO2@4,ppCO2@5,
& ppH2O@1,ppH2O@2,ppH2O@3,ppH2O@4,ppH2O@5,
& T gas@1,T gas@2,T gas@3,T gas@4,T gas@5,
& T bed@1,T bed@2,T bed@3,T bed@4,T bed@5,
& Twall@1,Twall@2,Twall@3,Twall@4,Twall@5)
43 FORMAT(1X,26(E15.5,'.'))
44 FORMAT(5X,5(E15.5X))
45 FORMAT(5X,5(E15.5X))
46 FORMAT(5X,5(E15.3X))
STOP
END
C
C
SUBROUTINE INITIAL_Z
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4),M_AVE,M_W(4),C_FO(4),IN_L1,IN_L2,IN_L3,IN_L4,
• Y(14,14),G(14),N,N'TPRT,1TCNT,F(I4),P(I4D.01),Z, U F1
COMMON/PROP_B_Z/D_LD_E,S_B ,CON_WA,
• CON_W'I Q,CON_WI_K.
• CP_WA,CP_WI_Q,CP_WI_K,RO_WA,RO_WI_Q,RO_WI_K,KX_WA.X_WI_Q,
• X_WI_KD_LMD_LMA
COMMON/PROP_S_Z/CP_S,RO_S,AINT,R_P,D_P,CON_S,HEAT(MW)
COMMON/D_Z/DDEL1,DELT1,DELT,DELZ,NC,ILLITEST1,K_F
COMMON/BOUN_CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC.C(4),TO
COMMON/PR_OLD_Z/VISC_P(201)
COMMON/INDXC/LI a.2,k3,L,t,12,L6
COMMON/NCY/NCI
COMMON/GAS/INERT,NCOMP
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA
DATA INERT,NCOMP/1,3/
C
C INITIALIZATON

C DATA Z,D_ID_E_S,B_CON WA,CON WI_Q,CON WI_K,CP_WA.
• CP_WI_Q,CP_WI_K,RO_WA,RO_WI_Q,RO_WI_K,KX_WA,X_WI_Q,X_WI_K
• /1.4,0.5412D0,0.5620DO,0.46D0,32.875D0,
• .29DD.D0,109848D0..21D0..21D0,489.00D0.35D0,16.0D0,
• 5.41666667D-3,4.1666667D-2/ DATA PT,RA,RAV,EPSEX,EPSIN,RHOS,ALPHA
• /202.014,4.724.41E-3,4.724.41E-3,.373,.375,.575/ DATA AINT,CP_S,RO_S,R_P,D_P,CON_S,HEAT
• /635.D0,0.2D0,70.0,4.72410D-3,9.44882D-3/ DATA G_F,PT,TOT,TO
• /58.6,15.28,538.0D0/ DATA BC_C/17.0,3.1481,0.0/ DATA BC_L1,BC_L2,BC_L3,BC_L5,BC_L6
• /538.,538.,538.,25.25./ DATA IN_L1,IN_L2,IN_L3,IN_L4,IN_L5,IN_L6
• /538.,538.,0.790.20415,0.790,20415/ DATA M_W/44.,18.,28.32/ DATA NC,NJ,DELZ1,DELT1/4.169,.00833333,1.0E-5/ DATA NC,NCI,DELT1/4.51,.01666667,0.001/

C DATA R.PI/555.0,3.141593D0/
DATA K_F/617.,0035.,05.,05/ NC1=NC
N1=NC*2+5 ALF=(1.0D0-EPSEX)/EPSEX
PT=P_TOT SUM_Y=0
DO 10 I=1,NC
• Y_F=BC_C(I)/P_TOT SUM_Y=SUM_Y+Y_F
• R_CRT=BC_L5/IN_L5 IF(R_CRT.LT.0.53) THEN
• BC_L5=0.53*IN_L5 10 CONTINUE

L1=2*NC+1
L2=L1+1
L3=L2+1
L4=L3+1
L5=L4+1
L6=1
BC_L5=BC_L5
VISC_F=VISC(IN_L1)*60
R_CRT=BC_L5/IN_L5 IF(R_CRT.LT.0.T0.53) THEN
BC_L5=.53*IN_L5
ENDIF
DO 413 I2=1,NJ
  C1(I2)=0.0
  P1(I2)=0.0
  C1(12)=BC_L5
  P1(12)=IN_L5
  C1(3,12)=IN_L1
  P1(3,12)=IN_L1
VISC_P(I2)=VISC_F
413 CONTINUE
CALL DIFEQ1(C1,P1,NJ,2)
N=N1
DO 423 I2=1,NJ
  C1(I2)=C1(1,12)
  C1(12)=C1(2,12)
423 CONTINUE
U_FI=C(L4,1)
DELTZ=DELZ1/Z
DELT=U_FI*DELT1/Z
DO 22 I1=1,NC
  C(I1,1)=C_FO(I1)
22 CONTINUE
DO 24 I2=1,NC
C(I2,1)=C_FO(I1)
P(I2,1)=IN_L1
P(I2,2)=IN_L2
P(I2,3)=IN_L3
P(I2,4)=IN_L4
P(I2,5)=IN_L5
P(I2,6)=IN_L6
C(L1,1)=BC_L1
C(L1,2)=BC_L2
C(L2,1)=BC_L3
C(L2,2)=BC_L4
24 CONTINUE
CALL IST_Z(1,C(L2,1),P(LS,1),C(1,1),C(2,1),C(3,1),C(4,1),Q2)
DO 40 I=NC+1,NC+NC
  DO 40 II=I,NJ
    C(LII)=Q2(I-NC)*RO_S
    P(LII)=C(II)
40 CONTINUE
RETURN
END
SUBROUTINE FUNCT(J)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4),M_AVE,M_W(5),KGAS,K_FP(4,201),C1(14,201),
  P1(14,201),REY_P(201),KEFF,D_L(4),YO(4)
DIMENSION Q2(4),C2(14,201),PE_N_M(4)
COMMON/PR_OLD_Z/VISC_P(201),RO_P(201),CP_P(201),CON_FPP(201),
  CON_LPP(201),I) LPP(4.201),H_FP(201),H_TFP(201),H_TPP(201),H_TIP(201),
  H_FWPP(201),Q(4,201),RATE_C1(201),AMOL_W(201),
  D_LAV(201)
COMMON/NBN/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
  Y(14,14),G(14),N,NJ,JPRT,TNC,NCVT,F(14),P(14,201),ZU_F1
COMMON/PROP_B_Z/D_LD_ES_B,CON_WA,CON_WI_Q,CON_WI_K,CP_WA,
  CP_WL,CP_WL_K,RO_WA,RO_WI_Q,RO_WI_K,RO_WI_KX,WA_X,WI_X,WI_K,
  D_LMD_LMA
COMMON/PROP_S_Z/CP_S,RO_S,AMNT,R_H,P,H,CON_S,G,F,HEAT(4),M_W
C C
C MASS TRANSFER FROM THE BULK OF GAS STREAM TO THE SURFACE OF ABSORBENT
C
C ESTABLISHED COEFFICIENT MATRIX

IF (TIME.GE.6.0) GO TO 501
IF (ITEST.EQ.0) THEN
   D_T=D_E+D_I
   X_W=D_E-D_I
   A_C=2*D_I/((D_I+D_E)*X_W)
   A_INS=2*D_E/((D_I+D_E)*X_W)
   ITEST=1
   U_F=C(L4,1)
   H_FW=6.0
   H_OW=0.1
ENDIF
IF (I.EQ.1 .AND. ITEST1 .NE. ITCNT) THEN
   RO_F=C(L5,1)/(C(L1,1)*R)
   DO 10 I=1,NJ
      DO 11 II=I,NC
         YO(I1)=C(I1,1)
      END DO
      M_AVE=0.
      DO 11 II=I,NC
         M_AVE=M_AVE+M_W(II)*YO(I1)
      END DO
      AMOL_W(I)=M_AVE
      RO_F=C(L5,1)/(C(L1,1)*R)
      TEMP=C(L1,1)
      GN=C(L4,1)*RO_F/60.
      VISC_P(I)=VISC(TEMP)*60
      REY=RE(TEMP,AMOL_W(I))
      IF (REY.LT.1.0) GO TO 10
      CP_P(I)=CPGAS(TEMP,YO)
      H_FP(I)=HFLM(AMOL_W,TEMP,REY,CP_P(I))*60.
      PP=C(L5,1)
      CON_LPP(I)=EFFK(GN,TEMP,CP_P(I),RO_F,PP,YO)*60.
      DO 11 II=1,NC
         D_LPP(I1,1)=EFFD(1,GN,TEMP,RO_F,PP,YO)*60.
         IF (D_LPP(I1,1).LT.0) THEN
            D_LPP(I1,1)=D_LPP(I1,1-1)
         END IF
      END DO
   GO TO 502
501 DO I=1,NC
      YO(I)=C(I1,1)
   END DO
   M_AVE=0.
   DO I=1,NC
      CONTINUE
      ITEST=ITCNT
   END IF
END IF
GO TO 502

F-5
M_AVE = M_AVE + M_W(I1) * YO(I1)
END DO
AMOL_W(I1) = M_AVE
502 R_CRT = BC_LS5/C(LS, NI)
IF(R_CRT < 0.53) THEN
   BC_LS5 = 0.53 * C(LS, NI)
ELSE
   BC_LS5 = BC_LS5
END IF
RO_F = C(LS, J)/(C(L1, J) * R)
CP_F = CP_P(I)
H_FS = H_PP(I)
CON_L = CON_LPP(I)
D_L_AVE = D_L_AVE + D_L(I1)
SUM = SUM + 1
D_L_AVE = D_L_AVE / SUM
END DO
D_L(1) = D_LPP(1, J)
IF(D_L(1).NE.0) THEN
   SUM = SUM + 1
   D_L_AVE = D_L_AVE + D_L(11)
END IF
END DO
D_LAV(J) = D_L_AVE
VISC_F = VISC_P(I)
PE_N_S = U_F1 * RO_S * CP_S * Z/CON_S
PE_N_P = U_F1 * RO_P * CP_P * Z/CON_L
F3 = ALP_H * H_FS * AINT / (RO_P * CP_F * U_F1)
F4 = H_FW * Z * 4 / (U_F1 * D_L * EPSEX * RO_F * CP_F)
F5 = H_FS * AINT * Z / (U_F1 * RO_S * CP_S)
F6 = AINT * Z / (RO_S * CP_S * U_F1)
F7 = Z * H_FW * A_C / RO_WA * CP_WA
F8 = Z * H_OW * A_INS * U_F1 / RO_WA * CP_WA
F9 = Z / ((1 - EPSEX) * RO_S * CP_S * U_F1 * PI * D_L / D_J / D_J / Z)
CALL IST_Z(1, C(L2, J), C(LS, J), C(1, J), C(2, J), C(3, J), C(4, J), Q2)
DO 20 J = 1, NC
   Q(J) = Q2(J) * RO_S
20 CONTINUE
IF(J.EQ.1) THEN
   DO 50 M1 = 1, NC
      F1 = K_F(M1) * AINT * Z / U_F1
      F(NC + M1) = F1 * (Q(M1, J) - C(NC + M1, J)) - (C(NC + M1, J) - P(NC + M1, J)) / DELT
50 CONTINUE
   FLUX1 = 0
   FLUX2 = 0
   DO 60 M1 = 1, NC
      FLUX1 = FLUX1 + HEAT(M1) * (K_F(M1) * (Q(M1, J) - C(NC + M1, J)))
      FLUX2 = FLUX2 + AINT * K_F(M1) * (Q(M1, J) - C(NC + M1, J))
60 CONTINUE
RATE_C1(J) = FLUX2
TOT_C = 0.
DO 40 M1 = 1, NC - 1
   F(M1) = (-D_L(M1) / DELT ** 2 * (C(M1, J + 1) - 2 * C(M1, J) + C(M1, J - 1)) +
            (C(L4, J) / (2.0 * DELT) * (C(M1, J + 1) - C(M1, J - 1)) + 1.0 / DELT ** 2 * (C(M1, J) -
            P(M1, J)) * ALF / RO_F * (C(M1, J) * RATE_C1(J) - AINT * K_F(M1) * (Q(M1, J) -
            C(NC + M1, J)))
   TOT_C = TOT_C + C(M1, J)
40 CONTINUE
   F(NC) = 1.0 / TOT_C * C(NC, J)
   F(L1) = 1.0 / DELT ** 2 * (C(L1, J + 1) - 2 * C(L1, J) + C(L1, J - 1)) +
            1.0 / (2.0 * DELT * U_F1) * (C(L1, J) - C(L1, J)) +
               F3 * (C(L1, J) - C(L1, J) - F3 * (C(L1, J) - C(L1, J)))
F5*(C(L1.J)-P(L2J)+F6*FLUX1+DELH*F9*(C(L2.J)-
P(L2.J))/DELT
P(L3.J))/DELT
F(L4)=C(L5.J)-P(L5.J)/DELZ+DELZ1**2*(C(L5.J)+1)
.150*(1-EPSEX)**2*VISC_F*C(L4.J)/D_P/
. EPSEX+RO_F*M_AVE*(C(L4.J)-P(L4.J))/DELT1
F(L5)=-(C(L5.J)-P(L5.J))/DELZ1-D_L_AVE/DELZ**2*(C(L5.J)+1)
. RATE(C1(J))
C
C THE LAST ROW
C
ELSE IF(1.EQ.NJ) THEN
DO 90 M=1,NC
F1=K_F(MI)*AINT*Z_U_F1
F(NC+M1)=-F1*(Q(MI,J)-(NC+M1,J)-(C(NC+M1.J)-P(NC+M1.J))/DELT
90 CONTINUE
FLUX1=0
FLUX2=0
DO 100 M=1,NC
FLUX1=FLUX1+HEAT(MI)*(K_F(MI)*(Q(MI,J)-(NC+M1.J))
FLUX2=FLUX2+AINT*K_F(MI)*(Q(MI,J)-(NC+M1.J))
100 CONTINUE
RATE(C1(J)=FLUX2
TOT_C=C:0
DO 80 M=1,NC
. C(NC+M1.J))
TOT_C=TOT_C+C(M1.J)
80 CONTINUE
F(NC+1)=_=1.0D0/PE_N_S/DELZ**2*(C(L1.J)+2*C(L1.J)+C(L1.J)+1)
F(L2)=1.0D0/PE_N_S/DELZ**2*(C(L2.J)+2*C(L2.J)+C(L2.J)+1)
P(L2.J))/DELT
P(L3.J))/DELT
F(L4)=(C(L5.J)-1.0D0/PE_N_S/DELZ**2*(C(L5.J)+1)
F(L5) = (C(L5,J) - P(L5,J))/DELZ1 - D_L_AVE/DELZ1**2 * (BC_L5 - 2 * C(L5,J) + C(L5,J-1))/DELZ1 + C(L5,J)**2 * (C(L4,J) - C(L4,J-1))/DELZ1 - C(L5,J)/C(L1,J)**2 * (C(L1,J) - C(L1,J-1)) + P(L1,J)/DELZ1 - D_L_AVE/DELZ1**2 * (C(L1,J) - 2 * C(L1,J) + C(L1,J-1)) + C(L4,J)**2 * (C(L1,J-1) - C(L1,J-1))/DELZ1) + R1 * C(L1,J) * ALF

RATE_C1(J)

C INTERIOR ROWS

ELSE
DO 130 MI=1,NC
  F1 = K_F(M1) * AINT * Z/DELT
  F(NC+M1) = F1 * (Q(M1,J) - C(NC+M1,J) - (C(NC+M1,J) - P(NC+M1,J))/DELZ1)
130  CONTINUE
FLUX1 = 0
FLUX2 = 0
DO 140 MI=1,NC
  FLUX1 = FLUX1 + HEAT(M1) * (K_F(M1) * (Q(M1,J) - C(NC+M1,J)) - C(NC+M1,J))/DELZ1
  FLUX2 = FLUX2 + AINT * K_F(M1) * (Q(M1,J) - C(NC+M1,J))/DELZ1
140  CONTINUE
RATE_C1(J) = FLUX2
TOT_C = 0
DO 120 MI=1,NC
  F(M1) = (-D_L(M1)/DELZ1 - D_L_AVE/DELZ1**2 * (C(M1,J+1) - 2 * C(M1,J) + C(M1,J-1)) + C(L4,J)**2 * (C(L1,J-1) - C(L1,J))/DELZ1 + C(L1,J)* (C(L1,J) - C(L1,J))/DELZ1 - D_L_AVE/DELZ1**2 * (C(L1,J) - 2 * C(L1,J) + C(L1,J))/DELZ1)
  F(L2) = 1.0D0/PE_N_H/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + 1.0D0/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + F1*FLUX1 + DELH*F1*P(L2,J)/DELZ1
  F(L3) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L4) = F1*FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L5) = F1*FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(12) = 1.0D0/PE_N_H/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + 1.0D0/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + F1*FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L2) = 1.0D0/PE_N_S/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + 1.0D0/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + F1*FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L3) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L4) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L5) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(12) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L2) = 1.0D0/PE_N_S/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + 1.0D0/DELZ1*2*(C(L1,J) - C(L1,J-1))/DELZ1 + F1*FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L3) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L4) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(L5) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
  F(12) = FLUX1 + DELH*F1 * P(L2,J)/DELZ1
ENDIF
END

SUBROUTINE DIFEQ
IMPLICIT REAL*8(A-H,O-Z)

C GENERALIZED CALLING PROGRAM FOR BAND(J) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY

C CALLED BY: MAIN CALLING PROGRAM

C SUBROUTINES CALLED:
WRTOUT (FOR DATA OUTPUT)
BAND (TO SOLVE BANDED TRIDIAGONAL COEFFICIENT MATRIX)
FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
FOR A VARIABLE)

C LIST OF IMPORTANT VARIABLES:
A  A coefficient described in Newman, Appendix C
AA first AA is F(WORKC*CU). Later AA is the
   value of the derivative df/dc used in Newton's
   method
B  B coefficient described in Newman, Appendix C
C  variables to be solved for
CD  multiplication factor used in obtaining
     numerical derivatives
COLD value of C from previous iteration
CU  2.0 - CD
D  D coefficient described in Newman, Appendix C
ERR convergence criterion
F  value of function f(C), calculated in FUNCT
G  residual of f(C) calculated with updated C value
I  index used for equation number
ITCNT index for iteration number
ITPRT flag used for determining whether intermediate
calculations are output; for ITPRT=0 only
   converged results are output; for
   ITPRT=1 results of each iteration are printed.
J  index for node number
K  index for equation number
M  index used in working through nodes used to
calculate numerical derivatives
MM used to determine starting node (in relation to
   J) for estimation of numerical derivatives
N  number of equations (no. of variables)
NJ  number of node points
SAVEC saved value of C
SUM intermediate value used in calculating G
TINIER criterion used to avoid working with small numbers
TINY criterion used to avoid working with small numbers
TNIEST criterion used to avoid working with small numbers
WORKC saved value of C; modified when C less than Tinier
X  X value described in Newman, Appendix C
Y  Y value described in Newman, Appendix C

C DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
C IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
C IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT, AND CHANGE THE SECOND
C DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
C NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
C WHATEVER YOU desire.

F-9
COMMON/OLD/ AA(14),SUM(14),COLD(14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),X(14,14),
.Y(14,14),G(14),N,NJ,ITPRT,ITCNT,F(14),P(14,201)
DATA TINY,TINIER,TNIEST,ERR/1.0D-10,1.0D-15,1.0D-20,1.0D-4/
DATA CU,CD/1.0001,.9999/

C ITCNT INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT
C IF ITPRT=1.
C
ITPRT=0
IF (ITPRT.GT.0) CALL WRTOUT2
C
C LOOP BEGUN FOR ITERATIONS
C
DO 75 ITCNT=1,10
C
C COLD ARRAY SET UP
C
DO 10 K=1,N
DO 10 J=1,NJ
COLD(K,J)=C(K,J)
10 CONTINUE
C
C LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
C PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F(I).
C
DO 60 J=1,NJ
CALL FUNCT(J)
DO 15 I=1,N
SUM(I)=0.0
G(I)=-F(I)
15 CONTINUE
C
C THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
C TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
C (IN RELATION TO J).
C
IF (J.EQ.1) THEN
   MM=0
ELSE IF (J.LT.NJ) THEN
   MM=1
ELSE
   MM=2
ENDIF
DO 50 M=MM,MM+2
C
C ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC
C
DO 50 K=1,N
SAVEC=C(K,J+M)
WORKC=SAVEC
C
C DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)
C
IF (ABS(WORKC).LT.TINY) THEN
   IF(ABS(WORKC).LT.TINIER) WORKC=SIGN(TINIER,WORKC)
   C(K,J+M)=1.2*WORKC
   CALL FUNCT(J)
   DO 20 I=1,N
      AA(I)=-F(I)
20   CONTINUE
   C(K,J+M)=1.1*WORKC
   CALL FUNCT(J)
   DO 25 I=1,N

F-10
AA(I)=AA(I)+4.0*F(I)
CONTINUE
C(K,J+M)=WORKC
CALL FUNCT(J)
DO 30 I=1,N
AA(I)=(AA(I)-3.0*F(I))/(0.2*WORKC)
30 CONTINUE
C
C DERIVATIVES CALCULATED FOR LARGER VALUES OF C (GREATER THAN TINY)
C
ELSE
C(K,J+M)=WORKC*CU
CALL FUNCT(J)
DO 35 I=1,N
AA(I)=F(I)
35 CONTINUE
C(K,J+M)=WORKC*CD
CALL FUNCT(J)
DO 40 I=1,N
AA(I)=(AA(I)-F(I))/((CU-CD)*WORKC)
40 CONTINUE
ENDIF
C(K,J+M)=SAVEC
C
C VALUES FOR A, B, D, X AND Y GIVEN. SUM IS ALSO INCREMENTED
C
DO 45 I=1,N
SUM(I)=SUM(I)+AA(I)*C(K,J+M)
IF (M.EQ.-2) Y(I)=AA(I)
IF (M.EQ.-1) A(L)=AA(I)
IF (M.EQ.0) B(L)=AA(I)
IF (M.EQ.1) D(L)=AA(I)
IF (M.EQ.2) X(L)=AA(I)
45 CONTINUE
50 CONTINUE
DO 55 I=1,N
G(I)=G(I)+SUM(I)
55 CONTINUE
C
C BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(J)
60 CONTINUE
C
C CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO 65 K=1,4,2
DO 65 J=1,NJ
IF (DABS(C(K,J)).GT.TNIEST) THEN
IF (DABS((C(K,J)-COLD(K,J))/C(K,J)).GT.ERR) GO TO 70
ENDIF
65 CONTINUE
GO TO 80
70 IF (FRPT .GT. 0) CALL WRTOU
75 CONTINUE
80 CONTINUE
RETURN
END
SUBROUTINE FUNCT1(J)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 D_L(2),M_AVE

F-11
C MASS TRANSFER FROM THE BULK OF GAS STREAM TO THE SURFACE OF ABSORBENT
C ESTABLISHED COEFFICIENT MATRIX
C THE FIRST ROW

RATE_C=RATE_CI(J)
VISC_F=VISC_P(J)
C_K=2.7845/(150*1*EPSSEX)**2*VISC_P/D_P/D_P/
EPSSEX/EPSEX/GC
D_L_AVE=D_LAV(J)

IF(I.EQ.1)THEN
F(L5)=(C(L5,J)-P(L5,J))/DELT1-D_L_AVE/DELZ1**2*(C(L5,J+1)-
2*C(L5,J)-C(L5,J-1)+C_K*(C(L5,J-1)-C(L5,J))**2/DELZ1/DELZ1-
. C*K*(C(L5,J)-C(L5,J-1)-2*C(L5,J)+C(L5,J+1))/DELZ1/DELZ1-
. C*(C(L5,J)+C(L5,J-1)*P(L5,J))/DEL1-D_L_AVE/DELZ1**2*
. (C(L1+1)-2*C(L1,J)+C(L1,J-1))+C(L4,J)*(C(L1,J+1)-C(L1,J))/
. (2*DELZ1))+R1*C(L1,J)*ALP*RATE_C

F(L4)=(C(L5,J+1)-C(L5,J))/DELZ1+(150*1*EPSSEX)**2*VISC_P*-
. C(L4,J)/D_P/D_P/EPSEX/EPSEX/GC/2.7845)

C--------------------------------------------
C ELSE IF(I.EQ.N)THEN
F(L5)=(C(L5,J)-P(L5,J))/DELT1-D_L_AVE/DELZ1**2*(C(L5,J-1)-
.2*C(L5,J)-C(L5,J-1)-C_K*(C(L5,J+1)-C(L5,J))**2/DELZ1/DELZ1-
. C_K*(C(L5,J)-C(L5,J-1)-2*C(L5,J)+C(L5,J+1))/DELZ1/DELZ1-
. C*(C(L5,J)+C(L5,J-1)*P(L5,J))/DEL1-D_L_AVE/DELZ1**2*
. (C(L1+1)-2*C(L1,J)+C(L1,J-1))+C(L4,J)*(C(L1,J+1)-
. C(L1,J))(2*DELZ1)+R1*C(L1,J)*ALP*RATE_C

F(L4)=(BC_L5*CONV-C(L5,J))/DELZ1+(150*1*EPSSEX)**2*VISC_P*-
. C(L4,J)/D_P/D_P/EPSEX/EPSEX/GC/2.7845)

C--------------------------------------------
C ELSE
F(L5)=(C(L5,J)-P(L5,J))/DELT1-D_L_AVE/DELZ1**2*(C(L5,J+1)-
.2*C(L5,J)-C(L5,J-1)-C_K*(C(L5,J+1)-C(L5,J))**2/DELZ1/DELZ1-
. C_K*(C(L5,J)-C(L5,J-1)-2*C(L5,J)+C(L5,J+1))/DELZ1/DELZ1-
. C*(C(L5,J)+C(L5,J-1)*P(L5,J))/DEL1-D_L_AVE/DELZ1**2*
. (C(L1+1)-2*C(L1,J)+C(L1,J-1))+C(L4,J)*(C(L1,J+1)-
. C(L1,J))(2*DELZ1)+R1*C(L1,J)*ALP*RATE_C
SUBROUTINE DIFFEQ1(CL,P1,NJ1,N1)

IMPLICIT REAL*8(A-H,O-Z)

C GENERALIZED CALLING PROGRAM FOR BAND(I) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY
C
C CALLED BY: MAIN CALLING PROGRAM
C
C SUBROUTINES CALLED:
C WRTOUT (FOR DATA OUTPUT)
C BAND (TO SOLVE BANDED TRIAGONAL COEFFICIENT MATRIX)
C FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
C FOR A VARIABLE)
C
C LIST OF IMPORTANT VARIABLES:
C
A A coefficient described in Newman, Appendix C
AA first, AA is F(WORKC*CU). Later AA is the
value of the derivative df/dc used in Newton's
method
B B coefficient described in Newman, Appendix C
C variables to be solved for
CD multiplication factor used in obtaining
numerical derivatives
COLD value of C from previous iteration
CU 2.0 - CD
D D coefficient described in Newman, Appendix C
ERR convergence criterion
F value of function f(C), calculated in FUNCT
G residual of f(C) calculated with updated C value
I index used for equation number
ITCNT index for iteration number
ITPRT flag used for determining whether intermediate
calculations are output; for ITPRT=0, only
converged results are output; for
ITPRT=1, results of each iteration are printed.
J index for node number
K index for equation number
M index used in working through nodes used to
calculate numerical derivatives
MM used to determine starting node (in relation to
J) for estimation of numerical derivatives
N number of equations (no. of variables)
NJ number of node points
SAVEC saved value of C
SUM intermediate value used in calculating G
TINIER criterion used to avoid working with small numbers
TINY criterion used to avoid working with small numbers
TNIEST criterion used to avoid working with small numbers
WORKC saved value of C; modified when C less than Tinier
X X value described in Newman, Appendix C
DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT, AND CHANGE THE SECOND
DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
WHATEVER YOU WANT.

REAL*8 C(14,201),P(14,201)
COMMON/OLD/AA(14),SUM(14),COLD(14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
Y(14,14),G(14),N,NJ,ITPRT,ITCNT,F(14),P(14,201)
DATA TINY,TINIER,TNIE,S/1.0D-10,1.0D-15,1.0D-20,1.0D-8/
DATA CU,CD/1.0001,-9999/

ITCNT INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT
IF ITPRT=1.

ITPRT=0
ITCNT=0
NJ=N1
N=N1
IF (ITPRT.GT.0) CALL WRTOUT2
DO 5 I1=1,N1+1
DO 5 I2=1,N1
C(I1,I2)=C(I1,I2)
P(I1,I2)=P(I1,I2)
5 CONTINUE

LOOP BEGUN FOR ITERATIONS
DO 75 ITCNT=1,10

COLD ARRAY SET UP
DO 10 K=1,N
DO 10 J=1,NJ
COLD(K,J)=C(K,J)
10 CONTINUE

LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F(I).
DO 60 J=1,NJ
CALL FUNCTJ(J)
DO 15 I=1,N
SUM(I)=0.0
G(I)=-F(I)
15 CONTINUE

THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET
TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED
(IN RELATION TO J).
IF (J.EQ.1) THEN
MM=0
ELSE IF (J.LE.NJ) THEN
MM=1
ELSE
MM=-2
END IF
DO 50 M=MM,MM+2

F-14
C ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC
C
DO 50 K=1,N
SAVEC=C(K,J+M)
WORKC=SAVEC
C
C DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)
C
IF (ABS(WORKC).LT.TINY) THEN
   IF (ABS(WORKC).LT.TINIER) WORKC=SIGN(TINIER,WORKC)
   C(K,J+M)=1.2*WORKC
   CALL FUNCT1(I)
   DO 20 I=1,N
      AA(I)=-F(I)
      CONTINUE
   C(K,J+M)=1.1*WORKC
   CALL FUNCT1(I)
   DO 25 I=1,N
      AA(I)=AA(I)+4.0*F(I)
      CONTINUE
   C(K,J+M)=WORKC
   CALL FUNCT1(I)
   DO 30 I=1,N
      AA(I)=(AA(I)-3.0*F(I))/(0.2*WORKC)
      CONTINUE
ELSE
   C(K,J+M)=WORKC*CU
   CALL FUNCT1(I)
   DO 35 I=1,N
      AA(I)=F(I)
      CONTINUE
   C(K,J+M)=WORKC*CD
   CALL FUNCT1(I)
   DO 40 I=1,N
      AA(I)=(AA(I)-F(I))/((CU-CD)*WORKC)
      CONTINUE
ENDIF
C(K,J+M)=SAVEC
C
C VALUES FOR A,B,D,X AND Y GIVEN. SUM IS ALSO INCREMENTED
C
DO 45 I=1,N
   SUM(I)=SUM(I)+AA(I)*C(K,J+M)
   IF (M.EQ.-2) Y(I,K)=AA(I)
   IF (M.EQ.-1) A(I,K)=AA(I)
   IF (M.EQ.0) B(I,K)=AA(I)
   IF (M.EQ.1) D(I,K)=AA(I)
   IF (M.EQ.2) X(I,K)=AA(I)
   CONTINUE
50 CONTINUE
DO 55 I=1,N
   G(I)=G(I)+SUM(I)
   CONTINUE
C
C BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX
C
CALL BAND2(I)
C
CONTINUE
C
C CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
C FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
C ITERATION IS BEGUN
C
DO 65 K=1,N
   DO 65 J=1,N
      IF(DABS(C(K,J)).GT.TNIT*Vr) THEN
         IF(DABS((C(K,J)-COLD(K,J))/C(K,J)).GT.ERR) GO TO 70
      ENDIF
   CONTINUE
GO TO 80
70 IF(TPRINT.LT.0) CALL WRTOU2
75 CONTINUE
80 CONTINUE
   DO 85 I=1,N
      DO 85 J=1,N
      CONTINUE
85 RETURN
END

SUBROUTINE WRTOU2

C***************************************************************************
IMPLICIT REAL*8(A-H,O-Z)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),
,Y(14,14),G(14),N,NJXrPRT,ITCNT,F(14)
IF (ITCNT.NE.0) WRITE (*,99)ITCNT
WRITE (*,100)
DO 1 K=1,N
   WRITE(*,101)K,E(C(L,K),L=1,N)
1 CONTINUE
99 FORMAT('ITCNT=',I2)
100 FORMAT('J C1 C2 C3 C4 C5 C6/)
101 FORMAT(1X,I3,6(1PE16.8))
RETURN
END

C BLOCK TRIDIAGONAL MATRIX SUBROUTINE
SUBROUTINE BAND20
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION E(14,14,201)
COMMON/BND/A(14,14),B(14,14),C(14,201),D(14,29),X(14,14),Y(14,14),
,G(14),N,NJXrPRT,ITCNT,F(14)
101 FORMAT('ITCNT=0 DETERM=0 AT J=,I4')
IF (J.EQ.1) THEN
   DETERM=0
   DO 2 I=1,N
      D(L*2*N+1)=G(I)
      DO 2 L=1,N
         D(LL+N)=X(LL)
      CONTINUE
2 CONTINUE
   CALL MATINV2(N,2*N+1,DETERM)
   IF(DETERM.EQ.0) WRITE (2,101) J
   DO 5 K=1,N
      E(K,NP1)=D(K,2*N+1)
      DO 5 L=1,N
         E(K,L)=D(K,L)
         X(K,L)=D(K,L+N)
      CONTINUE
5 CONTINUE
RETURN
ELSE IF(J.EQ.2) THEN
   DETERM=0
   DO 7 I=1,N
      DO 7 K=1,N
         DO 7 L=1,N
            D(L)=D(L)+A(LL)*X(L,K)
         CONTINUE
7 CONTINUE

F-16
ELSE IF(J.EQ.NJ) THEN
  DO 10 I=1,N
  DO 10 L=1,N
  G(I)=G(I)-Y(IL)*E(L,NP1,J-2)
  DO 10 M=1,N
  A(LL)=A(LL)+Y(IM)*E(M,LJ-2)
  CONTINUE
  ENDIF
  DO 12 I=1,N
  D(I,NP1)=-G(I)
  DO 12 L=1,N
  IXLNPI=IXI.NP I)+A(I,L)*_IJ- I)
  DO 12 K=1,N
  B(I,K)=B(I,K)+A(I,K)*E(K,LJ-1)
  12 CONTINUE
ENDIF
DO 15 K=1,N
  DO 15 M=1,N
  EfK,MJ)=-IXICM)
RETURN
ENDIF
ID/JCOL=1
IF(JCOL.NE.IROW) THEN
  DO 10 J=1,N
    SAVE=B(IROW,J)
    B(IROW,J)=B(JCOL,J)
    B(JCOL,J)=SAVE
  CONTINUE
  DO 11 K=1,M
    SAVE=D(IROW,K)
    D(IROW,K)=D(JCOL,K)
    D(JCOL,K)=SAVE
  CONTINUE
ENDIF
FF = 1.0/B(JCOL,J)
DO 13 J=1,N
  B(JCOL,J)=B(JCOL,J)**FF
  DO 14 K=1,M
    D(JCOL,K)=D(JCOL,K)**FF
  CONTINUE
  IF(I.NE.JCOL) THEN
    FF = B(I,J)
    DO 16 J=1,N
      B(J) = B(J)**FF*B(JCOL,J)
      DO 17 K=1,M
        D(L,K) = D(L,K)**FF*D(JCOL,K)
      CONTINUE
    ENDIF
CONTINUE
RETURN
END

FUNCTION RE (G,TEMP,MW)
  THIS FUNCTION CALCULATES THE PARTICLE REYNOLDS NUMBER ASSUMING THAT
  THE MOLECULAR WEIGHT OF THE GAS IS EQUAL TO THAT OF CARRIER GAS.
  IMPLICIT REAL*8(A-H,O-Z)
  REAL*8 LEN,MW
  COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSEIN,ALF,RHOS
  COMMON/GAS/INERT,NCOMP
  DATA IFLAG/0/
  IF (IFLAG.EQ.0) THEN
    CONST=2.*RA
    IFLAG=1
  ENDIF
RE=CONST*MW*ABS(G)/VIS(TEMP)
RETURN
END

SUBROUTINE MST_Z(METHOD,T,PTOT,Y11,Y12,Y13,Y14,Q1)
  IMPLICIT REAL*8(A-H,O-Z)
  COMMON/EQLIB/PP(4),B(4),V(4),PO(4),PI(4),XI(4),X1(4),Y1(4)
  COMMON/NCY/NC1
  REAL*8 Q(4)
  INTEGER LNLIM
  EXTERNAL FCN,FDER
  DATA XTOL,FTOL,JILIM/1.0E-2,1.0E-10,0.f0/
  DATA PO(4)/1.0E-12,1.0E-10,0.50/
  DATA R/5.55/
  T_G=T
  NC=NC1
  Y1(1)=Y11
  Y1(2)=Y12
  Y1(3)=Y13
  Y1(4)=Y14

F-18
DO I=1,NC
  PP(I)=Y(I)*PTOT
END DO
Z=1.0E-32
  DO I=1,NC
    Q1(I)=0.
  END DO
RETURN
END IF
V(1)=(81.2983138-21118560043*T+1.587732293D-4*T^2)/44/100
V(2)=1.69.035
V(3)=1.637879912E-5*T+.00961297026
V(4)=V(3)
B(1)=6864.9000131*EXP(-.019625791466*T)
IF(T.LT.610.) THEN
  B(2)=4.559728759E-7*EXP(9628.9555743/T)
ELSE
  B(2)=5.8089066684E-7*EXP(9115.734593/T)
END IF
IF(T.LE.532) THEN
  B(3)=3.2694515539E-5*T-.59988799E-4
ELSE
  B(3)=7.90864008E-5*T-4.14400420E-2
END IF
B(4)=B(3)
TERM1=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    TERM1 =B(I)*PP(I)^*PO(I)*TERM1
  END IF
ENDDO
SUM=0.
DO I=1,NC
  IF(PP(I).LE.0.) THEN
    Q1(I)=0.
  ELSE
    Q1(I)=V(I)*B(I)*PP(I)*PO(I)/(1+TERM1)
  END IF
  SUM=SUM+Q1(I)
END DO
IF(METHOD.EQ.1) THEN
  RETURN
END IF
DO I=1,NC
  XI(I)=Q1(I)/SUM
END DO
IF(XI(I).GT.0) THEN
  PI(I)=PP(I)/XI(I)
ELSE
  PI(I)=0.
END IF
END DO
DO I=1,NC
  IF(PP(I).LE.0.) THEN
    X1(I)=0.
  ELSE
    X1(I)=V(I)/PO(I)*LOG(1+B(I)*PI(I)*PO(I))
  END IF
END DO
X=X1(1)
DO I=2,NC
  IF(X1(I).LT.X) THEN
    X=X1(I)
  END IF
END DO
END DO
IF (X .LE. 1.0E-17) GO TO 80
CALL NEWT(FCN,FDER,X,XTOL,FTOL,NLIM,I)
DO I=1,NC
IF (PP(I), LE.0) THEN
   XI(I)=0.
ELSE
   PART1=PO(I)*X/V(I)
   IF (PART1.GT.73) PART1=73
   PI(I)=(EXP(PART1)-1)/B(I)
   XI(I)=PP(I)/PI(I)
END IF
END DO
TOT_Q=0
DO I=1,NC
IF (PP(I), LE.0) THEN
   QI(I)=0.
ELSE
   QI(I)=V(I)*B(I)*PI(I)**(1+B(I)*PI(I)**PO(I))
   TOT_Q=TOT_Q+XI(I)/QI(I)
END IF
END DO
DO I=1,NC
QI(I)=1/TOT_Q*XI(I)
END DO
80 RETURN
END

REAL FUNCTION FCN(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLM/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
IF (PP(I), GT.0) THEN
   PART1=PO(I)*X/V(I)
   IF (PART1.GT.73) PART1=73
   SUM=SUM+PP(I)/((EXP(PART1)-1)/B(I))**(1/PO(I))
END IF
END DO
FCN=SUM-1
RETURN
END

REAL FUNCTION FDER(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLM/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
IF (PP(I), GT.0) THEN
   PART3=PO(I)*X/V(I)
   IF (PART3.GT.32) THEN
      PART1=-PP(I)/B(I)/V(I)*EXP(PART3)
      PART2=((EXP(PART3)-1)/B(I))**(1+PO(I)/PO(I))
      SUM=SUM+PART1/PART2
   END IF
   END IF
END DO
FDER=SUM
RETURN
END
SUBROUTINE NEWTN(FCN,FDER,X,XTOL,FTOL,NLIM,IF)
IMPLICIT REAL*8(A-H,O-Z)
INTEGER NLIM,IF
FX=FCN(X)
DO J=1,NLIM
DELex=FX/FDER(X)
X=X-DELex
FX=FCN(X)
IF (ABS(DELex).LE.XTOL)THEN
RETURN
ENDIF
ENDIF
ENDDO
I=-I
PRINT 200, NLIM,X,FX
200 FORMAT(/=TOLERANCE NOT MET '.14, ITERATIONS X=', 2E12.5, 'F(X)=',E12.5)
RETURN
END

FUNCTION CPGAS(TEM,Y)
C THIS FUNCTION CALCULATES THE HEAT CAPACITIES OF CMRIER GAS IN BTU/#MOLE/R
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 A(4),B(4),C(4),D(4),E(4)
COMMON/GAS/INERT,NCOMP
COMMON/NCY/NC1
C CO2
DATA A/36.11,33.46,29.1/
C H2O
DATA B/4.233E-2,6860E-2,2199E-2,1.158E-2/
C N2
DATA C/-2.887E-5,.7604E-5,.5723E-5,-.6076E-5/
C O2
DATA D/7.464E-9,-3.593E-9,-2.8715E-9,1.311E-9/
NC=NC1
T=TEM/1.8-273.15
IF (INERT.EQ.1) THEN
CPGAS=0.
DO I=1,NC
CP=+A(I)+B(I)*T+C(I)*T*T+D(I)*T*T*T
CPGAS=CP*Y(I)/4.18669+CPGAS
END DO
ELSE
CPGAS=4.97
ENDIF
RETURN
END

FUNCTION CPS(TEMP)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE HEAT CAPACITY
C BTU/LB/R.
CPS=0.2
RETURN
END

REAL FUNCTION KGAS(TEMP)
C THIS FUNCTION CALCULATES THE THERMAL CONDUCTIVITY OF CARRIER GAS ASSUMING
C A LINEAR FUNCTION OF TEMPERATURE AND BASED ON VALUES AT 492 AND 672 R.
C BTU/FT/R
IMPLICIT REAL*8(A-H,O-Z)
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
  KGAS=3.88E-7*TEMP+0A052F.-4
ELSE
  KGAS=1.667E-6*TEMP+6.1E-4
ENDIF
RETURN
END

FUNCTION VIS(TEMP)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE VISCOSITY OF CARRIER GAS AS A LINEAR FUNCTION
C OF TEMPERATURE (LB/MIN/FT).
COMMON/GAS/INERT,NCOMP
IF (INERT.EQ.1) THEN
  VIS=1.0E-6*TEMP+1.65E-4
  VIS=-0.0102007812+5.384663937E-5*TEMP-8.7973727E-8*TEMP*TEMP+
  2 4.81138495E-11*TEMP*TEMP TEMP
ELSE
  VIS=0.9444E-6*TEMP+2.863E-4
ENDIF
RETURN
END

FUNCTION RHOG(TR,P)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
C THIS FUNCTION CALCULATES THE MOLAR DENSITY OF AN IDEAL GAS IN
C LB MOLES/CV FS.
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSPIN,ALF,RHOS,ALPHA1
DATA R/555./
RHOG=P/RffR
RETURN
END

FUNCTION EFFD_ICOMP(G,T,TEMP,RHO,PT,YO)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL DIFFUSIVITIES IN A PACKED BED
C USING THE EDWARDS AND RICHARDSON CORRRELATION. (FT2/FT/MIN)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LAMBD2A1,LAMDBA2,LEN,YO(4)
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSPIN,ALF,RHOS,ALPHA1
DATA IFLAG/0.,LAMBDA1/0.73/
IF(IFLAG.EQ.0)THEN
  CONST=2.*RA/EPSEX
  IFLAG=1
ENDIF
DIF=DIFF_ICOMP(TEMP,P,YO)
EFFD=LAMDBA1*DIF+CONST*ABS(G)*LAMDBA2(G,DIF,RHO)/RHO
RETURN
END

FUNCTION EFFK(G,T,CP,RHO,P,YO)
IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE EFFECTIVE AXIAL THERMAL CONDUCTIVITY OF A
C PACKED BED IN BTU/FT/MIN/F.
COMMON/NCY/NC1
REAL*8 YO(4)
NC=NC1
EFFK=0.
KK=0
DO II=1,NC
  SUM=CP*RHO*EFFD(II,G,T,RHO,P,YO)
  IF(SUM.GT.0)KK=KK+1
  EFFK=SUM+EFFK
ENDDO
RETURN
END
REAL FUNCTION LAMDA2(G,DIF,RHO)
C THIS FUNCTION CALCULATES THE DIMENSIONLESS PARAMETER OF THE EDWARDS AND
C RICHARDS Correlation modified for small diameter particles.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
DATA IFLAG/0/
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA
IF(IFLAG.EQ.0)THEN
  IF(RA.GT.0.00492)THEN
    PE=2.
  ELSE
    PE=406.4*RA
  ENDIF
CONST=2.*RA_PSKX
ENDIF
LAMBDA2=1./PE/(1.+9.5*CONST/ABS(G)*RHO)
RETURN
END

FUNCTION DIFP(ICOMP,TEM,PI.YO)
C THIS FUNCTION CALCULATES THE MOLECULAR DIFFUSION COEFFICIENTS BY CORRECTING
C FOR PRESSURE AND TEMPERATURE (FT*FT/MIN).
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN,VO(4),V(4),DIF(4)
COMMON/GAS/INERT,NCOMP
COMMON/NCY/NC1
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA
DATA V/26.9,12.7,17.9,16.6/
DATA MW/,_.01,18.016,28.013,31.999/
NC=NC1
K=ICOMP
P=P1/760.
T=TEM/1.8
DO I=1,NC
  PART1=((MW(K)+MW(I))/MW(K)/MW(I))**.5
  PART2=(V(K)**(1.3)+V(I)**(1.3))**2
  DIF(I)=PART1/PART2*T**1.75/P*1.0E-3
END DO
SUM=0.
DO I=1,NC
  IF(I.NE.K)THEN
    SUM=SUM+YO(I)/DIF(I)
  ENDIF
END DO
DIFF=(1.-YO(K))/SUM**.5*8745/60.
RETURN
END

FUNCTION HFLM(MW,TEMP,REY,CP)
C THIS FUNCTION CALCULATES THE FLUID FILM HEAT TRANSFER COEFFICIENT
C IN BTU/SQ FT/FT/MIN/R USING THE CORRELATION OF PETROY AND THODOS.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 ID,KGAS,KG,LEN,MW
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA
COMMON/GAS/INERT,NCOMP
FUNCTION DHCAR(TEMP,P)
C THIS SUBROUTINE Calculates HEAT OF ADSORPTION OF CARRIER GAS ONTO THE
C ACTIVATED CARBON TIMES THE TEMPERATURE DERIVATIVE OF THE SOLID PHASE
C CARRIER GAS CONCENTRATION AT THE BED PRESSURE (BTU/# SOLID/R).
C IMPLICIT REAL*8(A-H,O-Z)
C REAL*8 LEN
C COMMON/GAS/INEKT.NCOMP
C COMMON/PRIME/GN2.RA,RAV,EPSEX,ALF,RHOS,ALPHA1
C DATA R/1.9872/,A/1.28E-9/,B/3151 /
C IF(INERT.EQ.1) THEN
DHN2=RH*A*B*EXP(B/TEMP)*P/TEMP/TEMP
C ELSE
DHN2=0.
C ENDIF
C RETURN
C END

FUNCTION DHADS(ICOMP,T)
C THIS FUNCTION Calculates THE ISOTERIC HEAT OF ADSORPTION. (BTU/#MOLE)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
COMMON/PRIME/GN2.RA,RAV,EPSEX,EPSINJU,ALF,RHOS,ALPHA1
IF(ICOMP.EQ.2) THEN
DHADS=20400.0
ELSE
DHADS=20000.0
END IF
RETURN
END
APPENDIX G
FLOW3MOL FORTRAN CODE

A BED WITH THREE DIFFERENT MATERIALS. IN THIS CASE, 13X, SILICA GEL, AND 13X

C this is the main routine, the initial values of matrix C and parameters are
C called by "INITIAL\_Z" subroutine, the main routine then calls the "FUNCT2\_Z"
C subroutine to solve the discretized partial differential equations (pde's).
C after convergence, the routine calls the "DIFEQ1" subroutine, which is
C the main routine for solving the momentum and the pressure equations,
C if it is desire to solve these two equations as the time progresses.C
IMPLICIT REAL*8(A-H,O-Z)
REAL*4 PL(11,201),QP(14,201),PL\_TIME,T\_TIME
COMMON/BND\_Z/P(14,201),C(14,201),U\_F1,Z
COMMON/PROP\_D\_Z/DELZ1,DELZ1,DELZ,DELZ,NC,NJ,JFULL
COMMON/INDIC/L1,L2,L3,L4,L5,L6
COMMON/IND1/IND(4)
OPEN (30,FILE='ASCII.DAT',STATUS='NEW',RECL=32766)
OPEN (66,FILE='CON\_CO2.DAT',STATUS='NEW')
OPEN (88,FILE='CON\_H2O.DAT',STATUS='NEW')
OPEN (99,FILE='TEM.DAT',STATUS='NEW')
C WRITE HEADER DATA TO ASCII FILE
WRITE(50,42)
C
C INITIALIZE THE C ARRAY WITH THE INITIAL GUESSES OF THE SOLUTION
C
CALL INITIAL\_Z
ICOT=1
T\_TIME=0
C start marching through time
DO 301 LL=1,9000
C call funct2\_Z subroutine to solve the PDE's by numerical method
CALL FUNCT2\_Z
C accumulate the time steps
T\_TIME=T\_TIME+DELZ*U\_F1*60.
DO 74 M2=1,NJ
QP(1,M2)=C(1,M2)*10.73DO*C(L1,M2)*760/14.696
QP(2,M2)=C(2,M2)*10.73DO*C(L2,M2)*760/14.696
QP(3,M2)=C(3,M2)*DELZ*460.
QP(4,M2)=C(4,M2)*DELZ*460.
QP(5,M2)=C(5,M2)*DELZ*460.
74 CONTINUE
WRITE(\*,*)W0.LL\_LL_T\_TIME
WRITE(\*,*)QP(1,1),QP(1,25),QP(1,50),QP(1,75),QP(1,101)
WRITE(\*,*)QP(2,10),QP(2,25),QP(2,50),QP(2,75),QP(2,101)
WRITE(\*,*)QP(3,10),QP(3,25),QP(3,50),QP(3,75),QP(3,101)
WRITE(\*,*)QP(4,10),QP(4,25),QP(4,50),QP(4,75),QP(4,101)
WRITE(\*,*)W0.LL\_LL_T\_TIME
C
WRITE(\*,*)Q0(1,1),Q0(1,137),Q0(1,175),Q0(1,112),Q0(1,150)
C
WRITE(\*,*)Q0(2,3),Q0(2,37),Q0(2,75),Q0(2,112),Q0(2,150)
C
WRITE(\*,*)Q0(3,3),Q0(3,37),Q0(3,75),Q0(3,112),Q0(3,150)
DO 520 J=1,151
PL(1,J)=QP(1,J)
PL(2,J)=QP(2,J)
PL(3,J)=QP(3,J)
PL(4,J)=QP(4,J)
520 PL(5,J)=QP(5,J)
PL\_TIME=T\_TIME
ISAMP=25
IF(LL/ISAMP*ISAMP.EQ.LL) THEN
WRITE(50,43)PL_TIME,PL(1,6),PL(1,25),PL(1,50),PL(1,75),PL(1,101)
& .PL(2,6),PL(2,25),PL(2,50),PL(2,75),PL(2,101)
& .PL(3,6),PL(3,25),PL(3,50),PL(3,75),PL(3,101)
& .PL(4,6),PL(4,25),PL(4,50),PL(4,75),PL(4,101)
& .PL(5,6),PL(5,25),PL(5,50),PL(5,75),PL(5,101)
ENDIF
DO 78 II=1,N
DO 78 I=1,NJ
P(I,J)=C(I,J)
CONTINUE
200 CONTINUE
301 CONTINUE
42 FORMAT(IX,TIM,ppCO2_1,ppCO2_2,ppCO2_3,
& ,ppCO2_5',
& ,ppH20_1,ppH20_2,ppH20_3,ppH20_4,ppH20_5',
& ,T gas_1,T gas_2,T gas_3,T gas_4,T gas_5',
& ,T bed_1,T bed_2,T bed_3,T bed_4,T bed_5',
& ,T wall_1,T wall_2,T wall_3,T wall_4,T wall_5')
43 FORMAT(1X,26(E15_3X))
44 FORMAT(/IS.S.3X))
45 FORMAT(/5)LS(EIS .S.3X))
c number of component
NC1=NC

c number of equations
N=NC+5
ALFI=(1.0D0-EPSEX1)/EPSEX1
ALF2=(1.0D0-EPSEX2)/EPSEX2

PT=P_TOT*760/14.696
SUM_Y=0
G_F1=G_F
G_F2=G_F

c calculate the mole fraction
DO 10 I=1,NC
    Y_F=BC_C(I)/P_TOT
    SUM_Y=SUM_Y+Y_F
    BC_C(I)=P_TOT*Y_F/R/BC_L1
10 CONTINUE

c calculate fluid density
RO_FO=P_TOT/(BC_L1*R)

c calculate superficial velocity
GN=Q_P*RO_FO/60.
U_F1=G_F/(S_B*EPSEX1)

BC_L1=U_F1

c grid size in dimensionless
DELT=Z/DELZ1

c time step in dimensionless
DELTA=U_F1*DELTA1

c L1 is the gas temp, L2 is the solid temp, L3 is the wall temp, L4 is the
c velocity, L5 is the total pressure, and L6 is the total pressure without

c thermal effect

c L1=2*NC+1
L2=L1+1
L3=L2+1
L4=L3+1
L5=L4+1
L6=L5+1

c set the initial guess and the old value of C array; P
DO 20 I1=1,N
    DO 20 I2=1,NJ
    P(I1,I2)=0.0D0
    C(I1,I2)=0.0D0
20 CONTINUE

c set the the first grid to the boundry
DO 22 I1=1,NC
    C(I1,1)=BC_C(I1)
22 CONTINUE

d 24 I1=1,2
    DO 24 I2=2,NJ
        C(I1,I2)=0.
        C(I1+2,I2)=BC_C(I1+2)
24 CONTINUE

c set the initial temperature and pressure
DO 30 I1=1,NJ
    P(I1,1)=BC_L1
30 CONTINUE
P(L2j) = BC_L2
P(L3j) = BC_L3
P(L4j) = U_F1
P(L5j) = BC_L5
P(L6j) = BC_L6
C(L1j) = BC_L1
C(L2j) = BC_L2
C(L3j) = BC_L3
C(L4j) = U_F1
C(L5j) = BC_L5
C(L6j) = BC_L6
30 CONTINUE
RETURN
END

C this subroutine is being called by maine routine to compute the variable in
C matrix, in this routine first velocity profile is being determined, the
C conductivity, diffusivity, porosity, etc. are being calculated in this
C routine by calling the appropriate subroutine, the routine obtained the
C matrix in axial and radial directions, it iterates till it converges to the
C allowable error
C
SUBROUTINE FUNCTION2_Z
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 K_F(4), M_AVE, M_W(5), KGAS,K_FP(4,201),C1(14,201),
P(14,201),REY_P(201),KEFF_SIL,KEFF(4),D_L(4),A(4),Y(4),SS(4)
DIMENSION Q2(4),C2(14,201),PE_N_M(4),DWDX(4),DWDY(4)
COMMON/PRIME_I/GN
1,RAI,RAV1,EPSEX,EPSIN1,ALF1,RHOS1,ALPHA1
COMMON/PRIME_2/GN2,RA2,RAV2,EPSEX2,EPSIN2,ALF2,RHOS2,ALPHA2
COMMON/PROP_S_Z_1/CP_S1,RO_S1,AINT1,R_P1,D_P1,CON_S1,
G_F1,HEAT1(4),M_W
COMMON/PROP_S_2/CP_S2,RO_S2,AINT2,R_P2,D_P2,CON_S2,
G_F2,HEAT2(4)
COMMON/PR_OLD_Z/RO_P(201),CP_P(201),CON_FFP(201),
CON_LPP(201),D_LPP(4,201),H_PP(201),H_TPP(201),H_IIP(201),
H_OWPP(201),H_FWPP(201),Q(4,201),VISC_P(201),RATE_C1(201),
WM_AVE(201)
COMMON/BND_Z/P(14,201),C(14,201),U_F1,Z
COMMON/PROP_B_Z/DD_E,S,CON_WA,CON_W1,Q,CON_W1,K,CP_WA,
CP_W1,Q,CP_W1,K,RO_WA,RO_W1,Q,RO_W1,K,RO_W1,K,RO_W1,K,
D_LMLD_LMA
COMMON/PROP_D_Z/DELZ1,DEL1,DEL,D,DELZ2,NC,NJ1,ILL
COMMON/INDIC/L1.12/,L4,1-5,1.6
COMMON/BOUND/CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC_C(4),TO
COMMON/DELZ_DIFF/D01,D11,D21,D32,D12,D22,FR
COMMON/LAYERS/LAYER1,LAYER2
COMMON/GAS/NERT,NCOMP
COMMON/NCY,NC1
COMMON/IND1,IND(4)
COMMON/PRIME/GN,RAD,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
DATA R.PI/3.14D0,1.0D0/10.73D0,3.141593D0/
IIO=100
C set the number of grids for different material in the bed
IF(LL.EQ.1)THEN
IPORE=0
LAYER1=6
LAYER2=50
EPSP=.52
DELZ_OLD=DELZ
C set the under-relaxation coeff
WO=.2
W1=.2
W2=.2

G-4
W3=.2
ENDIF
IF(W0.LE.0.5)W0=W0*.002
IF(W1.LE.0.5)W1=W1+.002
IF(W2.LE.0.5)W2=W2+.002
IF(W3.LE.0.5)W3=W3+.002
ITEST=0
ICOUNT=1
ICONV=0

c calculate the surface area for the heat transfer
ERROR=1.0E-3
D_T=D_E+D_I
X_W=D_E-D_I
A_C=2*D_I/(D_I+D_E)*X_W
A_INS=2*D_E/(D_I+D_E)*X_W
RO_F=C(L5,1)/(C(L1,1)*R)
G_F=G_F1
G_N=G_F*RO_F/S_B/60

c compute parameters for all the grids
DO 199 J=1,NJ

c set parameters for middle material, silica gel
IF(J.GE.Layer1.AND. J.LE.Layer2)THEN
RA=RA2
EPSEX=EPSEX2
EPSIN=EPSIN2
R_P=R_P2
D_P=D_P2
DO 211 II=1,NC
HEAT(II)=HEAT2(II)
211 CONTINUE
ELSE
RA=RA1
EPSEX=EPSEX1
EPSIN=EPSIN1
AINT=AINT1
R_P=R_P1
D_P=D_P1
DO 213 II=1,NC
HEAT(II)=HEAT1(II)
213 CONTINUE
ENDIF

IF(LL.EQ.1) THEN
RO_F=C(L5,J)/(C(L1,J)*R)
YTOT=0.
c calculate the mole fraction
DO II=1,NC-1
YO(II)=C01J)/RO_F
YTOT=YO(II)+YTOT
END DO
YO(NC)=1-YTOT

c calculate the average molecular weight
M_AVE=0.
DO II=1,NC
M_AVE=M_AVE+M_W(II)*YO(II)
END DO
WM_AVE=1.0=M_AVE
TEMP=C(L1,J)
GN=G_F*RO_F/S_B/60.
c calculate viscosity
VISC_P(J)=VIS(TEMP)*60
c calculate reynolds number
REY=RE(GN,TEMP)
REY_P(J)=REY
c calculate heat capacity
CP_P(J)=CPGAS(TEMP,YO)
c calculate heat transfer coefficient between the pellet and fluid
H_FP(J)=HFILM(M_AVE TEMP,REY,CP_P(J))*60.
c converge pressure
PP=(C(L5,J)*760.)*14.696
c calculate the thermal dispersion
CON_LPP(J)=EFFK(GN,TEMP,CP_P(J),RO_F,PP,YO)*60.
c calculate mass diffusivity
DO II=1,NC
   D_LPP(I1,J)=EFFD(I1,GN,TEMP,RO_F,PP,YO)*60.
   IF(D_LPP(I1,J).LT.0) THEN
      D_LPP(I1,J)=D_LPP(I1,J-1)
   END IF
ENDDO
C ENDIF
199 CONTINUE
c heat transfer coefficient between the fluid and the wall
H_FW=4.0
c heat transfer coeff between the wall and outside
H_OW=0.05
c start iteration
IF(I.EQ.1)II_OLD=3000
   DO 220 II=1,II_OLD
DO 30 II=1,II93
   DO 30 I2=1,NJ
      C(I2)=C(I2)-C(I2)
   END DO
30 CONTINUE
34 DO 190 J=1,NJ
   c since there are different sizes of grids at the boundaries of two adjacent
   c materials, the equations must be revised.
   IF(J.EQ.LAYER1) THEN
      ITESTJ=1
   END IF
   c fraction of actual grid size
   FR=3.7550015
   FR=1.0
   c PDE's coefficients
   DO1=FR/(1+FR)
   D11=(1-DR)/FR
   D21=1.0/FR/(1+FR)
   D02=1.0/(1+FR)
   D12=1.0/FR
   D22=1.0/FR/(1+FR)
   ELSE IF(J.EQ.LAYER2) THEN
      ITESTJ=1
      FR=.2666666
   END IF
   ELSE
      ITESTJ=0
   END IF
   c fix the grid size
   IF(J.L.EQ.LAYER1) THEN
      DELZ=2666666*DELZ_OLD
      DELZ=DELZ_OLD
   ELSE IF(J.GT.LAYER2) THEN
      DELZ=2666666*DELZ_OLD
      DELZ=DELZ_OLD
   END DO
G-6
ELSE
    DELZ=DELZ_OLD
ENDIF

C set bed and pellet parameter for each material
IF(J.GE.LAYER1 .AND. J.LT.LAYER2)THEN
    RA=RA2
    RAV=RAV2
    EPSEX=EPSEX2
    EPSIN=EPSIN2
    ALF=ALF2
    RHOS=RHOS2
    ALPHA1=ALPHA12
    CP_S=CP_S2
    RO_S=RO_S2
    AINT=AINVT2
    R_P=R_P2
    D_P=D_P2
    CON_S=CON_S2
    DO 111 I=1,NC
        HEAT(I)=HEAT2(I)
    111 CONTINUE
ELSE
    RA=RA1
    RAV=RAV1
    EPSEX=EPSEX1
    EPSIN=EPSIN1
    ALF=ALF1
    RHOS=RHOS1
    ALPHA1=ALPHA11
    CP_S=CP_S1
    RO_S=RO_S1
    AINT=AINVT1
    R_P=R_P1
    D_P=D_P1
    CON_S=CON_S1
    DO 113 I=1,NC
        HEAT(I)=HEAT1(I)
    113 CONTINUE
ENDIF

C set fluid parameters
    RO_F=C(L5,J)/(C(L1,J)*R)
    CP_F=CP_F(J)
    H_FS=H_FP(J)
    CON_L=CON_LPP(J)
    DO 11=I,NC
        D_L(I)=D_LPP(I,J)
    END DO

C peclet number for solid
    PE_N_S=U_F1*RO_S*CP_S*Z/CON_S

C peclet number for heat in gas
    PE_N_H=U_F1*RO_P*CP_P*Z/CON_L

C coefficient in PDE's after making them dimensionless
    F3=ALPHA*H_FS*Z*AINVT(RO_F*CP_F*U_F1)
    F4=H_FW*Z*4/(U_F1*D_P*EPSEX*RO_P*CP_F)
    F5=H_FS*AINVT_Z(U_F1*RO_S*CP_S)
    F6=Z(RO_S*CP_S*U_F1)
    F7=Z*(H_FW*A_C/U_F1/RO_WA/CP_WA)
    F8=Z*(H_FW*A_INS/U_F1/RO_WA/CP_WA)

C CO2 partial pressure
    PCO2=C(5,J)*R*C(L2,J)

C H2O partial pressure
    PH20=C(6,J)*R*C(L2,J)

C set dynamic parameters for each section
IF(J.GE.LAYER1 .AND. J.LT.LAYER2)THEN
CALL DWDXDT_SIL(PCO2,PH2O,C(L1,J),C(L2,J),C(L5,J),
REY_P(J),DWDX(2),DWDT(2))
DWDX(1)=0.
DWDT(1)=0.
K_F(1)=0.
K_F(2)=3
K_F(3)=0.
K_F(4)=0.
ELSE
IF(IPORE.EQ.1) THEN
CALL to compute the solid amount in equilibrim with gas phase for silica
CALL DWDXDT_13X(PCO2,PH2O,C(L1,J),C(L2,J),C(L5,J),
REY_P(J),DWDX,DWDT)
K_F(1)=3
K_F(2)=3
ELSE
DO I=1,NC
SS(I)=C(I,J)
END DO
CALL to compute the solid amount in equilibrim with gas phase for 13X
CALL IST.Z(LCg,J),SS,Q2)
DO 3 I=1,NC
Q(LJ)=(Q2(I)*RO_S
3 CONTINUE
ENDIF
K_F(1)=.017
K_F(2)=.0035
K_F(3)=.05
K_F(4)=.05
ENDIF
ELSE
ENDIF
IF(J.LE.LAYER1 .AND. J.EQ.LAYER2) THEN
F=0.0
ELSE
W0=W0
ENDIF
ELSE
W0=W0
ENDIF
ELSE
ENDIF
ENDIF
CALL to compute the amount adsorbed in pore of pellet for silica gel
IF(J.LE.LAYER1 .AND. J.LE.LAYER2) THEN
F1=15.*K_F(M1)/R_P/R_P*Z/U_F1
A1=(EPS/DELT+F1)*RO_S*DWDX(M1)/DELT
C(1,J)=C(NC+M1,J)-W0*(-C(NC+M1,J)+A1*(Q1*C(M1,J)+
(DWDX(M1)*RO_S+EPS)*P(NC+M1,J)/DELT-DWDT(M1)*C(L1,J)-
P(L1,J)/DELT))
ENDIF
CALL to compute total heat of adsorption
FLUX1=FLUX1+HEAT(M1)*F1*U_F1/Z*(C(M1,J)-C(NC+M1,J))
ENDIF
CALL to compute total amount adsorbed
FLUX2=FLUX2+F1*U_F1/Z*(C(M1,J)-C(NC+M1,J))
ELSE
ENDIF
CALL to compute the amount adsorbed in solid phase for 13X
F1=K_F(M1)*AINT*Z/U_F1
A2=1/DELT+F1
C(NC+M1,J)=C(NC+M1,J)+W0*(-C(NC+M1,J)+1/A2*(Q1*Q(M1,J)+
P(NC+M1,J)/DELT))
ENDIF
CALL to compute total heat of adsorption
FLUX1=FLUX1+HEAT(M1)*3.0/R_P*K_F(M1)*(Q(M1,J)-C(NC+M1,J))
ELSE
ENDIF
CALL to compute the amount adsorbed in solid phase for 13X
G-8
FLUX2 = FLUX2 + 3.0/R_P*K_F(M1)*(Q(M1,J)-C('NC+M1,J))
ENDIF
70 CONTINUE
RATE_CJ(J)=FLUX2
DO 85 M=1,NC
PE_N_M(M1)=U_FI*Z/D_L(M1)
A(M1)=1.0DO/DELT+2/PE_N_M(M1)/DELZ**2+1/U_FI/DELZ*C(L4,J)
85 CONTINUE

C compute molar concentration in the gas phase
DO 90 M=1,NC
IF(M.EQ.1)THEN
W1=W0
ELSE
W1=W1
ENDIF
IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN
F2=15.*ALF*K_F(M1)/R_P/R_P*Z/U_F1
PART1=F2*(C(M1,J)-C('NC+M1,J))
ELSE
F2=ALF*K_F(M1)*3./R_P/R_P*Z/U_F1
PART1=F2*(Q(M1,J)-C('NC+M1,J))
ENDIF
C(M1,J)=C(M1,J)+W11*(-C(M1,J)+1.0DO/A(M1)*(1.0DO/PE_N_M(M1)/
DELZ**2*(BC_C(J)+C(M1,J+1))-1.0DO/U_F1/DELZ*(-BC_C(J)*
BC_L1)*PART1+P(M1,J)/DELT))
90 CONTINUE

C compute gas temperature
AL1=1./DELT+2./PE_N_H/DELZ**2+C(L4,J)/DELZ/U_F1+F3+F4
C(L1,J)=C(L1,J)+W3*(-C(L1,J)+1./AL1*(1.0DO/PE_N_H/DELZ**2*
. (BC_L1+C(L1,J+1))-1.0DO/(DELZ*U_F1)*(-BC_L1*BC_L4)*F3*
(-C(L2,J))+F4*(-C(L3,J))+P(L1,J)/DELT))

C compute solid temperature
C(L2,J)=C(L2,J)+W3*(-C(L2,J)+1.0DO/PE_N_S/DELZ**2*
. *(BC_L2+2*C(L2,J)+C(L2,J+1))-F5*(C(L1,J)-C(L2,J))-F6*FLUX1)
. +P(L2,J)

C compute wall temperature
C(L3,J)=DELT*(F7*(C(L1,J)-C(L3,J))-F8*(C(L3,J)-TO))+P(L3,J)

C THE LAST ROW
C computation of C array for the last grid

C ELSE IF(J .EQ. NJ) THEN
FLUX1=0
FLUX2=0
DO 87 M=1,NC
IF(M.EQ.1)THEN
IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN
W00=0
ELSE
W00=W1
ENDIF
ELSE
W00=W1
ENDIF

C compute amount adsorbed in the pore of pellet, silical gel
IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN
F1=15.*K_F(M1)/R_P/R_P*Z/U_F1
A1=1./EPSP/DELT+F1+RO_S*DWDX(M1)/DELT
C(NC+M1,J)=C(NC+M1,J)+W00*(-C(NC+M1,J)+A1*(F1*C(M1,J)+
. (DWDX(M1)*RO_S*EPSP)*P(NC+M1,J)/DELT-DWDT(M1)*P(C(L1,J)-
. P(L1,J)/DELT))

C compute total heat of adsorption, silical gel
FLUX1=FLUX1+HEAT(M1)*FLUX1/U_F1/Z*(C(M1,J)-C(NC+M1,J))
c compute total amount adsorbed, silica gel
   FLUX2=FLUX2+F1*U_F1/Z*(C(M1,J)-C(NC+M1,J))
ELSE
   c compute amount adsorbed in the solid of pellet, 13X
   F1=K_F(M1)*AMNT*Z/U_F1
   A2=1./DELT+F1
   C(NC+M1,J)=C(NC+M1,J)+W00*(-C(NC+M1,J)+1/A2*(F1*Q(M1,J)+
               P(NC+M1,J)/DELT))
   c compute total heat of adsorption, 13X
   FLUX1=FLUX1+HEAT(M1)*3.0/R_P*K_F(M1)*(Q(M1,J)-C(NC+M1,J))
   c compute total amount adsorbed, 13X
   FLUX2=FLUX2+3.0/R_P*K_F(M1)*(Q(M1,J)-C(NC+M1,J))
ENDIF
87 CONTINUE
   RATE(C1,J)=FLUX2
   c compute molar concentration of each component
   DO 125 M1=1,NC
      PE_N_M(M1)=U_F1*Z/D_L(M1)
      A(M1)=1.0D0/DELT+2.0D0/PE_N_M(M1)/DELZ**2+1/U_F1/DELZ*C(L4,J)
   125 CONTINUE
   DO 130 M1=1,NC
      IF(M1.EQ.1)THEN
         W11=W0
      ELSE
         W11=W1
      ENDIF
      IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN
         F2=15.*ALP*K_F(M1)/R_P*S/Z/U_F1
         PART1=F2*(C(M1,J)-C(M1+NC,J))
      ELSE
         F2=ALP*K_F(M1)/R_P*S/Z/U_F1
         PART1=F2*(Q(M1,J)-C(NC+M1,J))
      ENDIF
      C(M1,J)=C(M1,J)+W11*(-C(M1,J)+1.0D0/A(M1)*(1.0D0/PE_N_M(M1)/
                        DELZ**2*2*(C(M1,J)+C(M1+NC,J)))+
                        1.0D0/U_F1/DELZ*(-C(M1,J)))*
                        (C(L4,J)+PART1+P(M1,J)/DELT))
   130 CONTINUE
   c gas temperature
   AL1=1./DELT+2./PE_N_H/DELZ**2+C(L4,J)/DELZ/U_F1+F3+F4
   C(L1,J)=C(L1,J)+W2*(-C(L1,J)+1./AL1*(1.0D0/PE_N_H/DELZ**2*2*
                    (C(L1,J)+C(L1+1,J))-1.0D0/DELZ*U_F1)*(-C(L1,J)+C(L4,J))-
                    F3*(-C(L2,J)+F4*(-C(L3,J)+P(L1,J)/DELT))
   c solid temperature
   C(L1,J)=C(L1,J)+W3*(-C(L1,J)+DEL2*(1.0D0/PE_N_S/DELZ)**2*
                     *((C(L2,J)-2+C(L2,J)+C(L2+1,J)+F5*(C(L1,J)-C(L2,J)))
                     -F6*FLUX1)+P(L2,J))
   c wall temperatur
   C(L3,J)=DEL8*(F7*(C(L1,J)-C(L3,J))-F8*(C(L3,J)-TO)+P(L3,J)

C
C computation of C array for interior grids
C INTERIOR ROWS
C
ELSE
   FLUX1=0
   FLUX2=0
   DO 198 M1=1,NC
      IF(M1.EQ.1)THEN
         IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN
            W00=0
         ELSE
            W00=W0
         ENDIF
ELSE
  W00=W1
ENDIF

\textbf{compute amount adsorbed in pore of pellet, silica gel}

\textbf{IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN}
  \textbf{F1=15.0*K_F(M1)/R_P/R_P*Z/U_F1}
  \textbf{A1=1/DELT+F1}
  \textbf{C(NC+M1,J)=C(NC+M1,J)+W00*(-C(NC+M1,J)+A1*(F1*C(M1,J)-}
    \textbf{(DWX(M1)*RO_S*EPS+P(NC+M1,J)*DELWDT(M1)*C(L1,J)-}
    \textbf{P(L1,J)/DELT))}
\textbf{ENDIF}

\textbf{compute total heat of adsorption}

\textbf{FLUX1=FLUX1+HEAT(M1)*F1*U_F1/Z*(C(M1,J)-C(NC+M1,J))}

\textbf{compute total amount adsorbed}

\textbf{FLUX2=FLUX2+F1*U_F1/Z*(C(M1,J)-C(NC+M1,J))}

\textbf{c compute amount adsorbed in pore of pellet, 13X}

}\textbf{ELSE}
  \textbf{F1=K_F(M1)*AINT*Z/U_F1}
  \textbf{A2=1/DELT+F1}
  \textbf{C(NC+M1,J)=C(NC+M1,J)+W00*(-C(NC+M1,J)+1/A2*(F1*Q(M1,J)+
    P(NC+M1,J)/DELT))}
\textbf{ENDIF}

\textbf{c compute total heat of adsorption}

\textbf{FLUX1=FLUX1+HEAT(M1)*3.0/R_P*K_F(M1)*(Q(M1,J)-C(NC+M1,J))}

\textbf{c compute total amount adsorbed}

\textbf{FLUX2=FLUX2+3.0/R_P*K_F(M1)*(Q(M1,J)-C(NC+M1,J))}

\textbf{END IF}

198 \textbf{CONTINUE}

\textbf{RATE_C1(f)=FLUX2}

\textbf{c if the computation is where two different sizes of grids are adjacent then}

\textbf{IF(TTESTI.EQ.1) THEN}
  \textbf{DELZ=DELZ_OLD}
  \textbf{DO 165 MI=1,NC}
    \textbf{PE_N_M(MI)=U_F1*Z/DELZ(MI)}
    \textbf{A(MI)=1.0D0/DELZ+2.0D0/PE_N_M(MI)/DELZ**2*D12+1.0D0/U_F1/DELZ*}
    \textbf{C(L4,J)*D11*0}
  \textbf{165 CONTINUE}

\textbf{DO 170 MI=1,NC}
  \textbf{IF(M1.EQ.1)THEN}
    \textbf{W11=W0}
  \textbf{ELSE}
    \textbf{W11=W1}
  \textbf{ENDIF}

\textbf{IF(J.GE.LAYER1 .AND. J.LE.LAYER2)THEN}
  \textbf{F2=15.0*ALP*K_F(M1)/R_P/R_P*Z/U_F1}
  \textbf{PART1=F2*(C(M1,J)-C(M1,J))}
  \textbf{ELSE}
    \textbf{F2=ALP*K_F(M1)*3.0/R_P*Z/U_F1}
    \textbf{PART1=F2*(Q(M1,J)-C(NC+M1,J))}
  \textbf{ENDIF}

\textbf{c compute molar concentration of gas}

\textbf{END IF}

\textbf{C(M1,J-C(M1,J))+W11*(-C(M1,J)+1.0D0/A(M1)*(2.0D0/PE_N_M(M1)/}
    \textbf{DELZ**2*(C(M1,J-1)*D02+C(M1,J-1)*D22)-1.0D0/U_F1/DELZ*}
    \textbf{(-C(M1,J-1)*D01+C(M1,J-1)*D21-C(M1,J)*D11)*C(L4,J-1)-PART1+}
    \textbf{P(M1,J)/DELZ)}

170 \textbf{CONTINUE}

\textbf{AL1=1.0D0/DELZ+2.0D0/PE_N_H/DELZ**2*D12+C(L4,J)/DELZ*U_F1*D11*0+}

\textbf{F3+F4}

\textbf{c gas temperature}

\textbf{C(L1,J)=C(L1,J)+W2*(-C(L1,J)+1.0D0/PE_N_H/DELZ**2*}
  \textbf{(-C(L1,J-1)*D02+C(L1,J-1)*D22)-1.0D0/DELZ*U_F1*(-C(L1,J-1)*}
  \textbf{D01+C(L1,J-1)*D21-D11*C(L1,J))*C(L4,J-1)-F3*(-C(L2,J)-}
  \textbf{F4*(-C(L3,J)+P(L1,J)/DELZ))}

\textbf{c solid temperature}

\textbf{C(L2,J)=C(L2,J)+W3*(-C(L2,J)+DELT*(2.0D0/PE_N_S/DELZ**2*}
  \textbf{(-C(L2,J-1)*D02-C(L2,J-1)*D22)-F5*(-C(L1,J)-}
C(L2,J)=-F6*FLUX1)+P(L2,J))

if the adjacent grids are the same sizes
ELSE
  DO 161 M1=1,NC
  PE_N_M(M1)=U_F1*Z/D_L(M1)
  A(M1)=1.0D0/DELT+2.0D0/PE_N_M(M1)/DELZ**2+1.0D0/U_F1/DELZ*
  C(L4,J)
  161 CONTINUE
DO 171 M1=1,NC
IF(M1.EQ.1)THEN
  W1=W0
ELSE
  W1=W1
ENDIF
IF(I.GE.LAYER1 .AND. J.L.E.LAYER2)THEN
  F2=15.*ALF*K_F(M1)/R_P/R_P*Z/U_F1
  PART1=F2*(C(M1,J)-C(M1+NC,J))
ELSE
  F2=ALF*K_F(M1)*3./R_P*Z/U_F1
  PART1=F2*(Q(M1,J)-C(NC+M1,J))
ENDIF
ENDIF
DO 190 I1=1,NC
IF(I.GE.LAYER1 .AND. I.L.E.LAYER2)THEN
  F2=15.*ALF*K_F(M1)/R_P/R_P*Z/U_F1
  PART1=F2*(C(M1,J)-C(M1+NC,J))
ELSE
  F2=ALF*K_F(M1)*3./R_P*Z/U_F1
  PART1=F2*(Q(M1,J)-C(NC+M1,J))
ENDIF
END IF
IF(I1.GE.LAYER1 .AND. I1.L.E.LAYER2)THEN
  F2=15.*ALF*K_F(M1)/R_P/R_P*Z/U_F1
  PART1=F2*(C(M1,J)-C(M1+NC,J))
ELSE
  F2=ALF*K_F(M1)*3./R_P*Z/U_F1
  PART1=F2*(Q(M1,J)-C(NC+M1,J))
ENDIF
C(molar concentration in the gas phase)
C(M1,J)=C(M1,J)+W1*(-C(M1,J)+1.0D0/PE_N_M(M1)/
  DELZ**2*(C(M1,J-1)+C(M1,J+1))-1.0D0/U_F1/DELZ*(-C(M1,J-1)*
  C(L4,J-1)-PART1+P(M1,J)/DELT))
  171 CONTINUE
C(gas temperature)
  ALI=1./DELT+2.*PE_N_H/DELZ**2+C(L4,J)/DELZ/U_F1+F3+F4
  C(L1,J)=C(L1,J)+W2*(-C(L1,J)+1./AL1*(1.0D0/PE_N_H/DELZ**2* 
  (C(L1,J-1)+C(L1,J+1))-1.0D0/(DELZ**2*U_F1)*(C(L1,J-1)*C(L4,J-1))
  +F5*(C(L2,J)-F4*(-C(L3,J))+P(L1,J)/DELT))
C(solid temperature)
  C(L2,J)=C(L2,J)+W3*(-C(L2,J)+DELT*(1.0D0/PE_N_S/DELZ**2*
  *(C(L2,J-1)+C(L2,J+1))+F5*(C(L1,J)-C(L2,J))
  -F6*FLUX1)+P(L2,J))
ENDIF
C(wall temperature)
  C(L3,J)=DELT*(F7*(C(L1,J)-C(L3,J))-F8*(C(L3,J)-TO))+P(L3,J)
C
END IF
190 CONTINUE
IF(I1.LT.100)THEN
  GO TO 220
ENDIF
IF(check for convergence)
  DO 200 I1=1,NC
  DO 200 I2=1,NJ
  IF(C(I1,I2).NE.0) THEN
    IF(ABS(C(I1,I2)-C2(I1,I2))C(I1,I2).GT.ERROR) GO TO 220
  END IF
  200 CONTINUE
  IF(I1.LT.100)GO TO 220
DO 300 I1=1,NC
C1(I1,I2)=C(L4,I2)
P1(I1,I2)=P(L4,I2)
C1(1,12)=C(L5,I2)+760.14.696
P1(1,12)=P(L5,I2)+760.14.696
C1(2,12)=C(L6,I2)+760.14.696
P1(2,12)=P(L6,I2)+760.14.696
C1(3,12)=C(L7,I2)+760.14.696
P1(3,12)=P(L7,I2)+760.14.696
C1(4,12)=C(L8,I2)
P1(4,12)=P(L8,I2)
300 CONTINUE
CALL DIFFEQ(C1,P1,NL3)
G-12
DO 400 IZ=1,NJ
  C(I4,IZ)=C1(1.IZ)
  C(I5,IZ)=C1(2.IZ)*14.696/760.
  C(I6,IZ)=C1(3.IZ)*14.696/760.
400 CONTINUE
GO TO 210
220 CONTINUE
210 RETURN
END

c-------------------------c
c this subroutine compute the equilibrium amount adsorbed in the solid phase
of pellet, for silica gel
SUBROUTINE DWDXDT_SIL(PCO2,PH2O,TS,P,REY,DWDX2,DWDT3)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 KF,LEN,MW
COMM/PRIMEGN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
COMM/GAS/INERT,NCOMP
COMMON/P0/PH2O1,XP
COMMON/IND1/IND(4)
DATA MW/18/
DWDX1=DWDX_SIL(PH20,P,TS,1)
DWDX2=DWDX1*1545.12*TS/MW
DWDT3=DWDX1*PH2O1/TS*XP/TS
RETURN
END

C-------------------------c
this subroutine calculate the derivitive of pre concentration with respect,
to temperature and other component,silica gel
FUNCTION DWDX_SIL(PH2O,P,TS,1)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/IND1/IND(4)
COMMON/P0/PH2O1,XP
DATA R/1545.0/
DATA C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,C12,C13/-5674.5359,
-6.3925247,-9.677843-3.6,2215701-7.2,0747825-9,9.484024E-13,
4.1635019,-580,2206,1,3914993,-4.860239E-2,4.1764768E-5,
-1.4452093E-8,6.5459673/
DATA R/1545.0/
ITEST=1
T1=TS/1.8
IF(T1.LE.273.15)THEN
P0=EXP(C1+TS*C2+TS*C3+TS*C4+TS*C5+TS*C6+TS*C7+TS*C8+TS*C9+TS*C10+TS*C11+TS*C12+TS*C13+5674.5359,
-6.3925247,-9.677843-3.6,2215701-7.2,0747825-9,9.484024E-13,
4.1635019,-580,2206,1,3914993,-4.860239E-2,4.1764768E-5,
-1.4452093E-8,6.5459673/
ELSE
PH2O=PH20*144.0
IF((TEST.EQ.1))THEN
PH20=PH20
ELSE
PH20=1.0D-10
XP=TS*(LOG(P0/PH2O))
ENDIF
ENDIF
PART1=1.0D0+(XP/1200.)*XP/1200.
PART2=.177*ATAN(XP/1200.)
PART3=.7025E-7*XP*PART1**(-2.77)*EXP(PART2)
PART4=.20875E-5*PART1*EXP(PART2)*PART1**(-1.77)
DWDX_SIL=-(PART3+PART4)*TS/PH2O
ELSE
PH2O1 = PH2O
IF(PH2O1.LE.1.0E-10) PH2O1=1.0E-10
XP=TS*(LOG(P0/PH2O1))
W=354*(1.0+(XP/1200)**2)**(-1.77)*
EXP(-177*ATAN(XP/1200))
XP1=XP+10.0
W1=354*(1.0+(XP1/1200)**2)**(-1.77)*
EXP(-177*ATAN(XP1/1200))
DWDX_SI=-TS*(W1-W)/(XP1-XP)/PH2O1
END IF
RETURN
END

This subroutine compute the equilibrium amount adsorbed in the solid phase
SUBROUTINE DWDXDT_13X(PCO2,PH2O,P,TS,P,REY,DWDX,DWDT)
IMPLICIT REAL*8(A-ILO-Z)
REAL*8 Q0(4),B(4),N(4),PI(1),P1(4),W(4),DWDX(4),TERM(4),DWDT(4),
Q2(4),Q1(4)
DATA R.NC/555.2/
ITEST=0
10 Q0(1)=-0.0541863937*TSO+56.6418249)/100
B(1)=28.19709466,((1-TG'SO/9588.8566167)**1.418802_97)**(331.23533275
N(1)=4.24259381,+02210824511*TSO-3.5706432963D-5*TSO**TSO+
2.0564581055D-8*TSO**TSO
Q0(2)=0.15
B(2)=1.879094E-4*EXP(5467.4817024/TSO)
N(2)=-5
P1(1)=PCO2/14.696*760.0
P1(2)=PH2O/14.696*760.0
IF(PI(1).LT. 1.0E-10) PI(1)=1.0E-10
IF(PI(2).LT. 1.0E-10) PI(2)=1.0E-10
TERM1=0.
DO 20 I=1,NC
TERMI=TERM 1+TERM(I)
20 CONTINUE
IF(ITEST.EQ.0) THEN
DWDX(1)=Q0(1)*B(1)*N(1)*PI(1)**(N(1)-1.)*
(1+TERM(2))/(1+TERM1)**2
DWDX(2)=Q0(2)*B(2)*N(2)*PI(2)**(N(2)-1.)*
(1+TERM(1))/(1+TERM1)**2
DO 30 I=1,NC
Q1(I)=Q0(I)*B(I)*PI(I)**N(I)/(1+TERM1)
30 CONTINUE
IF(ITEST.EQ.0) THEN
DWDV(1)=-Q0(1)*B(1)*N(1)*PI(1)**(N(1)-1.)*
(1+TERM(2))/(1+TERM1)**2
DWDV(2)=-Q0(2)*B(2)*N(2)*PI(2)**(N(2)-1.)*
(1+TERM(1))/(1+TERM1)**2
DO 30 I=1,NC
Q1(I)=-Q0(I)*B(I)*PI(I)**N(I)/(1+TERM1)
30 CONTINUE
END
CONTINUE
TSO1=TSO
TSO=TSO+1.0
ITEST=1
GO TO 10
ELSE
DO 40 II=1,NC
   Q2(II)=Q0(II)*B(II)*PI(II)**N(II)/TERM1
40   CONTINUE
ENDIF
DO 50 II=1,NC
   DWDT(II)=(Q2(II)-Q1(II))/(TSO-TSO1)
50   CONTINUE
RETURN
END

C         subroutine compute the amount of adsorbed gas in equilibrium with gas
C         molar density, for single component uses Langmuir-fredrich isotherm. the
C         computation of equilibrium for multi component uses the Ideal Solution Theory
C         IST), since the equations are none linear and implicit a numerical method
C         was used to compute the adsorbed equilibrium amount. the method is by Forythe,
C         Computer Methods for Mathematical Computation. it is an bisect method with
C         quadratic convergence.
C
C B,V,PO arrays are single equilibrium constant
SUBROUTINE IST_Z1(METHOD,T,SS,Q1)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/NCY/NC1
COMMON/IND1/IND(4)
REAL*8 Q1(4),SS(4)
INTEGER LNLM
EXTERNAL FCN1
DATA XTOL,FT0L,LNLM/1.0E-5,1.0E-5,0,50/
DATA R/555/
T_G=T
NC=NC1
C the partial pressure
DO II=1,NC
   YI(II)=SS(II)
   END DO
DO I=1,NC
   PP(I)=YI(I)*T_G*R
   END DO
C no mole fraction return
Z=1.0E-32
   DO I=1,NC
      QI(I)=0.
   END DO
   RETURN
ENDIF
N1=1
C set the constant as a function of temperature
IF(IND(1).EQ.1)THEN
   C      V(N1)=(81.2983138-21118560043*T+1.587732293D-4*T**2)/100
   V(N1)=17.0/100
   C      B(N1)=6864.9000131*EXP(-.019625791466*T)
   B(N1)=5.323250566*EXP(-.5)*EXP(13948.544244/1.987/T)
   PO(N1)=8
   N1=N1+1
ENDIF

G-15
END IF
IF(IND(2).EQ.1) THEN
  VON1) = 1./69.035
  BON1) = 1.879094E-4 * EXP(5467.4817024/T)
END IF
IF(T.LT.610.) THEN
  BON1) = 4.5597278759E-7 * EXP(5467.4817024/T)
ELSE
  BON1) = 5.80890666E-7 * EXP(9115.734593/T)
ENDIF
NI = NI + 1
POf(N1) = 1.0
ENDIF
IF(IND(3).EQ.1) THEN
  V(N1) = 1.637879912E-5 * T + .00961297026
IF(T.LE.532) THEN
  B(N1) = 3.2694515539E-7 * T + 4.5998799E-4
ELSE
  B(N1) = 7.90864008E-5 * T - 4.1440042E-2
ENDIF
PO_1) = 1.0
END IF
ENDIF
IF(IND(4).EQ.1) THEN
  V(N1) = 1.637879912E-5 * T + .00961297026
IF(T.LE.532) THEN
  B(N1) = 3.2694515539E-7 * T + 4.5998799E-4
ELSE
  B(N1) = 7.90864008E-5 * T - 4.1440042E-2
ENDIF
PO(N1) = 1.0
ENDIF
END IF
IF(NC.EQ.1) THEN
  Q1(1) = V(1) * B(1) * PP(1) ** PO(1) / (1 + B(1) * PP(1) ** PO(1))
RETURN
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0) THEN
  Q1(2) = V(2) * B(2) * PP(2) ** PO(2) / (1 + B(2) * PP(2) ** PO(2))
  Q1(1) = 0
RETURN
ELSE IF(NC.EQ.2 .AND. PP(2).EQ.0) THEN
  Q1(1) = V(1) * B(1) * PP(1) ** PO(1) / (1 + B(1) * PP(1) ** PO(1))
  Q1(2) = 0
RETURN
ENDIF
TERM1 = 0.
c calculate the equilbrium isotherm by Langmuir method
DO I=1, NC
  IF(P(1).GT.0) THEN
    TERM1 = B(1) * PP(1) ** PO(1) / (1 + B(1) * PP(1) ** PO(1))
  END IF
END DO
SUM = 0.
DO I=1, NC
  IF(P(1).LE.0.) THEN
    Q1(I) = 0.
  ELSE
    Q1(I) = V(I) * B(I) * PP(I) ** PO(I) / (1 + TERM1)
  END IF
SUM = SUM + Q1(I)
END DO
c if the Langmuir method is asked for then returned
IF(METHOD.EQ.1) THEN
  RETURN
ENDIF
c if not, take the result as the first guess for IST theory
DO I=1,NC
   X1(I)=Q1(I)/SUM
   IF(X1(I).GT.0) THEN
      P1(I)=PP(I)/X1(I)
   ELSE
      P1(I)=0.
   END IF
END DO

c calculate the spread pressure
DO I=1,NC
   IF(P1(I).LE.0) THEN
      X1(I)=0
   ELSE
      X1(I)=V(I)/PO(I)*LOG(1+B(I)*P1(I)**PO(I))
   END IF
END DO
X=X1(1)
DO I=1,NC
   IF(X1(I).LT.X .AND. X1(I).GT.0) THEN
      X=X1(I)
   END IF
END DO
AX=X
DELX=AX
BX=AX
c call Zeroin subroutine to find the root to the IST equation
DO I=1,100
   BX=BX+DELX
   FUN=FCN1(BX)
   IF(FUN.LT.0) GO TO 113
END DO
113 X=ZERON(FCN1,AX,BX,TOL)
c root was found
DO I=1,NC
   IF(P1(I).LE.0) THEN
      P1(I)=1.0E-32
   END IF
c calculate the fraction in the solid phase
   PART1=PO(I)*X/V(I)
   IF(PART1.GT.73)PART1=73
   P1(I)=(EXP(PART1)-1)/B(I)
   X1(I)=P1(I)/P1(I)
END DO
TOT_Q=0
c calculate the total amount adsorbed
DO I=1,NC
   Q1(I)=V(I)*B(I)*P1(I)**PO(I)/(1+B(I)*P1(I)**PO(I))
   TOT_Q=TOT_Q+X1(I)*Q1(I)
END DO
c calculate the amount adsorbed for each component
DO I=1,NC
   Q1(I)=1./TOT_Q*X1(I)
END DO
80 RETURN
END

c IST function
REAL FUNCTION FCN1(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC
NC=NCY
SUM=0.
DO I=1,NC
   SUM=Q1(I)
END DO
G-17
IF(PP(I).GT.0) THEN
  PART1=PO(I)*X/V(I)
  IF(PART1.GT.73) PART1=73
  SUM=SUM+PP(I)*((EXP(PART1)-1)/B(I))**(1./PO(I))
END IF
C  IF(PP(I).LE.0)PP(I)=1.0E-32
C  PART1=PO(I)*X/V(I)
C  IF(PART1.GT.73) PART1=73
C  SUM=SUM+PP(I)*((EXP(PART1)-1)/B(I))**(1./PO(I))
END DO
FCN1=SUM-1
RETURN
END

------------------------------------------------------------------------

C subroutine to find the root of equation by bisect method

REAL FUNCTION ZEROIN(FCN1,AX,BX,TOL)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/IND1/IND(4)
REAL*8 AX,BX,FCN1,TOL
REAL*8 A,B,C,D,E,EP$,FA,FB,FC,TOL
I ,XM,P,Q,P,,S
EPS=L0
EPS_/Z
TOL=I.0+EPS
IF(TOLLGT.I.0) GO TO 10
C initialization
  A=AX
  B=BX
  FA=FCNI(A)
  FB=FCNI(B)
C begin step
20  C=A
    FC=FA
    D=B-A
    E=D
30  IF(ABS(FC) .GE. ABS(B)) GO TO 40
    A=B
    B=C
    C=A
    FA=FB
    FB=FC
    FC=FA
C convergence test:
40  TOL=2.*EPS*ABS(B)+.5*TOL
    XM=.5*(C-B)
    IF(ABS(XM).LE.TOL)GO TO 90
    IF(FA.EQ.0.0) GO TO 90
C is bisection necessary
70  IF(ABS(E),LE,TOL)GO TO 70
    IF(ABS(FA).LE.ABS(FB)) GO TO 70
C is quadratic interpolation possible
   IF(A.NE.C)GO TO 50
C linear interpolation
  S=FB/FA
  P=2.0*XM*S
  Q=1.0-S
  GO TO 60
C inverse quadratic interpolation
50  Q=FA/FC
    R=FB/FC
    S=FB/FA

G-18
P=S*(2.*XM*Q*(Q-R)-(B-A)*(R-1.0))
Q=(Q-1.0)*(R-1.0)*(S-1.0)

C adjust signs
60 IF(P.GT.0.0)Q=-Q
P=ABS(P)
C is interpolation acceptable
IF((2.0*P).GE.0.0*XM*Q-ABS(TOL1*Q)) GO TO 70
IF(P.GE.ABS(5.0*Q)) GO TO 70
E=D
D=P/Q
GO TO 80
C bisection
70 D=XM
E=D
C complete step
80 A=B
FA=FB
IF(ABS(D).GT.TOL1)B=B+D
IF(ABS(D).LE.TOL1)B=B+SIGN(TOL1,XM)
FB=FCN(B)
IF((FB-ABS(FC))).GT.0.0 GO TO 20
GO TO 30
C done
90 ZEROIN=B
RETURN
END
C
C
C
C the second method, this method is faster but the initial guess must be near
C the root of the equation.
C
C this subroutine compute the amount of adsorbed gas in equilibrium with gas
C molar density, for single component uses Langmuir-fredrich isotherm, the
C computation of equilibrium for multi component uses the Ideal Solution Theory
C (IST), since the equations are none linear and implicit, a numerical method
C was used to compute the adsorbed equilibrium amount, the method is Newton.
C
C B,V,PO arrays are sinle equilibrium constant
SUBROUTINE IST_Z(METHOD,T,SS,Q1)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4),PI(4),XI(4),XI(4),Y1(4)
COMMON/NCY/NC1
COMMON/INDI/IND(4)
REAL*8 Q1(4),SS(4)
INTEGER LN_LIM
EXTERNAL FCN,FDER
DATA XTOLFTOL._/1.0E-5,1.0E-5,0.50/
DATA R/555.0/
DATA T_G=T
NC=NC1
DO II=1,NC
Y1(II)=SS(II)
END DO
DO I=1,NC
PP(I)=Y1(I)*T_G*R
END DO
C no mole fraction return
Z=1.0E-32
DO I=1,NC
Q1(I)=0.
END DO
G-19
RETURN
END IF

N1=1

c set the constant as a function of temperature
IF((IND(1),EQ,1))THEN

! 13x by l.grace
  c point=1567.1205874+9.00256903*t+.0172347*t*t+1.100806e-5*t*t*t
  c if(pp(n1),.gt,.point.or.t.gt.627)then
    c V(N1)=(8.12983138-21118560043*T+1.587732293D-4*T*T)/44/100
    c B(N1)=6864.9000131*EXP(-.019625791466*T)
    c po(n1)=1.0
  c else

! 13x by l.grace
  v(n1)=23.32228444/100
  b(n1)=9.639763e-4*T**(-.5)*EXP(9233.33778/1.987/T)
  po(n1)=2.9138991288+.017181761178*T-2.584903257e-5*T*T-
      1.622511757e-8*T*T*T
  c end if

  c from Finn data 5A
  c if(pp(n1),.lt,.1.0) then
    c b(N1)=2.37022397e-6*T**(-.5)*EXP(14907.6535/1.987/T)
    c v(N1)=16.644/100
    c po(n1)=.80
  c else
    c v(n1)=(25.9713508-6.084518e-3*T-2.1799516646e-5*T*T)/44/100
    c b(n1)=1.88663393e-5*T**(-.5)*EXP(12170.875335/1.987/T)
    c po(n1)=1.
  c end if

5A BY GRACE, BY L.F
  v(N1)=17.01100/44
  b(N1)=2.341477E-4*T**(-.5)*EXP(10257.166145/1.987/T)
  po(N1)=3.830450111E-4*T**(-.5)*EXP(10719.0/1.987/T)
5A BY GRACE, BY L.F BETWEEN 0-75 C
  v(N1)=(399.3942-1.938428896*T+3.515e-3*T*T-1.8226211899e-6*T*T*T)/100/18
  b(N1)=35.358072159-.17016733*T+2.7458762E-4*T*T-T*
  p0(N1)=29.3861075+.1533898497*T-2.61225877E-4*T*T*
  1.478184694*7*T**3
  c linde 5a
  v(n1)=.005
  b(n1)=1.129015193e-5*EXP(5055.015089/T)
  po(n1)=.6
  N1=N1+1
END IF

c h20 on 5a by grace l1
IF((IND(2),EQ,1))THEN
  if(lle.46)then
    v(n1)=(39.914452-8.87103e-2*T-6.839502987e-5*T*T)/100/18
  else
    v(n1)=(873.44464-3.867834937*T+5.80375049e-3*T*T-
      2.9346685e-6*T*T*T)/100/18
    end if
  b(n1)=29690.66923-137.837129*T+.214456126*T*T*
  po(n1)=1
  else
    b(n1)=48.56639771-2.2620239975e-1*T+3.9101703168e-4*T*T-
      2.379098497e-7*T**3
    end if
v(n) = (95.093824733 - 21725775358*t + 1.4628603e-4*t^2)/100/18
p(n) = 1
end if
IF(T.LT.610.) THEN
B(2) = 4.5597278759E-7*EXP(9628.9655743/T)
ELSE
B(2) = 5.808906684E-7*EXP(9115.734593/T)
ENDIF
V(2) = 0.015
PO(2) = 1.0

END IF

IF(N(I).EQ.1) THEN
V(N) = 1.637879912E-5*T + 0.00961297026
IF(T.LE.532) THEN
B(N) = 3.2694515539E-7*T + 4.59988799E-4
ELSE
B(N) = 7.90864008E-5*T - 4.4400420E-2
ENDIF
PO(N) = 1.0
N = N + 1
ENDIF

IF(N(D).EQ.3) THEN
Q1(1) = V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
RETURN
ELSE IF(NC.EQ.2 .AND. PP(1).EQ.0) THEN
Q1(2) = V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
Q1(1) = 0
RETURN
ELSE IF(NC.EQ.2 .AND. PP(3).EQ.0) THEN
Q1(1) = V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
Q1(2) = 0
RETURN
ELSE IF(NC.EQ.3) THEN
if(pp(1).le.0 .and. pp(2).le.0) then
Q1(3) = V(3)*B(3)*PP(3)**PO(3)/(1+B(3)*PP(3)**PO(3))
Q1(1) = 0
Q1(2) = 0
end if
else if(pp(1).le.0 .and. pp(3).le.0) then
Q1(2) = V(2)*B(2)*PP(2)**PO(2)/(1+B(2)*PP(2)**PO(2))
Q1(1) = 0
Q1(3) = 0
end if
else if(pp(2).le.0 .and. pp(3).le.0) then
Q1(1) = V(1)*B(1)*PP(1)**PO(1)/(1+B(1)*PP(1)**PO(1))
END IF
Q1(2)=0
Q1(3)=0
return
end if
END IF
TERM1=0.
c calculate the equilibrium by Langmuir isotherm
DO I=1,NC
IF(PP(I).GT.0.)THEN
TERM1=B(I)*PP(I)**PO(I)+TERM1
END IF
END DO
SUM=0.
DO I=1,NC
IF(PP(I).LE.0.) THEN
Q1(I)=0.
ELSE
Q1(I)=V(I)*B(I)*PP(I)**PO(I)/(1+TERM1)
SUM=SUM+Q1(I)
END IF
END DO
c if the Langmuir method is asked for, then return. If not use it as first guess
c for IST theory
IF(METHOD.EQ.1)THEN
RETURN
END IF
DO I=1,NC
X1(I)=Q1(I)/SUM
IF(X1(I).GT.0.) THEN
PI(I)=PP(I)/X1(I)
ELSE
PI(I)=0.
END IF
END DO
c set the initial guess for the spreading pressure
DO I=1,NC
IF(PP(I).LE.0.) THEN
X1(I)=0
ELSE
X1(I)=V(I)/PO(I)*LOG(1+B(I)*PP(I)**PO(I))
END IF
END DO
X=X1(1)
DO I=2,NC
IF(X1(I).LT.X AND. X1(I).GT.0)THEN
X=X1(I)
END IF
END DO
c call newton method to the rout to IST equation
IF(X .LE. 1.0E-17) GO TO 80
CALL NEWTN(FCN,FDER,X,XTOL,FTOL,NLIM,1)
c rout was found, calculate the fraction in the solid phase
DO I=1,NC
IF(PP(I).LE.0.) THEN
X1(I)=0.
ELSE
PART1=PO(I)*X/V(I)
IF(PART1.GT.73)PART1=73
PI(I)=(EXP(PART1)-1)/B(I)
X1(I)=PP(I)/PI(I)
END IF
END DO
c calculate the total amount in the solid phase
TOT_Q=0
DO I=1,NC
  IF(PP(I).LE.0) THEN
    Q(I)=0.
  ELSE
    Q(I)=V(I)*B(I)*PI(I)**PO(I)/(1+B(I)**PI(I)**PO(I))
    TOT_Q=TOT_Q+X(I)/Q(I)
  END IF
END DO
END

DO calculate the amount in equilibruim with the gas phase for each component
DO I=1,NC
  Q(I)=1/TOT_Q*X(I)
END DO
80 RETURN
END

c IST final equation

REAL FUNCTION FCN(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/NCY/NC1
COMMON/IND1/IND(4)
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART1=PO(I)*X/V(I)
    IF(PART1.GT.73)PART1 = 73
    SUM=SUM+PP(I)*((EXP(PART1)-1)/B(1))**(1/PO(I))
  END IF
END DO
FCN=SUM-1
RETURN
END

c IST final derivative

REAL FUNCTION FDER(X)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/EQLIB/PP(4),B(4),V(4),PO(4)
COMMON/IND1/IND(4)
COMMON/NCY/NC1
NC=NC1
SUM=0.
DO I=1,NC
  IF(PP(I).GT.0) THEN
    PART3=PO(I)*X/V(I)
    IF(PART3.LT.35)THEN
      PART1=-PP(I)/B(I)**((1+PO(I))/(1+PO(I))**((1+PO(I))/(1+PO(I)))
      SUM=SUM+PART1/PART2
    ELSE IF(PART3.LT.73) THEN
      SUM=SUM-B(1)**((1+PO(I))/(1+PO(I)))*PP(I)/B(I)/V(I)*
        EXP(-PART3/PO(I))
    ELSE
      PART3=73
      SUM=SUM-B(1)**((1+PO(I))/(1+PO(I)))*PP(I)/B(I)/V(I)*
        EXP(-PART3)
    END IF
  END IF
END DO
FDER=SUM
RETURN
SUBROUTINE NEWTN(FCN,FDER,X,XTOL,FTOL,NLIM,I)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/IND1/IND(4)
INTEGER NLIM,IJ
FX=FCN(X)
XI=X
DO J=1,NLIM
DELX=FX/FDER(X)
X=X-DELX
FX=FCN(X)
IF (ABS(X-X1)/X.I.,E.XTOL) THEN
  RETURN
END IF
IF(FX.NE.0)'n-mN
IF(ABS(FX-FX1)/FX.LE.FTOL) THEN
  RETURN
END IF
XI=X
FX1=FX
END DO
I=I+1
PRINT 200, NLIM,X,FX
200 FORMAT(I4,1X,4(E12.5,F12.3))
RETURN
END

FUNCTION CPGAS(TEM,Y)
C THIS FUNCTION CALCULATES THE HEAT CAPACITIES OF CMRIER GAS IN BTU/MOLE/R
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 A(4),B(4),C(4),D(4),Y(4)
COMMON/GAS/INERT,NCOMP
COMMON/NCY/NC1
COMMON/IND1/IND(4)
C CO2
DATA A/3.611,33.46,29,29.1/
C H2O
DATA B/4.233E-2,6880E-2,2199E-2,1.158E-2/
C N2
DATA C/-2.887E-5,7604E-5,5723E-5,6076E-5/
C O2
DATA D/7.464E-9,3.593E-9,2.871E-9,1.311E-9/
NC=NC1
T=TEM/1.8-273.15
IF (INERT.EQ.1) THEN
  CPGAS=0.
  DO I=1,NC
    CP=A(I)*B(I)*T+C(I)*T+D(I)*T*T
    CPGAS=CP*Y(I)/4.18669+CPGAS
  END DO
ELSE
  CPGAS=4.97
ENDIF
RETURN
END
FUNCTION CPS(TEMP)
  IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE HEAT CAPACITY
C BTU/LB/R.
  CPS=0.2
  RETURN
END

REAL FUNCTION KGAS (TEMP)
C THIS FUNCTION CALCULATES THE THERMAL CONDUCTIVITY OF CARRIER GAS ASSUMING
C A LINEAR FUNCTION OF TEMPERATURE AND BASED ON VALUES AT 492 AND 672 R.
C BTU/MIN/FT/R
  IMPLICIT REAL*8(A-H,O-Z)
  COMMON/GAS/INERT,NCOMP
  IF (INERT.EQ.1) THEN
    KGAS=3.88E-7*TEMP+0.4052E-4
  ELSE
    KGAS=1.667E-6*TEMP+6.1E-4
  ENDIF
  RETURN
END

FUNCTION RE (G,TEMP)
C THIS FUNCTION CALCULATES THE PARTICLE REYNOLDS NUMBER ASSUMING THAT
C THE MOLECULAR WEIGHT OF THE GAS IS EQUAL TO THAT OF CARRIER GAS.
  IMPLICIT REAL*8(A-H,O-Z)
  REAL*8 LEN,MW
  COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSP,ALF,RHOS,ALPHA1
  COMMON/GAS/INERT,NCOMP
  DATA IFLAG/0/
  IF (INERT.EQ.1) MW=28.0
  IF (INERT.EQ.2) MW=4.
  IF (IFLAG.EQ.0) THEN
    CONST=2.*KA
    IFLAG=1
  ENDIF
  RE=CONST*MW*ABS(G)/VIS(TEMP)
  RETURN
END

FUNCTION VIS(TEMP)
  IMPLICIT REAL*8(A-H,O-Z)
C THIS FUNCTION CALCULATES THE VISCOSITY OF CARRIER GAS AS A LINEAR FUNCTION
C OF TEMPERATURE (LB/MIN/FT).
  COMMON/GAS/INERT,NCOMP
  IF (INERT.EQ.1) THEN
    VIS=1.0E-6*TEMP+1.65E-4
    VIS=-0.0102007812+5.384663937E-5*TEMP-8.7973727E-8*TEMP**TEMP
    2 + 4.811397495E-11*TEMP**TEMP
  ELSE
    VIS=0.9444E-6*TEMP+2.863E-4
  ENDIF
  RETURN
END
FUNCTION RHOG(TR,P)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
C THIS FUNCTION CALCULATES THE MOLAR DENSITY OF AN IDEAL GAS IN
C LBMOL/CVFS.
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
DATA R555./
RHOG=P/R/TR
RETURN
END

FUNCTION EFFD(ICOMP,T,TEMP,P,&IO.FT,YO)
C FUNCTION _TES EFFECTIVE AXIAL DIFFUSIVITIES IN A PACED BED
C USING THE EDWARDS AND RICHARDSON CORRRELATION. (FT*FT/MIN)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LAMBDA1,LAMBDA2,LEN,YO(4)
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
COMMON/IND1/IND(4)
DATA IFLAG/0/,LAMBDA1/0.73/
IF(IFLAG.EQ.0)THEN
CONST=2.*RAJEPSEX
IFLAG=1
ENDIF
DIF=DIFF(ICOMP,TEMP,P,T,YO)
EFFD=LAMBDA1*DIF+CONST*ABS(G)*LAMBDA2(G,DIF,RHO)/RHO
RETURN
END

FUNCTION EFFK(G,T,CP,RHO,P,YO)
IMPLICIT REAL*8(A-H,O-Z)
C FUNCTION _TES THE EFFECTIVE AXIAL THERMAL CONDUCTIVITY
C OF A PACKED BED IN BTU_INF.
COMMON/NCY/NC1
COMMON/IND1/IND(4)
REAL*8 YO(4)
NC=NC1
EFFK=0.
KK=0
DO II=I,NC
SUM=CP*RHO*EFFD(II,G,T,RHO,P,YO)
IF(SUM.GT.0)KK=KK+1
EFFK=SUM+EFFK
END DO
EFFK=EFFK/KK
RETURN
END

REAL FUNCTION LAMBDA2(G,DIF,RHO)
C FUNCTION _TES THE DIMENSIONLESS PARAMETER OF THE EDWARDS AND
C RICHARDS CORRELATION MODIFIED FOR SMALL DIAMETER PARTICLES.
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 LEN
DATA IFLAG/0/
COMMON/PRIME/GN2,RA,RAV,EPSEX,EPSIN,ALF,RHOS,ALPHA1
IF(IFLAG.EQ.0)THEN
IF(RA.GT.0.00492)THEN
G=26
FUNCTION DIFFOCOMP, TEM, P1, YO)

This function calculates the molecular diffusion coefficients by correcting for pressure and temperature (ft*ft/Min).

IMPLICIT REAL*8(A-H.O-Z)
REAL*8 LEN, YO(4), V(4), MW(4), DIF(4)
COMMON/GAS/INERT,NCOMP
COMMON/NCY/NC1
COMMON/PRIME/GN2, RA, RAV, EPSEX, EPSIN, ALF, RHOS, ALPHA1
COMMON/IND1/IND(4)
DATA V/26.9, 12.7, 17.9, 15.6/
DATA MW/4.4, 01, 18.016, 28.013, 31.999/
NC=NC1
K=ICOMP
P=P1/760.
T=TEM/I.8
DO I=1, NC
PART1=((MW(K)+MW(I))/V(K)/MW(I))**.5
PART2=(V(K)**(1./3)+V(I)**(1./3))**2
DIF(I)=PART1/PART2*T**1.75/P**1.0E-3
END DO
SUM=0.
DO I=1, NC
IF (LNE, K) THEN
SUM=SUM+YO(I)/DIF(I)
ENDIF
END DO
DIFF=(1.-YO(K))/SUM*3.8745/60.
RETURN
END

FUNCTION HFI(M, MW, TEM, P, REY, CP)

This function calculates the fluid film heat transfer coefficient in BTU/SQ FT/Min/R using the correlation of Petrov and Thodos.

IMPLICIT REAL*8(A-H.O-Z)
REAL*8 ID, KGAS, KG, LEN, MW
COMMON/PRIME/GN2, RA, RAV, EPSEX, EPSIN, ALF, RHOS, ALPHA1
COMMON/GAS/INERT,NCOMP
COMMON/IND1/IND(4)
KG=KGAS(TEMP)
PR=CP/MW*VIS(TEMP)/KG
HFI=M=0.357/EPSIN*REY**0.64*PR**0.33*KG*0.5/RA
RETURN
END

FUNCTION DHCAR(TEMP, P)

This subroutine calculates heat of adsorption of carrier gas onto the activated carbon times the temperature derivative of the solid phase.
C CARRIER GAS CONCENTRATION AT THE BED PRESSURE (BTU/# SOLID/R).
C IMPLICIT REAL*8(A-H,O-Z)
C REAL*8 L
C COMMON/GAS/INERT,NCOMP
C COMMON/PRIME/GN2,RA,RAV,EPSEX,ALF,ROH,S,ALPHA1
C DATA R/1.9872/A/1.28E-9/B/3151/
C IF(INERT,EQ.1) THEN
C   DH=R*B
C ELSE
C   DHN2=0.
C ENDIF
C RETURN
C END

FUNCTION DHADS(ICOMP,T)
C THIS FUNCTION CALCULATES THE ISOTERIC HEAT OF ADSORPTION. (BTU/# MOLE)
IMPLICIT REAL*8(A-I-O-Z)
REAL*8 LEN
COMMON/PRIME/GN2,RA,RAV,EPSEX,ALF,ROH,S,ALPHA1
IF(ICOMP,EQ.2) THEN
   DHADS=2000.0
ELSE
   DHADS=20000.0
ENDIF
RETURN
END

C CHER SUBROUTINE IS BEING CALLED BY DIFFEQ! WHICH IS ALSO BEING CALLED BY
C SUBROUTINE FUNCT2_Z TO COMPUTE THE VELOCITY AND THE PRESSURE DROP IN THE BED.
C THE EQUATIONS ARE BEING SOLVED BY NEWMAN'S METHOD.

SUBROUTINE FUNCT1(I)
IMPLICIT REAL*8(A-H,O-Z)
REAL*8 D_L(2),M_AVE
COMMON/OLD/AA(I4),SUM(14),COLD(14201)
COMMON/BND/A(14,13),B(14,13),C(14,201),D(14,29),X(14,13),Y(14,13),G(14,21),N(14,14),P(I,14),IT,ITPRT,ITCNT,F(I,14),P(14,201),COMMON/PR_OLD.Z/RO_P(201),CP_P(201),H_FP(201),H_JIP(201),H_FWPP(201),H_FWPP(201),Q(4,201),VISC_P(201),RATE_C1(201),VW_AVE(201),COMMON/BOUN_CON/BC_L1,BC_L2,BC_L3,BC_L4,BC_L5,BC_L6,BC_C(4)
COMMON/PROP/DELZ1,DELZ1
COMMON/PROP_S_Z_1CP_S1,RO_S1,AINT1,R_P1,D_P1,CON_S1,
G_F1,HEAT1(4)
COMMON/PROP_S_Z_2CP_S2,RO_S2,AINT2,R_P2,D_P2,CON_S2,
G_F2,HEAT2(4)
COMMON/DELZ2,DELZ1
COMMON/INDI/IND(4)
COMMON/NCY/NC1
COMMON/IND1/IND(4)
COMMON/PRIME_1/GN1,RA1,RAV,EPSEX,ALF,ROH1,ALPHA11
COMMON/PRIME_2/GN2,RA2,RAV,EPSEX,ALF,ROH2,ALPHA12
COMMON/LAYERS/LAYER1,LAYER2
DATA L1,L4,L5,L6,L_1,ROV,CN/(4,1,2,3,555.0,51.714752314/
DATA FAC,GC/2.78450526316,416975040.0/.
C C THE FIRST ROW
C
C set variable values calculated in functe2_z subroutine

G-28
NC=NC1
RATE_C=RATE_C1(I)
VISC_F=VISC_P(I)
M_AVE=WM_AVE1(I)
KK=0
SUM1=0.
DO I=1,NC
D_L(I)=D_LPP(I)
IF(D_L(I).GT.0)THEN
  KK=KK+1
  SUM1=SUM1+D_L(I)
ENDIF
END DO
D_L_AVE=SUM1/KK
RO_F=C(L5,J)/(C(L1,J)*R1)
c set constants for material in between
IF(J.GE.LAYER1 AND J.LT.LAYER2)THEN
  EPSX=EPSX1
  D_P=D_P1
  ALF=ALF1
ELSE
  c set constant for material at two ends
  EPSX=EPSX1
  D_P=D_P1
  ALF=ALF1
ENDIF
C solve the pde's for the first grid
IF(J.EQ.1)THEN
  c velocity
  F(L4)=FAC*(C(L5,J)-BC_L5*CONV)/DELT1+1/GC*(RO_F*M_AVE*C(L4,J)
  *(C(L4,J)-BC_L4)/DELT1+150*(1-EPSEX)**2*VISC_P*C(L4,J)/
  D_P/D_P*EPSEX/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
  D_P*EPSEX+RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELT1
  c total pressure without the heat
  F(L5)=C(L5,J)-P(L5,J)/DELT1-D_L_AVE/DELT1**2*(BC_L5*CONV-
  2*C(L5,J)+C(L5,J+1))*C(L4,J)*C(L5,J-BC_L5*CONV)/DELT1+
  C(L5,J)*C(L4,J)-BC_L4)/DELT1+R1*C(L1,J)*ALF*RACE_C
  c total pressure with heat
  F(L6)=C(L6,J)-P(L6,J)/DELT1-D_L_AVE/DELT1**2*(BC_L6*CONV-
  2*C(L6,J)+C(L6,J+1)-C(L6,J-1))*C(L5,J)*C(L6,J-BC_L6*CONV)/DELT1+
  C(L6,J)*C(L5,J)-BC_L5)/DELT1+C(L1,J)*ALF*RACE_C
C last grid
ELSE IF(J.EQ.NJ)THEN
  c velocity
  F(L4)=FAC*(C(L5,J)-C(L5,J-1))/DELT1+1/GC*(RO_F*M_AVE*C(L4,J)
  *(C(L4,J)-C(L4,J-1))/DELT1+150*(1-EPSEX)**2*VISC_P*C(L4,J)/
  D_P/D_P*EPSEX/EPSEX+1.75*(1-EPSEX)*RO_F*M_AVE*C(L4,J)**2/
  D_P*EPSEX+RO_F*M_AVE*(C(L4,J)-P(L4,J))/DELT1
C total pressure without heat
  F(L5)=C(L5,J)-P(L5,J)/DELT1-D_L_AVE/DELT1**2*(C(L5,J-1)-
  2*C(L5,J)+C(L5,J+1))*C(L4,J)*C(L5,J-1)/DELT1+
  C(L5,J)*C(L4,J-1))/DELT1+R1*C(L1,J)*ALF*RACE_C
  c total pressure with heat
  F(L6)=C(L6,J)-P(L6,J)/DELT1-D_L_AVE/DELT1**2*(C(L6,J-1)-
  2*C(L6,J)+C(L6,J+1))*C(L5,J)*C(L6,J-1)/DELT1+
  C(L6,J)*C(L5,J-1))/DELT1+C(L1,J)*ALF*RACE_C
G-29
C

C interior grids
ELSE

C velocity
F(L4)=(FC*(C(L5,J)-C(L5,J-1))/DELZ1+1/((1-EPSEX)*RO*P=M_AV*(C(L4,J)*
               (C(L4,J)-C(L4,J-1))/DELZ1)+FAC*RO*P=M_AV*(C(L4,J)*
               .DELZ1*DELZ1+1.75*(1-EPSEX)*RO*P=M_AV*(C(L4,J)*2/D_P/
               .DELZ1*DELZ1+1.75*(1-EPSEX)*RO*P=M_AV*(C(L4,J)*2/D_P/
               .DELZ1)+R1*C(L1,J)*ALF*RATE_C
ENDIF

C total pressure without heat:
F(L5)=(C(L5,J)-P(L5,J))/DELZ1-D_L_AVE**2*(C(L5,J)-1-
               2*C(L5,J)+C(L5,J+1))=C(L4,J)*((C(L5,J)-C(L5,J-1))/DELZ1+
               C(L5,J)*(C(L4,J)-C(L4,J-1))/DELZ1+R1*C(L1,J)*ALF*RATE_C

C total pressure with heat:
F(L6)=(C(L6,J)-P(L6,J))/DELZ1-D_L_AVE**2*(C(L6,J)-1-
               2*C(L6,J)+C(L6,J+1))=C(L4,J)*((C(L6,J)-C(L6,J-1))/DELZ1+
               C(L6,J)*(C(L4,J)-C(L4,J-1))/DELZ1+R1*C(L1,J)*ALF*RATE_C

END IF

C---------------------------------------------------------------

210 RETURN
END

C

SUBROUTINE DIFFEQ(CI,P1,NJ1,N1)
IMPLICIT REAL*(A-H,O-Z)

C GENERALIZED CALLING PROGRAM FOR BAND(J) TO SOLVE DIFFERENTIAL
C EQUATIONS TAKING PARTIAL DERIVATIVES NUMERICALLY

C CALLED BY: MAIN CALLING PROGRAM

C---------------------------------------------------------------

C SUBROUTINES CALLED:

WRTOUT (FOR DATA OUTPUT)
BAND (TO SOLVE BANDED TRIDIAGONAL COEFFICIENT MATRIX)
FUNCT (TO OBTAIN VALUE FOR FUNCTION FOR A GIVEN VALUE
FOR A VARIABLE)

C---------------------------------------------------------------

C LIST OF IMPORTANT VARIABLES:

A A coefficient described in Newman, Appendix C
AA first AA is F(WORKC CU). Later AA is the value of the derivative df/dc used in Newton's
method
B B coefficient described in Newman, Appendix C
C variables to be solved for
CD multiplication factor used in obtaining numerical derivatives
COLD value of C from previous iteration
CU 2.0 - CD
D D coefficient described in Newman, Appendix C
ERR convergence criterion
F value of function f(C), calculated in FUNCT
G residual of f(C) calculated with updated C value
I index used for equation number
ITCNT index for iteration number
IFPR flag used for determining whether intermediate

G-30
calculations are output; for ITPRT=0, only
converged results are output; for
ITPRT=1, results of each iteration are printed.

J   index for node number
K   index for equation number
M   index used in working through nodes used to
calculate numerical derivatives
MM  used to determine starting node (in relation to
J) for estimation of numerical derivatives
N   number of equations (no. of variables)
NJ  number of node points
SAVEC saved value of C
SUM  intermediate value used in calculating G
TINIER criterion used to avoid working with small numbers
TINY criterion used to avoid working with small numbers
TNIEST criterion used to avoid working with small numbers
WORKC saved value of C; modified when C less than Tinier
X   X value described in Newman, Appendix C
Y   Y value described in Newman, Appendix C

DIMENSIONS HAVE BEEN SET FOR 6 EQUATIONS AND 101 NODE POINTS; IF
IT IS DESIRABLE TO INCREASE THE NUMBER OF EQUATIONS, CHANGE THE 6
IN THE DIMENSIONS TO WHATEVER NUMBER YOU WANT. AND CHANGE THE SECOND
DIMENSION OF D TO 2N+1, WHERE N IS THE NUMBER OF EQUATIONS. IF MORE
NODE POINTS ARE DESIRED, CHANGE THE 101 IN THE DIMENSION STATEMENTS TO
WHATEVER YOU罂罂

REAL*8 C1(14,201),P1(14,201)
COMMON/OLD/AA(14),SUM(14),COLD(14,201)
COMMON/BND/A(14,13),B(14,13),C(14,201),D(14,29),X(14,13),
.Y(14,13),G(14),N,J,ITPRT,ITCNT,F(14),P(14,201)
COMMON/INDI/IND(4)
DATA TINY,TNIER,TNIEST,ERR/I.0D-10,1.0D-15,1.0D-20,1.0D-6/
DATA CU,CD/I.0D01..999999/

ITCNT: INITIALIZED HERE, AND INITIAL VALUES FOR VARIABLES PRINTED OUT
IF ITPRT=1.

ITPRT=0
ITCCT=0
NJ=N1
N=N1
IF (ITPRT.GT.0) CALL WRTOIIr2
DO 5 I1=1,N1+1
   DO 5 I2=1,N1
      C(I1,I2)=C(I1,I2)
   5 CONTINUE

LOOP BEGUN FOR ITERATIONS

DO 75 ITCNT=1,50

COLD ARRAY SET UP

DO 10 K=1,N
   DO 10 J=1,NJ
      COLD(K,J)=C(K,J)
10 CONTINUE

C LOOP BEGUN TO MARCH THROUGH EACH NODE POINT. SUBSEQUENT CALCULATIONS
PERFORMED AT EACH NODE POINT. G VALUES ALSO SET AT -F().
CALL FUNCT1(J)
DO 15 I=1,N
SUM(I)=0.0
G(I)=-F(I)
CONTINUE
15 THIS IS THE PLACE THE DERIVATIVES ARE CALCULATED. MM IS SET TO INDICATE THE INTERVAL WHERE THE DERIVATIVES ARE TO BE CALCULATED (IN RELATION TO J).

IF (J.EQ.1) THEN
MM=0
ELSE IF (J.LT.NJ) THEN
MM=-1
ELSE
MM=-2
ENDIF
DO 50 M=MM,MM+2

ORIGINAL VALUES OF C STORED IN SAVEC AND WORKC

DO 50 K=1,N
SAVEC=C(K,J+M)
WORKC=SAVEC

DERIVATIVES CALCULATED FOR SMALL VALUES OF C (LESS THAN TINY)

IF (ABS(WORKC).LT.TINY) THEN
IF (ABS(WORKC).LT.TINY) WORKC=SIGN(TINY,WORKC)
C(K,J+M)=1.2*WORKC
CALL FUNCT1(J)
DO 20 I=1,N
AA(I)=-F(I)
CONTINUE
20 C(K,J+M)=1.1*WORKC
CALL FUNCT1(J)
DO 25 I=1,N
AA(I)=AA(I)+4.0*F(I)
CONTINUE
25 C(K,J+M)=1.0*WORKC
CALL FUNCT1(J)
DO 30 I=1,N
AA(I)=(AA(I)-3.0*F(I))/(CU-CD)*WORKC)
CONTINUE
30 ELSE
C(K,J+M)=WORKC*C
CALL FUNCT1(J)
DO 35 I=1,N
AA(I)=-F(I)
CONTINUE
35 C(K,J+M)=WORKC*CD
CALL FUNCT1(J)
DO 40 I=1,N
AA(I)=(AA(I)-F(I))/((CU-CD)*WORKC)
CONTINUE
40 ENDIF
C(K,J+M)=SAVEC

VALUES FOR A,B,D,X AND Y GIVEN. SUM IS ALSO INCREMENTED

DO 45 I=1,N
SUM(I) = SUM(I) + AA(I) * C(KJ + M)
IF (M.EQ.-2) Y(LK) = AA(I)
IF (M.EQ.-1) A(LK) = AA(I)
IF (M.EQ.0) B(LK) = AA(I)
IF (M.EQ.1) D(LK) = AA(I)
IF (M.EQ.2) X(LK) = AA(I)

CONTINUE

DO SS = 1,N
G(I) = G(I) + SUM(I)
CONTINUE

BAND CALLED TO SOLVE THE BLOCK TRIDIAGONAL MATRIX

CALL BAND2(J)

CONVERGENCE CRITERION CHECKED. IF ANY VALUE OF RELATIVE CONVERGENCE
FOR ANY VARIABLE IS GREATER THAN THE CONVERGENCE CRITERION, A NEW
ITERATION IS BEGUN

DO 65 K = 1,N
DO 65 J = 1,N
IF (DABS(C(K,J)).GT.TNINST) THEN
IF (DABS((C(K,J)-COLD(K,J))/C(K,J)).GT.ERR) GO TO 70
ENDIF
65 CONTINUE
GO TO 80
70 IF (ITPRT.GT.0) CALL WRTOUT2
CONTINUE
80 CONTINUE
DO 95 I = 1,N
DO 95 J = 1,N
C(I,J) = C(I,J)
95 CONTINUE
RETURN

SUBROUTINE WRTOUT2

C******************************************************************************
IMPLICIT REAL*8(A-H,O-Z)
COMMON/BND/A(14,13),B(14,13),C(14,201),D(14,29),X(14,13),
Y(14,13),G(14),N,N,ITPRT,ITCNT,F(14)
IF (ITCNT.NE.0) WRITE (*,99)ITCNT
WRITE (*,100)
DO 1 K = 1,N
WRITE(*,101)K,(C(I,K),I=1,N)
1 CONTINUE
99 FORMAT( ITCNT='12)
100 FORMAT( J C1 C2 C3
   & C4 C5 C6)
101 FORMAT(1X,I,6(1PE16.8))
RETURN

BLOCK TRIDIAGONAL MATRIX SUBROUTINE
SUBRO...TINE BAND2(J)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION E(14,14,201)
COMMON/BND/A(14,13),B(14,13),C(14,201),D(14,29),X(14,13),Y(14,13),
G(14),N,N,ITPRT,ITCNT,F(14)
101 FORMAT(0DETERM=0 AT J='I4)
IF (J.EQ.1) THEN
N+1 = N + 1
DO 2 J = 1,N

G-33
D(L2*N+I)=G(I)
DO 2 L=1,N
D(LL+N)=X(LL)
2 CONTINUE
CALL MATINV2(N,2*N+I,DETERM)
IF(DETERM.EQ.0) WRITE (2,101) J
DO 5 K=1,N
E(K,NP1,1)=D(K,2*N+I)
DO 5 L=1,N
E(K,L,1)=D(K,L,1)
X(K,L,1)=D(K,L)+N
5 CONTINUE
RETURN
ELSE IF(J.EQ.2) THEN
DO 7 I=1,N
DO 7 K=1,N
DO 7 L=1,N
D(I,K)=D(I,K)+A(I)*X(K)
7 CONTINUE
RETURN
ELSE IF(J.EQ.N) THEN
DO 10 I=1,N
DO 10 L=1,N
G(I)=G(I)-Y(LL)*E(LL,LP1LJ-2)
DO 10 M=1,N
A(LL)=A(LL)+Y(IM)*E(IM,LJ-2)
10 CONTINUE
ENDIF
DO 12 I=1,N
D(LNP1)=G(I)
DO 12 L=1,N
D(LNP1)=D(LNP1)+A(II)*E(LNP1LJ-1)
DO 12 K=1,N
B(LK)=B(LK)+A(I)*E(LKJ-1)
12 CONTINUE
CALL MATINV2(N,NP1,DETERM)
IF(DETERM.EQ.0) WRITE (2,101) J
DO 15 K=1,N
DO 15 M=1,N
E(K,M)=D(K,M)
15 CONTINUE
IF(J.EQ.N) THEN
DO 17 K=1,N
C(KJ)=E(K,NP1,J)
17 CONTINUE
DO 18 M=NLJ-1,1,-1
DO 18 K=1,N
C(K,M)=E(K,NP1,M)
DO 18 L=1,N
C(K,M)=C(K,M)+E(K,L,M)*C(L,M+1)
18 CONTINUE
DO 19 L=1,N
DO 19 K=1,N
C(K,L)=C(K,L)+X(K,L)*C(L3)
19 CONTINUE
ENDIF
RETURN
END
C
MATRIX INVERSION SUBROUTINE
SUBROUTINE MATINV2(N,M,DETERM)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION ID(14)
COMMON/BND/A(14,13),B(14,13),C(14,201),D(14,29)
DETERM=1.0
DO 1 I=1,N
   ID(I)=0
DO 18 NI=1,N
   BMAX=0.0
DO 6 I=1,N
   IF(ID(I).EQ.0)THEN
      DO 5 J=1,N
         IF(DABS(B(JLJ)).GT.BMAX)THEN
            BMAX=DABS(B(JLJ))
            IROW=I
            JCOL=J
         ENDIF
      ENDIF
   CONTINUE
   6 CONTINUE
   IF(BMAX.EQ.0.0)THEN
      DETERM=0.0
      RETURN
   ENDIF
   5 CONTINUE
   IF(JCOL.NE.IROW) THEN
      DO 10 J=1,N
         SAVE=B(IROW,J)
         B(IROW,J)=B(JCOL,J)
         B(JCOL,J)=SAVE
      CONTINUE
      DO 11 K=1,M
         SAVE=D(IROW,K)
         D(IROW,K)=D(JCOL,K)
         D(JCOL,K)=SAVE
      CONTINUE
      FF = 1.0/B(JCOL,JCOL)
      DO 13 J=1,N
         B(JCOL,J)=B(JCOL,J)*FF
      DO 14 K=1,M
         D(JCOL,K)=D(JCOL,K)*FF
      DO 18 I=1,N
         IF(I.NE.JCOL)THEN
            FF = B(I,JCOL)
            DO 16 J=1,N
               B(JLJ) = B(JLJ) - FF*B(JCOL,J)
            DO 17 K=1,M
               D(LK) = D(LK) - FF*D(JCOL,K)
            ENDIF
         CONTINUE
      RETURN
      END