INTERACTIVE COMPUTER MODELING OF COMBUSTION CHEMISTRY
and
COALESCENCE-DISPERSION MODELING OF TURBULENT COMBUSTION

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The goals of this research project are as follows:

1. Develop an interactive computer code for simulation of a high-intensity turbulent combustor as a "single point" inhomogeneous stirred reactor [1]. This will be developed from an existing batch processing computer code CDPSR [2].

2. Use the interactive CDPSR code as a guide for interpretation and direction of DOE-sponsored companion experiments utilizing Xenon tracer with optical laser diagnostic techniques to experimentally determine the appropriate mixing frequency, and for validation of CDPSR as a mixing-chemistry model for a laboratory jet-stirred reactor.

3. Incorporate the coalescence-dispersion model for finite rate mixing into an existing interactive code AVCO-MARK I, to enable simulation of a combustor as a modular array of stirred flow and plug flow elements, each having a prescribed finite mixing frequency, or axial distribution of mixing frequency, as appropriate.

4. Further increase the speed and reliability of the batch kinetics integrator code CREKID [3] by rewriting in vectorized form for execution on a vector or parallel processor, and by incorporating numerical techniques which enhance execution speed by permitting specification of a very low accuracy tolerance [4].

REFERENCES


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Figure 1. Jet-stirred reactor with optical access (2). Details:
(a) annular reactor wall; (b) reactor feed tube; (c) spring-loaded window holder; (d) exhaust ports; and (e) sapphire window.

Figure 2. Measured and homogeneous PSR predicted (CHN), and uncorrected thermocouple temperature for combustion of CHN-air at $\Delta P = 19$ kg/cm². (2)
Circles are values predicted from CUBAR code with $NT = 20$. 252
Figure 3. Measured IDI normalized by D-OH equilibrium, and (homogeneous PSR) predicts IDI for combustion of CH/air at D/V = 19 kg/cu ft. Crosses are predicted values from CDR code with NT = 20.

**Figure 4.1**

- **FEED 1 POPULATION** = N₁
- **COMBUSTOR POPULATION** = N
- **MASS FLOW RATE**
- **MIXING AND FLOW**
- **FEED 2 POPULATION** = N₂

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OF POOR QUALITY

FEED 1 POPULATION = \( N_1 \)

COMBUSTOR POPULATION = \( N \)

FEED 2 POPULATION = \( N_2 \)

\[ k = K K-1 K-2 \cdots \]

MASS FLOW RATE \( \dot{n} \)

MIXING FLOW

\[ \alpha \]

\[ L \]

\[ z \]

\[ i \]

\[ 0 \]

\[ \text{GAUSSIAN DISTRIBUTION FUNCTION} \]

\[ 05 \quad 10 \quad 15 \quad 20 \]

LOCAL FUEL AIR EQUIVALENCE RATIO

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \quad 120 \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \quad 120 \]

\[ n=1 \quad n=2 \quad n=3 \quad n=4 \]

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MARKII

"MARKII" IS AN INTERACTIVE VERSION OF THE MARK-II COMBUSTOR MODEL. THIS IS A PRELIMINARY DESIGN TOOL. A MEANS OF GAINING INTUITIVE INSIGHT INTO EFFECTS OF CHANGES IN FUEL-AIR MIXING OR PARTITIONING ON TURN-DOWN RATIO, COMBUSTION EFFICIENCY AND POLLUTANT FORMATION RATES.

AN INITIAL DATA SET IS TAKEN FROM DATA FILE "MARK2.DAT" BUT CAN BE ALTERED INTERACTIVELY, AND USED IN CONSECUTIVE RUNS.

MARK-II REPRESENTS A SIMPLE BRAZED COMBUSTOR CONSISTING OF A MAXIMUM OF 9 FLOW ELEMENTS WITH THE ADDITION OF A SINGLE RECYCLE ELEMENT. FLOW ELEMENT TYPES MAY INCLUDE:
1) NON-REACTING MIXERS ("MIX"), IN WHICH THE CHEMICAL REACTIONS ARE ASSUMED TO HAVE STOPPED DURING THE MIXING PROCESS;
2) PERFECTLY STIRRED REACTORS ("PSR"), WITHIN WHICH INTENSE SELF- OR BACK-MIXING IS ASSUMED TO OCCUR, SO THAT THERE ARE NO AXIAL GRADIENTS;
3) FLUG FLOW REACTORS ("FFR").

THE USER MAY DEFINE THE MODEL AS HAVING UP TO 9 ELEMENTS IN SERIES WITH AIR AND FUEL INLET JETS AT EACH ELEMENT. THE RECYCLE ELEMENT MAY BE ANY OF THE THREE FLOW TYPES, AND MUST RECYCLE FROM A HIGHER NUMBERED ELEMENT TO A LOWER. COOLING BOUNDARY LAYER EFFECTS AND CHEMICAL REACTIONS WITHIN THE BOUNDARY LAYER ARE NOT CONSIDERED.

--- PLEASE WAIT A MOMENT WHILE INITIALIZATION IS COMPLETED ---

--- INITIALIZED -- PRESS *RETURN* TO BEGIN ---

--- INPUT DATA ---

<table>
<thead>
<tr>
<th>FLOW ELEMENT</th>
<th>LENGTH (INCHES)</th>
<th>FLOW TYPE</th>
<th>INLET AIR (LDM/S)</th>
<th>INLET FUEL (LDM/S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.4405E02</td>
<td>4.0000E-01</td>
<td>FSR</td>
<td>1.3350E00</td>
</tr>
<tr>
<td>2</td>
<td>1.4400E02</td>
<td>1.0000E-01</td>
<td>MIX</td>
<td>0.0000E-01</td>
</tr>
<tr>
<td>4</td>
<td>1.4500E00</td>
<td>2.0000E-01</td>
<td>MIX</td>
<td>0.0000E-01</td>
</tr>
<tr>
<td>RECYCLE</td>
<td>1.4400E02</td>
<td>1.0000E+00</td>
<td>MIX</td>
<td>0.0000E+00</td>
</tr>
</tbody>
</table>

AIR TEMP = 2.1000E02 F
FUEL TEMP = 0.0000E01 F

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET
-1- CHANGE AIR TEMPERATURE
-2- CHANGE FUEL TEMPERATURE
-3- CHANGE LOWER HEATING VALUE
ACTION? (0-7) 7

MARKII MODEL SCHEMATIC LAYOUT

--- PRESS RETURN TO CONTINUE ---