FAST COMPUTATIONAL KINETICS PROGRAM

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1. Introduction

This project has two goals: First, to develop very fast algorithms for solution of the transient and stationary-state equations describing combustion chemical kinetics in batch and stirred-tank chemical reactors, for imbedding in larger hydrodynamic codes which model mixing, heat transfer and chemical change in gas turbine combustors and other combustion devices. The second goal is to develop "user-friendly" interactive computer programs which combine the fast kinetics algorithms with graphics and user selection menus to create a dynamic environment for parametric variation, preliminary design, and in general permitting the user to gain an improved understanding of the thermal-chemical-physical behavior of combustion processes, without being hampered by considerations of numerical methods, stability, convergence or computational efficiency.

2. Batch Kinetics (1-D) Algorithm Development

A typical batch combustion problem at constant pressure consists of three distinctly different chemical-physical regimes, each of which requires a unique algorithm for the peculiar form of stiffness of the governing set of ordinary differential equations. (The term "stiff", coined by Hirschfelder, means that the characteristic time constants of the coupled set of equations differ by many orders of magnitude, so that integration of the equations by conventional methods would require time-steps very much smaller than desired, resulting in excessively large computational work. [1])

A single-step integration algorithm was developed which automatically identifies equations as having either positive or negative time constants, and then approximates the unstable equations (positive time constants) with the trapezoidal rule, and the stable equations (negative time constants) with a decaying exponential function. This "exponential-fitted trapezoidal rule" was adapted form the work of Liniger and Willoughby [2] and of Brandon [3].

During induction and early heat-release regime, the species equations are dominated by positive time constants, and the temperature also exhibits a positive time constant. Since very small steps are required for integration of unstable equations, a simple predictor-corrector scheme with functional iteration assures the least computational work possible. However, during late heat release and equilibration, when the temperature and species equations exhibit negative time constants, large stepsizes are now possible, so that Newton-Raphson iteration with calculation of the full Jacobian matrix is the optimal convergence method. At the present level of development, the batch kinetics code CREK-1D (for "combustion reaction kinetics, one-dimensional") appears to be at least five times faster than LSODE, the Lawrence Livermore Laboratory implementation of the Gear-B algorithm [4]. Further details of the algorithm are given in Reference 5.

3. Stirred Reactor (0-D) Algorithm Development

An earlier packaged code, CREK [6], solved for time-stationary states of a perfectly-stirred chemical reactor. A major improvement has been made in the automatic estimate-generating feature of the CREK code. In this approach, the transient stirred-reactor equations are solved for the predictor step only, using the same techniques developed for the batch kinetics CREK-1D code. The resulting approximate solution gives a very good estimate of the steady-state solution, which is then solved for exactly using the original CREK algorithm. As a result, the speed and reliability of the "CREK-0D" program appears to have been increased by at least an order of magnitude over the original CREK code.

4. Interactive Computer Programs

Two "user-friendly", menu-driven programs have been written to date. The first program, EQLBRM, solves for chemical equilibrium states for combustion of arbitrary hydrocarbon fuels with air, at a specified constant pressure, fuel-air ratio and initial temperature of fuel and air. The second program, AVCO-M2, is a reactor-theoretic simulation of a gas turbine combustor [7]. The combustor is assumed to consist of up to nine "flow elements" connected in series, and optionally one flow element connected in recycle. Each flow element may be a zero-dimensional or perfectly-stirred reactor (PSR), a one-dimensional or plug-flow reactor (PFR), or a non-reacting mixer (MIX). The user is prompted to select the order, type and size of the flow elements, the recycle path, and the distribution of fuel and air into each individual flow element. On demand, the program also displays a crude graphic schematic of the combustor model under consideration.

1. Lambert, J. D., Computational Methods in Ordinary Differential Equations, John Wiley and Sons (1973).

2. Liniger, W. and Willoughby, R. A., "Efficient Integration Methods for Stiff Systems of Ordinary Differential Equations", SIAM J. Numer. Anal. 7, 47-66 (1970).

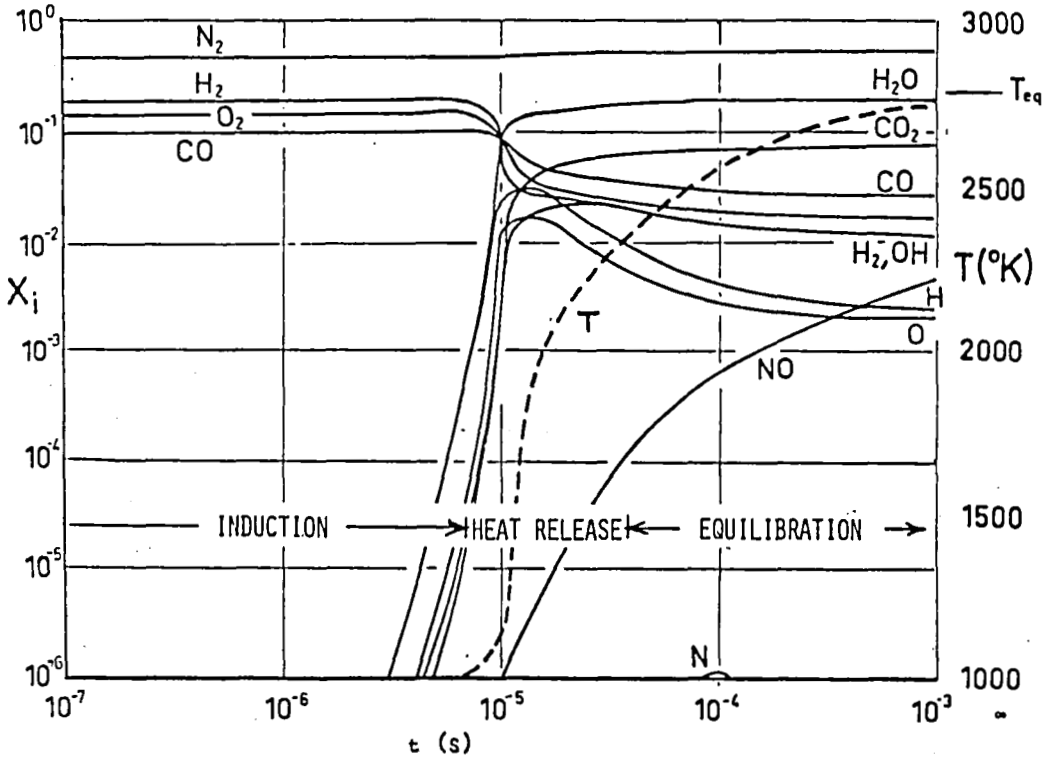
3. Brandon, D. M., Jr., "A New Single-Step Integration Algorithm with A-Stability and Improved Accuracy", Simulation 23, No. 1 (1974).

4. Hindmarsh, A. C., LSODE and LSODI, Two New Initial Value Ordinary Differential Equation Solvers, ACM-SIGNUM Newsletter 15, No. 4., 10-11 (1980).

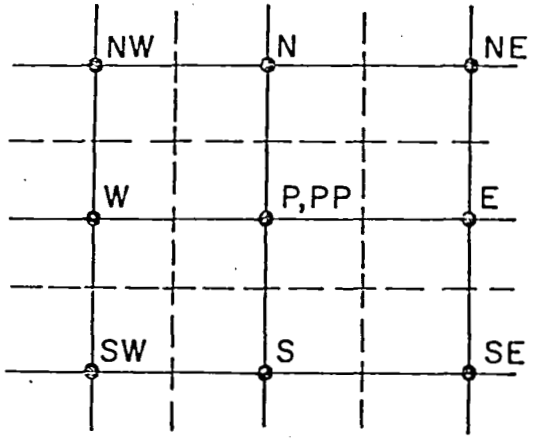
5. Pratt, D. T., Fast Algorithms for Combustion Kinetics Calculations, International Symposium on Stiff Computation, Park City, Utah, April 12-14 (1982).

6. Pratt, D. T. and Wormeck, J. J., CREK - A Computer Program for Calculation of Combustion Reaction Equilibrium and Kinetics in Laminar or Turbulent Flow, Report WSU-ME-TEL-76-1, Washington State University (1976).

7. Pratt, D. T., AVCO "Mark-11" Combustor Model, Program No. K140 MK2, IRAD Report, AVCO-Lycoming Division, Stratford, Connecticut, March (1980).



Variation with time of temperature and chemical species mole fraction in adiabatic batch reaction. (Pyrolized CH_4-air, Stoichiometric, T=1000K, P=10 atm)



Conventional staggered finite-difference grid for calculation within a flow domain. Points H ("high") and L ("low") are above and below the plane of E-W-N-S-P. PP refers to conditions at P at the previous time step.

HOMOGENEOUS, ADIABATIC, GAS-PHASE
REACTION AT CONSTANT PRESSURE

$$\frac{d\sigma_i}{dt} = -\frac{r_i}{\rho} + \frac{\dot{m}}{\rho V}(\sigma_i^* - \sigma_i) \qquad 1 \quad 2 \quad 3$$

Batch kinetics (1-D) $\quad 3 \longleftarrow 0$

Stirred-reactor kinetics (0-D) $\quad 1 \longleftarrow 0$

where

$$r_i = \sum_{j=1}^{J} (\alpha''_{ij} - \alpha'_{ij})(R_j - R_{-j})$$

$$R_j = k_j (\rho\sigma_m)^{\overline{\alpha_j}} \prod_{k=1}^{N} (\rho\sigma_k)^{\alpha'_{kj}}$$

$$k_j = 10^{B_j} T^{N_j} \exp(-T_j/T)$$

$$\rho = P/RT\sigma_m \qquad \sigma_m = \sum_{k=1}^{N} \sigma_i$$

$$H_o = \sum_{k=1}^{N} h_k\sigma_k = \text{const.}$$

"LOCALLY EXACT" SOLUTIONS
OF THE TRANSIENT EQUATIONS

1. Decoupling

$$\text{let } \frac{d\sigma_i}{dt} \equiv f_i\,(\sigma_k, T; P) = A_i + B_i\sigma_i$$

2. Integration

$$\sigma_i^{n+1} = -\frac{A_i}{B_i} + \left[\sigma_i^n + \frac{A_i}{B_i}\right] e^{B_i h}$$

$$\text{or } \sigma_i^{n+1} = \sigma_i^n + h f_i^n \left[\frac{e^{B_i h}-1}{B_i h}\right]$$

where $h = t^{n+1} - t^n$

3. Analysis

The locally exact solution is stable (for $h \to \infty$) if and only if $B_i \leq 0$.

FORMALLY DECOUPLING THE EQUATIONS: "L - FORMULATION" .

let $\frac{r_i}{\rho} = D_i - Q_i \quad ; \quad D_i = L_i \sigma_i$

then $\frac{d\sigma_i}{dt} = Q_i - L_i \sigma_i + \frac{\dot{m}}{\rho V} (\sigma_i^* - \sigma_i)$

$$= \left[Q_i + \frac{\dot{m}}{\rho V} \sigma_i^* - L_i + \frac{\dot{m}}{\rho V} \sigma_i \right]$$

$\Rightarrow$ $A_i = \left[Q_i + \frac{\dot{m}}{\rho V} \sigma_i^* \right]$

$B_i = - \left[L_i + \frac{\dot{m}}{\rho V} \right]$

. . . A_i is positive-definite; B_i negative-definite

$\therefore$ "L-formulated" equations are always

stable, but may be inaccurate.

FUNCTIONALLY DECOUPLING THE EQUATIONS : "Z-FORMULATION"

let $$\frac{d\sigma_i}{dt} = f_i = f_i^o + Z_i^o \, (\sigma_i - \sigma_i^o)$$

where $$Z_i \equiv \frac{df_i}{d\sigma_i} = \sum_{k=1}^{N} \frac{\partial f_i}{\partial \sigma_k} \cdot \frac{f_k}{f_i} + \frac{\dot{T}}{f_i} \frac{\partial f_i}{\partial T}$$

(and where $\dot{T} = - \sum_k h_k f_k \; / \; \sum_k C_{p_k} \sigma_k$)

then $$\frac{d\sigma_i}{dt} = [f_i^o - Z_i^o \sigma_i^o] + Z_i^o \sigma_i$$

$\Rightarrow$ $$A_i = [f_i^o - Z_i^o \sigma_i^o]$$

$$B_i = Z_i^o$$

. . . neither A_i nor B_i are positive-definite or negative-definite.

$\therefore$ "Z-formulated" equations are always <u>accurate</u>, but may be <u>unstable</u>.

```
        *** MARK2I ***
     'MARK2I' 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 BRAGG 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) PLUG FLOW REACTORS ('PFR').
     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 OF 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.

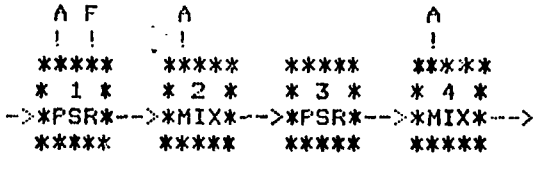
--- INITIALIZED -- PRESS <RETURN> TO BEGIN --
```

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR      INLET FUEL
 ELEMENT#      (SQ.IN)        (INCHES)       TYPE         (LBM/S)        (LBM/S)
    1       1.4600E+02     4.0000E-01        PSR      1.3450E+00     9.7200E-02
    2       1.4600E+02     1.0000E-01        MIX      6.9600E-01     0.0000E-01
    3       1.4600E+02     1.5000E+00        PSR      0.0000E-01     0.0000E-01
    4       1.4500E+00     2.0000E-01        MIX      7.9500E-01     0.0000E-01

 AIR TEMP =  2.1000E+02 F       COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  8.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET            -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE            -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE           -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE        -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 7
```

MARK-II MODEL SCHEMATIC LAYOUT



PRESS <RETURN> TO CONTINUE

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR       INLET FUEL
 ELEMENT#      (SQ.IN)       (INCHES)       TYPE         (LBM/S)         (LBM/S)
    1        1.4600E+02     4.0000E-01     PSR        1.3450E+00      9.7200E-02
    2        1.4600E+02     1.0000E-01     MIX        6.9600E-01      0.0000E-01
    3        1.4600E+02     1.5000E+00     PSR        0.0000E-01      0.0000E-01
    4        1.4500E+00     2.0000E-01     MIX        7.9500E-01      0.0000E-01

 AIR TEMP =  2.1000E+02 F       COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  8.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET          -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE          -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE         -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE      -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 5
```

```
RECYCLE ELEMENT STATUS:
CROSS-SECTIONAL AREA =  1.4600E+02 SQ.INCH
ELEMENT LENGTH       =  1.0000E+00 INCHES
FLOW TYPE            =  MIX
RECYCLES   0.00% OF ELEMENT # 1 OUTFLOW TO ELEMENT # 1 INFLOW

SELECT AN OPTION BY NUMBER:
0- NO MORE CHANGES TO RECYCLE ELEMENT
1- CHANGE AREA
2- CHANGE LENGTH
3- CHANGE FLOW TYPE
4- CHANGE RECYCLE INTAKE PERCENTAGE
5- CHANGE RECYCLE PATH
6- ELIMINATE RECYCLE

OPTION? (0-6) 4
ENTER PERCENT OF OUTFLOW TO BE RECYCLED: 20.
```

```
RECYCLE ELEMENT STATUS:
CROSS-SECTIONAL AREA =  1.4600E+02 SQ.INCH
ELEMENT LENGTH       =  1.0000E+00 INCHES
FLOW TYPE            =  MIX
RECYCLES  20.00% OF ELEMENT # 1 OUTFLOW TO ELEMENT # 1 INFLOW

SELECT AN OPTION BY NUMBER:
0- NO MORE CHANGES TO RECYCLE ELEMENT
1- CHANGE AREA
2- CHANGE LENGTH
3- CHANGE FLOW TYPE
4- CHANGE RECYCLE INTAKE PERCENTAGE
5- CHANGE RECYCLE PATH
6- ELIMINATE RECYCLE

OPTION? (0-6) 5
ENTER ELEMENT WHOSE OUTFLOW IS TO BE RECYCLED: (1- 4) 3
ENTER ELEMENT WHOSE INFLOW IS TO RECEIVE RECYCLE: (1- 3) 2
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```
RECYCLE ELEMENT STATUS:
CROSS-SECTIONAL AREA =  1.4600E+02 SQ.INCH
ELEMENT LENGTH       =  1.0000E+00 INCHES
FLOW TYPE            =  MIX
RECYCLES  20.00% OF ELEMENT # 3 OUTFLOW TO ELEMENT # 2 INFLOW

SELECT AN OPTION BY NUMBER:
0- NO MORE CHANGES TO RECYCLE ELEMENT
1- CHANGE AREA
2- CHANGE LENGTH
3- CHANGE FLOW TYPE
4- CHANGE RECYCLE INTAKE PERCENTAGE
5- CHANGE RECYCLE PATH
6- ELIMINATE RECYCLE

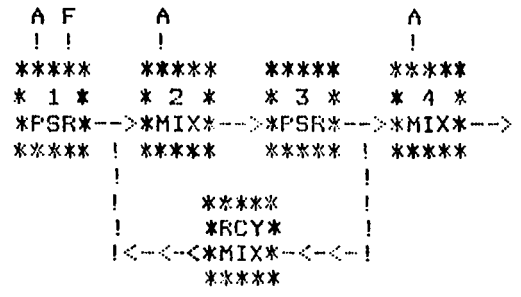
OPTION? (0-6) 0
```

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR       INLET FUEL
 ELEMENT#      (SQ.IN)        (INCHES)      TYPE          (LBM/S)         (LBM/S)
    1        1.4600E+02     4.0000E-01     PSR        1.3450E+00      9.7200E-02
    2        1.4600E+02     1.0000E-01     MIX        6.9600E-01      0.0000E-01
    3        1.4600E+02     1.5000E+00     PSR        0.0000E-01      0.0000E-01
    4        1.4500E+00     2.0000E-01     MIX        7.9500E-01      0.0000E-01
RECYCLE      1.4600E+02     1.0000E+00     MIX         RECYCLE  20.00% OF # 3
                                                      OUTFLOW TO # 2 INFLOW

 AIR TEMP =  2.1000E+02 F       COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  8.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET              -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE              -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE             -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE          -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 7
```

MARK-II MODEL SCHEMATIC LAYOUT



PRESS <RETURN> TO CONTINUE

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR      INLET FUEL
 ELEMENT#      (SQ.IN)       (INCHES)       TYPE         (LBM/S)        (LBM/S)
    1        1.4600E+02     4.0000E-01      PSR       1.3450E+00     9.7200E-02
    2        1.4600E+02     1.0000E-01      MIX       6.9600E-01     0.0000E-01
    3        1.4600E+02     1.5000E+00      PSR       0.0000E-01     0.0000E-01
    4        1.4500E+00     2.0000E-01      MIX       7.9500E-01     0.0000E-01

 AIR TEMP =  2.1000E+02 F       COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  8.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET              -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE              -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE             -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE          -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 6
```

```
TO CHANGE DATA, ENTER THE CODE AND ELEMENT #. (IE "B2" FOR #2'S LENGTH)

              CODE "A"      CODE "B"   CODE "C"      CODE "D"       CODE "E"
  FLOW          AREA         LENGTH      FLOW       INLET AIR      INLET FUEL
 ELEMENT#     (SQ.IN)       (INCHES)    TYPE        (LBM/S)        (LBM/S)
    1        1.4600E+02     4.0000E-01      PSR       1.3450E+00     9.7200E-02
    2        1.4600E+02     1.0000E-01      MIX       6.9600E-01     0.0000E-01
    3        1.4600E+02     1.5000E+00      PSR       0.0000E-01     0.0000E-01
    4        1.4500E+02     2.0000E-01      MIX       7.9500E-01     0.0000E-01
CODE "F" - REMOVE ENTIRE FLOW ELEMENT
CODE "G" - ADD ANOTHER FLOW ELEMENT (NO NUMBER NEEDED)
   (BLANK ENTRY RETURNS TO MAIN MENU)

ENTER CODE,ELEMENT# A4
ENTER CROSS-SECTIONAL AREA OF  ELEMENT # 4 (SQUARE INCHES): 2.00E2
ENTER CODE,ELEMENT# A4
ENTER CROSS-SECTIONAL AREA OF  ELEMENT # 4 (SQUARE INCHES): 1.45E2
ENTER CODE,ELEMENT#
```

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR      INLET FUEL
 ELEMENT#      (SQ.IN)       (INCHES)       TYPE         (LBM/S)        (LBM/S)
    1        1.4600E+02     4.0000E-01      PSR       1.3450E+00     9.7200E-02
    2        1.4600E+02     1.0000E-01      MIX       6.9600E-01     0.0000E-01
    3        1.4600E+02     1.5000E+00      PSR       0.0000E-01     0.0000E-01
    4        1.4500E+00     2.0000E-01      MIX       7.9500E-01     0.0000E-01
RECYCLE      1.4600E+02     1.0000E+00      MIX        RECYCLE  20.00% OF # 3
                                                      OUTFLOW TO # 2 INFLOW

 AIR TEMP =  2.1000E+02 F       COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  8.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET              -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE              -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE             -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE          -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 2

ENTER FUEL TEMPERATURE (DEG FAHRENHEIT): 90.
```

```
*** INPUT DATA ***
   FLOW          AREA          LENGTH        FLOW        INLET AIR       INLET FUEL
 ELEMENT#      (SQ.IN)       (INCHES)       TYPE         (LBM/S)         (LBM/S)
    1        1.4600E+02     4.0000E-01      PSR       1.3450E+00      9.7200E-02
    2        1.4600E+02     1.0000E-01      MIX       6.9600E-01      0.0000E-01
    3        1.4600E+02     1.5000E+00      PSR       0.0000E-01      0.0000E-01
    4        1.4500E+00     2.0000E-01      MIX       7.9500E-01      0.0000E-01
RECYCLE      1.4600E+02     1.0000E+00      MIX        RECYCLE  20.00% OF # 3
                                                      OUTFLOW TO # 2 INFLOW

 AIR TEMP =  2.1000E+02 F        COMBUSTOR PRESSURE =  2.2100E+00 ATM
FUEL TEMP =  9.0000E+01 F      LOWER HEATING VALUE =  1.8500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:
-0- RUN WITH THIS DATA SET              -4- CHANGE NOMINAL COMBUSTOR PRESSURE
-1- CHANGE AIR TEMPERATURE              -5- CHANGE RECYCLE ELEMENT STATUS
-2- CHANGE FUEL TEMPERATURE             -6- CHANGE FLOW ELEMENTS STATUS
-3- CHANGE LOWER HEATING VALUE          -7- INSPECT SCHEMATIC MODEL LAYOUT
OPTION? (0-7) 0
RUN WITH THIS DATA SET --- ARE YOU SURE? (Y/N) Y
```

```
*** OUTPUT: ***

TEMP AND COMPOSITION FOR MARK-II MODEL:
PRESSURE =  2.21 ATM        OVERALL E.R. =  0.4995
FUEL FLOW = 349.92 LBM/HR      AIR FLOW =      2.84 LBM/SEC

 20.0 PCT. OF FLOW RECYCLED FROM OUTLET OF
ELEMENT NO. 3 TO INLET OF ELEMENT NO. 2

OTHER OUTPUT: SELECT BY NUMBER -
0- QUIT / BEGIN NEXT INPUT DATA SET
1- INSPECT MOLE FRACTIONS
2- INSPECT MASS FRACTIONS
3- INSPECT EMISSIONS INDEX
4- INSPECT MISC. OTHER OUTPUT
5- INSPECT CURRENT INPUT DATA SET
OPTION? (0-4) 1
```

```
MOLE FRACTIONS X(I)
SPECES 'I'        *1*          *2*          *3*          *4*          EQL          RCY
C12H23        7.484D-05    4.070D-05    2.154D-07    1.572D-07    2.886D-19    2.154D-07
C2H2          1.080D-02    6.322D-03    2.300D-03    1.679D-03    2.886D-19    2.300D-03
C2H3          9.782D-04    5.327D-04    6.558D-06    4.785D-06    2.886D-19    6.558D-06
C2H4          7.447D-04    4.054D-04    4.625D-06    3.375D-06    2.886D-19    4.625D-06
CH2O          5.914D-05    3.298D-05    4.315D-06    3.149D-06    1.696D-18    4.315D-06
CH3           5.570D-05    3.092D-05    3.332D-06    2.431D-06    2.886D-19    3.332D-06
CH4           3.815D-12    2.590D-12    2.693D-12    1.965D-12    2.886D-19    2.693D-12
CO            1.428D-02    8.335D-03    2.902D-03    2.118D-03    1.694D-06    2.902D-03
CO2           9.676D-02    6.970D-02    8.616D-02    6.288D-02    6.858D-02    8.616D-02
HCO           1.064D-04    5.848D-05    3.366D-06    2.456D-06    5.752D-15    3.366D-06
H             1.246D-03    7.275D-04    2.554D-04    1.864D-04    1.814D-08    2.554D-04
H2            2.892D-03    1.681D-03    5.569D-04    4.064D-04    5.761D-07    5.569D-04
H2O           1.108D-01    7.716D-02    8.541D-02    6.233D-02    6.569D-02    8.541D-02
HO2           2.861D-04    1.724D-04    8.572D-05    6.255D-05    7.480D-08    8.572D-05
N             3.167D-07    1.751D-07    3.479D-08    2.539D-08    1.602D-13    3.479D-08
NO            3.253D-05    4.941D-05    5.814D-05    4.243D-05    1.201D-03    5.814D-05
NO2           1.374D-07    2.879D-07    4.442D-07    3.241D-07    5.285D-06    4.442D-07
N2            7.249D-01    7.469D-01    7.512D-01    7.617D-01    7.634D-01    7.512D-01
O             1.531D-03    1.022D-03    9.594D-04    7.001D-04    1.912D-06    9.594D-04
OH            4.489D-03    2.965D-03    2.651D-03    1.935D-03    7.152D-05    2.651D-03
O2            3.000D-02    8.386D-02    6.744D-02    1.060D-01    1.010D-01    6.744D-02
PRESS <RETURN> TO CONTINUE
```

```
*** OUTPUT: ***

TEMP AND COMPOSITION FOR MARK-II MODEL:
PRESSURE =  2.21 ATM        OVERALL E.R. =  0.4995
FUEL FLOW = 349.92 LBM/HR     AIR FLOW =      2.84 LBM/SEC

 20.0 PCT. OF FLOW RECYCLED FROM OUTLET OF
ELEMENT NO. 3 TO INLET OF ELEMENT NO. 2

OTHER OUTPUT: SELECT BY NUMBER -
0- QUIT / BEGIN NEXT INPUT DATA SET
1- INSPECT MOLE FRACTIONS
2- INSPECT MASS FRACTIONS
3- INSPECT EMISSIONS INDEX
4- INSPECT MISC. OTHER OUTPUT
5- INSPECT CURRENT INPUT DATA SET
OPTION? (0-4) 4
```

ELEMENT NO.	*1*	*2*	*3*	*4*	EQL	RCY
ELEMENT TYPE	PSR	MIX	PSR	MIX	EQL	RCY-MIX
EQUIV RATIO	1.053D+00	6.941D-01	6.941D-01	4.995D-01	4.995D-01	6.941D-01
RES TIME, SEC	5.647D-04	9.558D-05	1.261D-03	1.879D-06	0.000D-01	4.205D-03
AREA, SQ IN	1.460D+02	1.460D+02	1.460D+02	1.450D+00	0.000D-01	1.460D+02
VELO, FT/SEC	5.903D+01	8.719D+01	9.909D+01	8.872D+03	0.000D-01	-1.982D+01
FLOW, LBM/SEC	1.442D+00	2.673D+00	2.673D+00	2.933D+00	2.933D+00	5.346D-01
AXIAL LOC, IN	4.000D-01	5.000D-01	2.000D+00	2.200D+00	2.200D+00	4.304D+10
ENTH, BTU/LBM	-2.219D+01	-4.426D+00	-4.427D+00	5.530D+00	5.530D+00	-4.380D+00
TEMP EFF	8.192D-01	7.850D-01	9.317D-01	9.260D-01	1.000D+00	9.317D-01
TEMP, DEG F	3.105D+03	2.400D+03	2.810D+03	2.192D+03	2.350D+03	2.810D+03

```
PRESS <RETURN> TO CONTINUE
```

```
*** OUTPUT: ***

TEMP AND COMPOSITION FOR MARK-II MODEL:
PRESSURE =  2.21 ATM        OVERALL E.R. =  0.4995
FUEL FLOW = 349.92 LBM/HR     AIR FLOW =      2.84 LBM/SEC

 20.0 PCT. OF FLOW RECYCLED FROM OUTLET OF
ELEMENT NO. 3 TO INLET OF ELEMENT NO. 2

OTHER OUTPUT: SELECT BY NUMBER -
0- QUIT / BEGIN NEXT INPUT DATA SET
1- INSPECT MOLE FRACTIONS
2- INSPECT MASS FRACTIONS
3- INSPECT EMISSIONS INDEX
4- INSPECT MISC. OTHER OUTPUT
5- INSPECT CURRENT INPUT DATA SET
OPTION? (0-4) 3
```

```
EMISSION INDEX EI(I), GM I/KG FUEL
SPECES 'I'          *1*          *2*          *3*          *4*          EQL          RCY
C12H23         6.545D+00    6.552D+00    3.449D-02    2.759D-02    5.049D-14    6.897D-03
C2H2           1.470D+02    1.584D+02    5.731D+01    4.585D+01    7.858D-15    1.146D+01
C2H3           1.383D+01    1.386D+01    1.697D-01    1.358D-01    8.162D-15    3.394D-02
C2H4           1.092D+01    1.095D+01    1.241D-01    9.930D-02    8.466D-15    2.483D-02
CH2O           9.282D-01    9.530D-01    1.240D-01    9.918D-02    5.325D-14    2.479D-02
CH3            4.377D-01    4.473D-01    4.793D-02    3.834D-02    4.537D-15    9.586D-03
CH4            3.199D-08    3.999D-08    4.134D-08    3.307D-08    4.841D-15    8.267D-09
CO             2.091D+02    2.246D+02    7.778D+01    6.222D+01    4.963D-02    1.556D+01
CO2            2.226D+03    2.952D+03    3.628D+03    2.902D+03    3.156D+03    7.256D+02
HCO            1.614D+00    1.633D+00    9.344D-02    7.475D-02    1.745D-10    1.869D-02
H              6.565D-01    7.056D-01    2.463D-01    1.971D-01    1.912D-05    4.926D-02
H2             3.047D+00    3.262D+00    1.074D+00    8.592D-01    1.214D-03    2.148D-01
H2O            1.043D+03    1.338D+03    1.472D+03    1.178D+03    1.238D+03    2.944D+02
HO2            4.936D+00    5.476D+00    2.707D+00    2.166D+00    2.582D-03    5.414D-01
N              2.318D-03    2.361D-03    4.662D-04    3.730D-04    2.346D-09    9.325D-05
NO             5.102D-01    1.427D+00    1.669D+00    1.335D+00    3.770D+01    3.338D-01
NO2            3.303D-03    1.275D-02    1.955D-02    1.564D-02    2.542D-01    3.910D-03
N2             1.061D+04    2.013D+04    2.013D+04    2.238D+04    2.236D+04    4.027D+03
O              1.281D+01    1.574D+01    1.469D+01    1.175D+01    3.198D-02    2.937D+00
OH             3.990D+01    4.853D+01    4.314D+01    3.452D+01    1.272D+00    8.629D+00
O2             5.018D+02    2.582D+03    2.065D+03    3.557D+03    3.380D+03    4.130D+02
PRESS <RETURN> TO CONTINUE
```

```
*** OUTPUT: ***

TEMP AND COMPOSITION FOR MARK-II MODEL:
PRESSURE =  2.21 ATM        OVERALL E.R. =  0.4995
FUEL FLOW = 349.92 LBM/HR      AIR FLOW =      2.84 LBM/SEC

 20.0 PCT. OF FLOW RECYCLED FROM OUTLET OF
ELEMENT NO. 3 TO INLET OF ELEMENT NO. 2

OTHER OUTPUT: SELECT BY NUMBER -
0- QUIT / BEGIN NEXT INPUT DATA SET
1- INSPECT MOLE FRACTIONS
2- INSPECT MASS FRACTIONS
3- INSPECT EMISSIONS INDEX
4- INSPECT MISC. OTHER OUTPUT
5- INSPECT CURRENT INPUT DATA SET
OPTION? (0-4) 0
DO YOU WANT A HARD COPY OF THE INPUT AND OUTPUT DATA FOR THIS RUN? (Y/N) Y

DO YOU WANT ANOTHER RUN? (Y/N) N

--- QUIT --- ARE YOU SURE? (Y/N) Y


-- FORTRAN STOP
```

PRESENT STATUS OF PROJECT - OCTOBER 1982

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