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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 appopriate 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

1. Pratt, D. T.: Mixing and Chemical Reaction in Continuous Combustion, in Progress. Progress in Energy and Combustion Science, vol. 1, N. A. Chigier, Ed., Pergamon Press, 1976.

2. Pratt, D. T.: Coalescence/Dispersion Modeling of High Intensity Combustion, AIAA J. Energy, 3, 3, 177180, 1979.

3. Pratt, D. T.: CREK1D: A Computer Code for Transient, Gas-phase Combustion Kinetics, Paper No. WSCI 8321, Western States Section/The Combustion Institute, 1983.

4. Pratt, D. T.: Exponential-Fitted Methods for Integrating Stiff Systems of Ordinary Differential Equations: Applications to Homogeneous Gas-Phase Chemical Kinetics, paper presented at the 1984 JANNAF Propulsion Meeting, New Orleans, LA., February 1984.

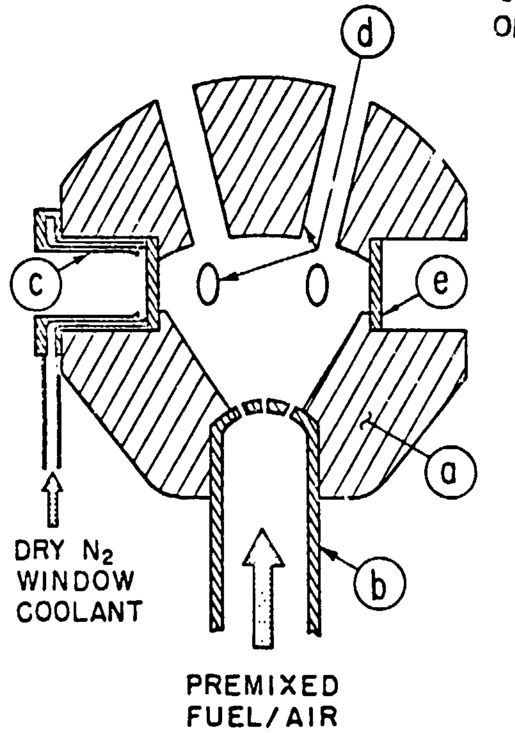


Figure 1. Jet-stirred reactor with optical access [2]. Details: (a) zirconia reactor wall; (b) reactant feed tube; (c) spring-loaded window holder; (d) exhaust ports; and (e) sapphire window

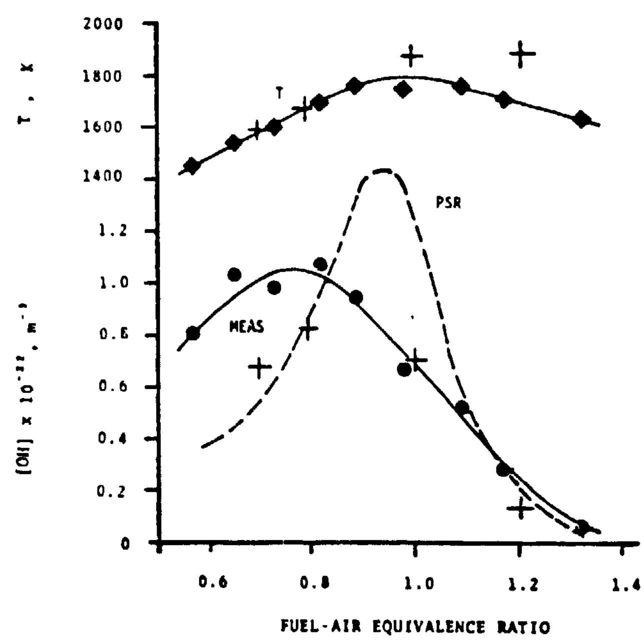


Figure 2. Measured and (homogeneous PSR) predicted [OH], and uncorrected thermocouple temperature for combustion of CH_4/air at $\dot{m}/V$ = 19 kg/cu m/sec. [2]
Crosses are values predicted from CDJSR code with NT = 20.

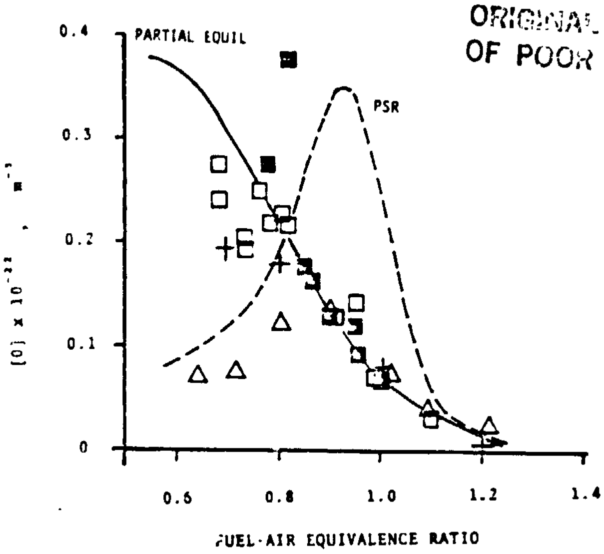


Figure 3. Measured [O] normalized by O-OH equilibrium, and (homogeneous PSR) predicted [O] for combustion of CH_4/air at $\dot{m}/V$ = 19 kg/cu m/s. Crosses are predicted values from CDJSR code with NT = 20.

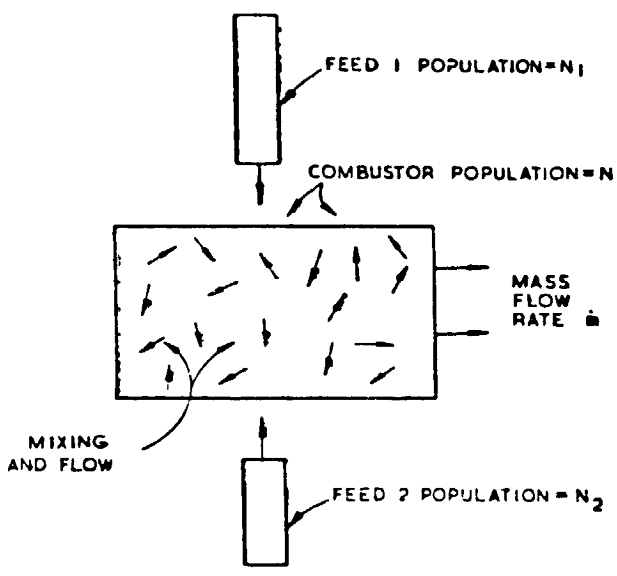
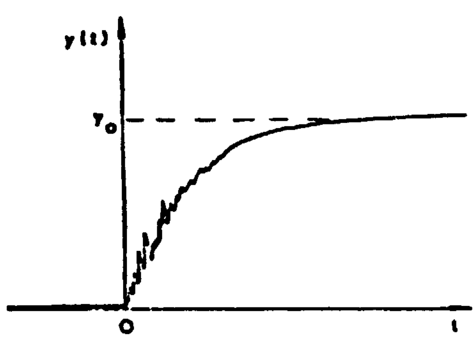


FIG 4 1



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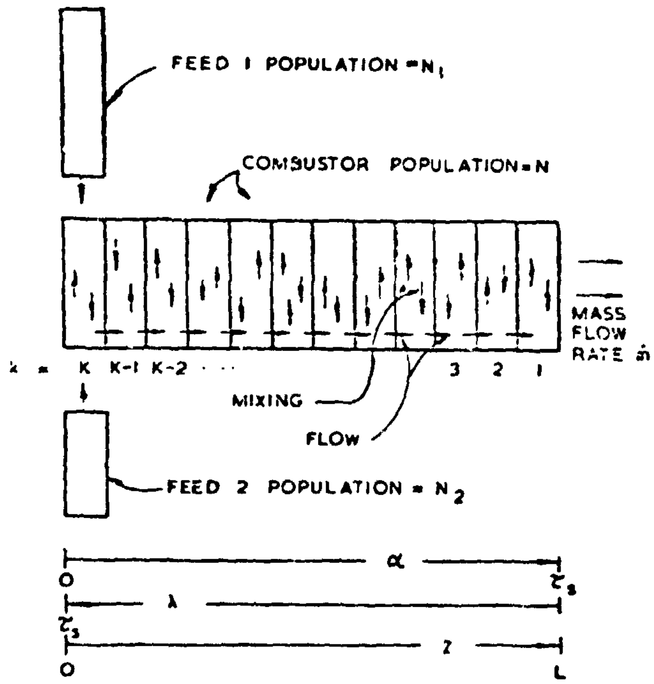

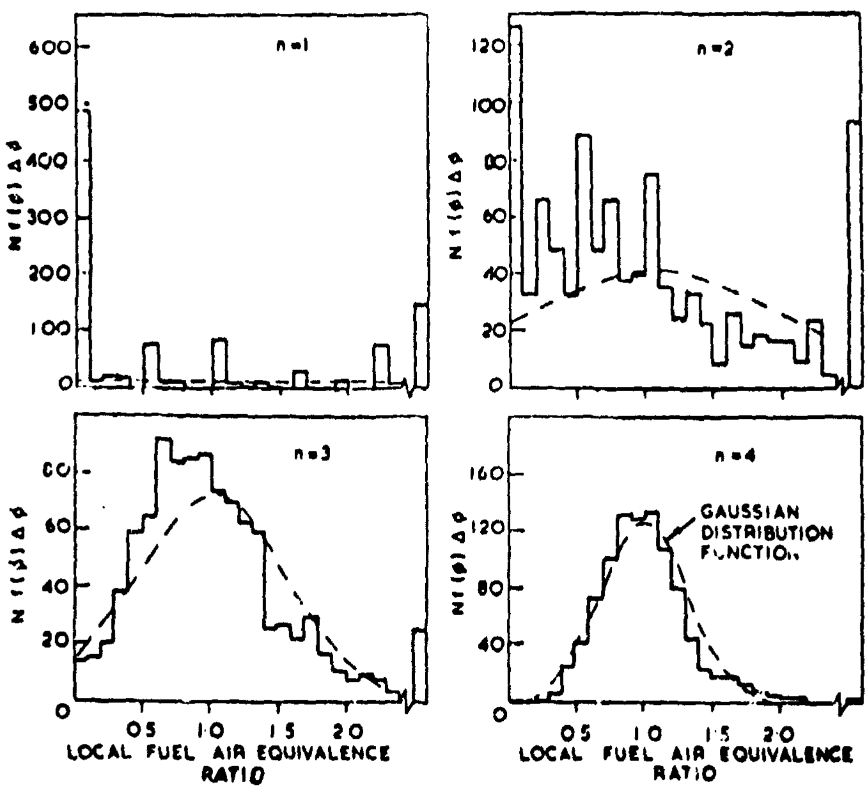

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            *** MARK2I ***
     'MARK2I' IS AN INTERACTIVE VERSION OF THE MARK-II COMBUSTOR MODEL.
THIS IS A PRELIMINARY DESIGN TOOL, A MEANS OF GAINING INTUITIVE INSIGHT
INTO EFFECTS OF CHANGES IN FUEL-AIR MIXING OR PARTITIONING ON TURN-DOWN
RATIO, 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 --
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*** 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
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              MARK-II MODEL SCHEMATIC LAYOUT

                A F     A                 A
                ! !     !                 !
               *****   *****   *****    *****
               * 1 *   * 2 *   * 3 *    * 4 *
               *PSR*-->*MIX*-- *PSR*--  *MIX*-->
               ***** ! *****   ***** !  *****
                     !               !
                     !     *****     !
                     !     *RCY*     !
                     !<--<*MIX*-<--!
                           *****

                PRESS  RETURN  TO CONTINUE
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