N84 20553

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.

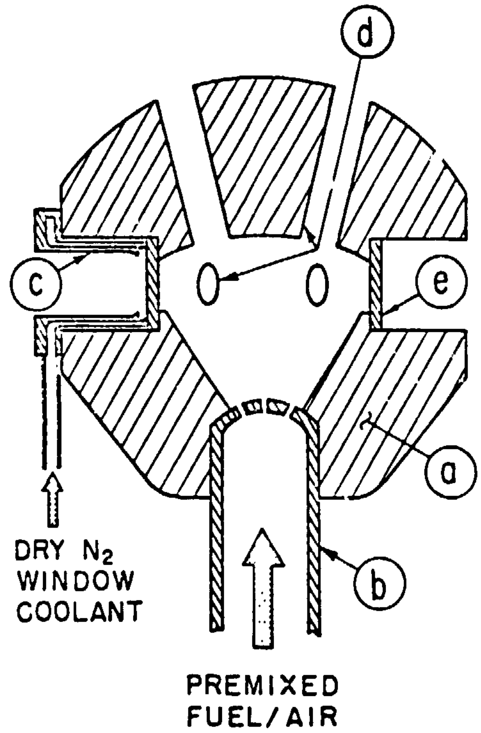


Figure 1. Jet-stirred reactor with optical access [2]. Details: (a) zirconia reactor wall; (b) reactant feed tube; (c) spring-loaded window holder; (d) exhaust ports; and (e) sapphire window

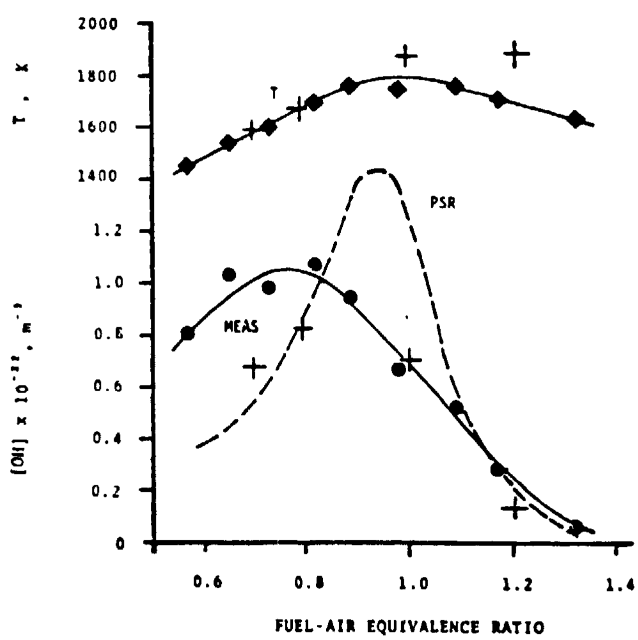


Figure 2. Measured and (homogeneous PSR) predicted [OH], and uncorrected thermocouple temperature for combustion of CH_4/air at $\dot{m}/V$ = 19 kg/cu m/sec. [2]
Crosses are values predicted from CDJSR code with NT = 20.

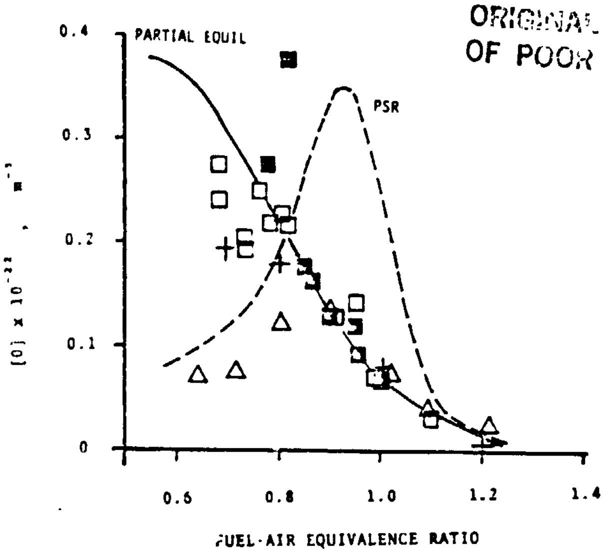


Figure 3. Measured [O] normalized by O-OH equilibrium, and (homogeneous PSR) predicted [O] for combustion of CH_4/air at $\dot{m}/V$ = 19 kg/cu m/s. Crosses are predicted values from CDJSR code with NT = 20.

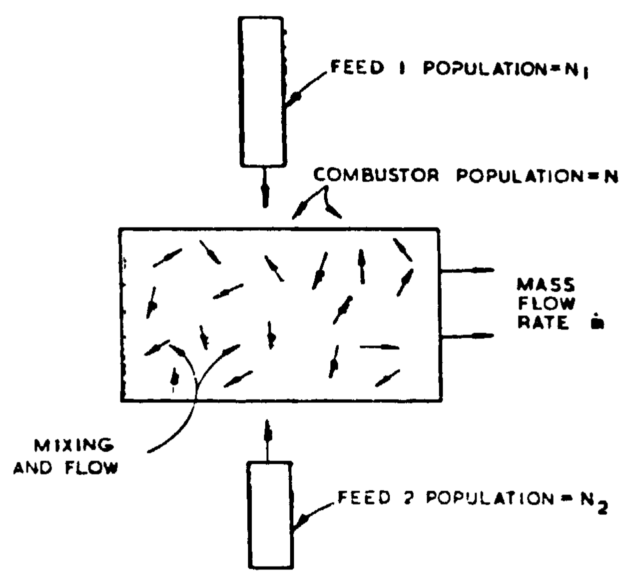
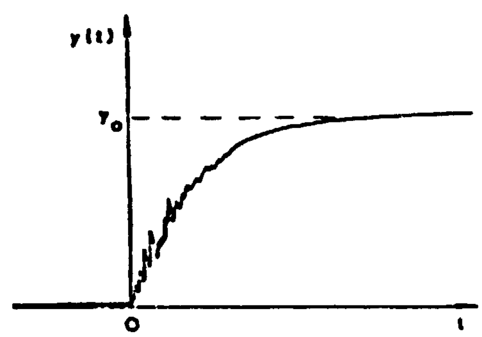
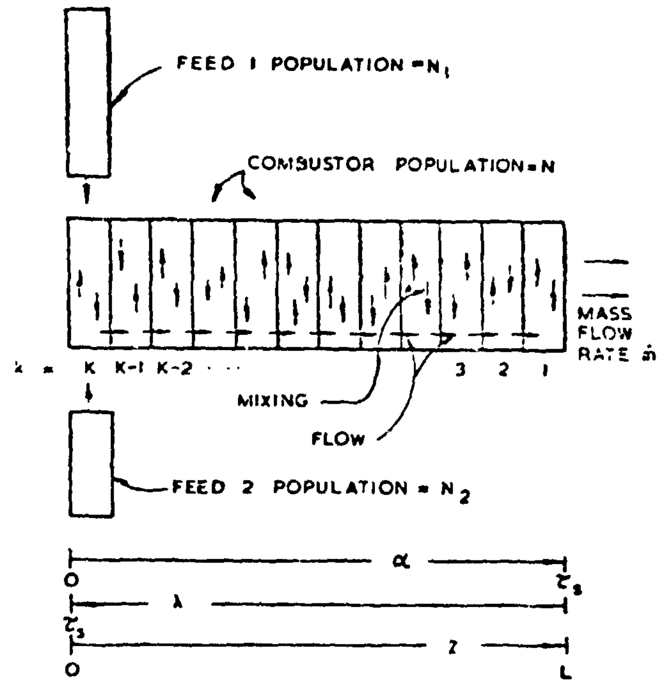
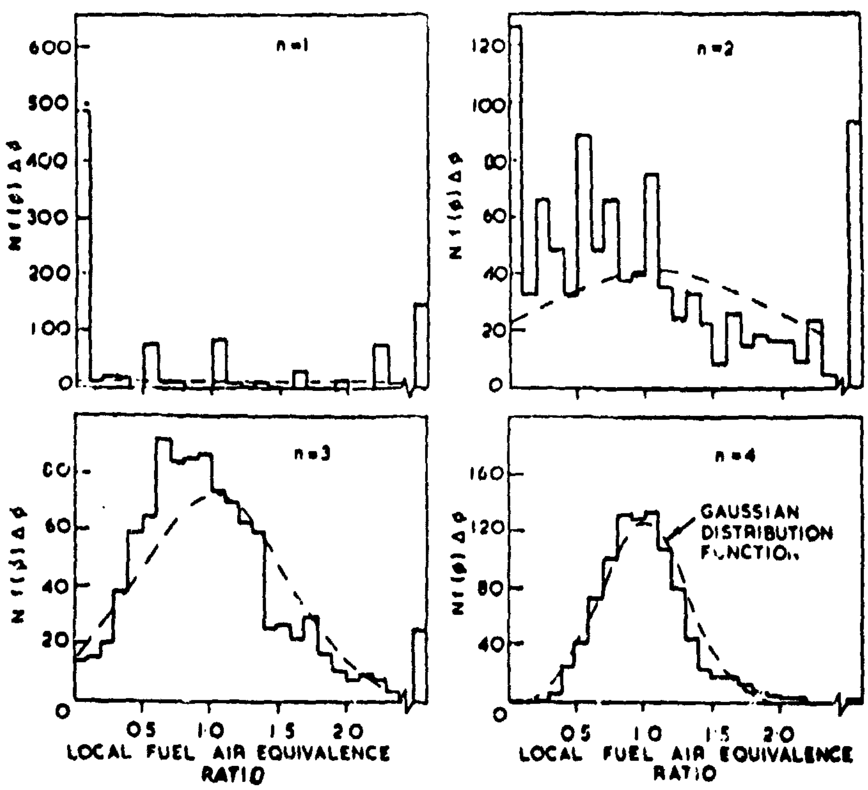


FIG 4 1




FEED 1 POPULATION = N1
COMBUSTOR POPULATION = N
MASS
FLOW
RATE ṁ
k = K K-1 K-2 ...
3 2 1
MIXING
FLOW
FEED 2 POPULATION = N2
α
λ
z
O
L


n=1
n=2
n=3
n=4
N f(φ) Δφ
GAUSSIAN
DISTRIBUTION
FUNCTION
LOCAL FUEL AIR EQUIVALENCE
RATIO

ORIGINAL PAGE IS
OF POOR QUALITY

*** 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 ELEMENT#	AREA (SQ.IN)	LENGTH (INCHES)	FLOW TYPE	INLET AIR (LBM/S)	INLET FUEL (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