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


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

Figure 2. Measured and homogeneous PSR predicted (CDH), and
uncorrected thermocouple temperature for combustion of CH₄/air at
$\Delta V = 10$ kg/sec sec. [2]
Crosses are values predicted from CUBR code with $NT = 20$. 

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Figure 3. Measured IDI normalized by D-OH equilibrium, and (homogeneous PSR) predicts IDI for combustion of CH4/air at 6V = 19 kg/cu ft. Crosses are predicted values from CCB code with NT = 0.6.

\[ p(t) \]

\[ T_0 \]
"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 "MARKII.DAT" but can be altered interactively, and used in consecutive runs.

MARKII represents a simple brick 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**

<table>
<thead>
<tr>
<th>ELEMENT</th>
<th>FLOW</th>
<th>LENGTH</th>
<th>FLOW</th>
<th>INLET AIR</th>
<th>INLET FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.44606E02</td>
<td>0.0000E+01</td>
<td>4.0000E-01</td>
<td>1.1300E+00</td>
<td>9.7000E-02</td>
</tr>
<tr>
<td>2</td>
<td>1.4460E02</td>
<td>0.0000E+01</td>
<td>1.0000E-01</td>
<td>4.9500E-01</td>
<td>0.0000E+01</td>
</tr>
<tr>
<td>3</td>
<td>1.4460E02</td>
<td>0.0000E+01</td>
<td>1.0000E-01</td>
<td>0.0000E+01</td>
<td>0.0000E+01</td>
</tr>
<tr>
<td>4</td>
<td>1.4500E00</td>
<td>0.0000E+01</td>
<td>2.0000E-01</td>
<td>0.0000E+01</td>
<td>0.0000E+01</td>
</tr>
<tr>
<td>RECYCLE</td>
<td>1.4460E00</td>
<td>1.0000E00</td>
<td>1.0000E+00</td>
<td>RECYCLE 20.00% of 3</td>
<td>OUTFLOW TO #2 INFLOW</td>
</tr>
</tbody>
</table>

AIR TEMP = 2.1000E02 F  COMBUSTOR PRESSURE = 2.7100E+00 ATM
FUEL TEMP = 0.0000E01 F  LOWER HEATING VALUE = 1.6500E+04 BTU/LBM

SELECT AN OPTION BY NUMBER:

1- Run with this data set
2- Change air temperature
3- Change fuel temperature
4- Change lower heating value
5- Change combustor pressure
6- Change recycle element status
7- Change flow elements status
8- Perform schematic model layout

ACTION? (0-7) 7

MARKII MODEL SCHEMATIC LAYOUT

```
A      A      A
|      |      |      
|      |      |      |
|      |      |      |
|      |      |      |
|      |      |      |
|      |      |      |
|      |      |      |
|      |      |      |
```

PRESS RETURN TO CONTINUE