

# PROPELLANT CHEMISTRY FOR CFD APPLICATIONS

R.C. Farmer, P.G. Anderson, Gary C. Cheng

SECA, Inc.  
Huntsville, AL

## ABSTRACT

Current concepts for Reusable Launch Vehicle design have created renewed interest in the use of RP-1 fuels for high pressure and tri-propellant propulsion systems. Such designs require the use of analytical methodology which accurately accounts for the effects of real fluid properties, combustion of large hydrocarbon fuel molecules, and the possibility of soot formation. These effects are inadequately treated in current computational fluid dynamics (CFD) codes which are used for propulsion system analyses.

The objective of this investigation is to provide an accurate analytical description of hydrocarbon combustion thermodynamics and kinetics which is sufficiently computationally efficient to be practical design tool when used with CFD codes such as the FDNS code.

A rigorous description of real fluid properties for RP-1 and its combustion products will be derived from the literature and from experiments conducted in this investigation. Upon the establishment of such a description, the fluid description will be simplified by using the minimum of empiricism necessary to maintain accurate combustion analyses and including such empirical models into an appropriate CFD code. An additional benefit from this approach is that the real fluid properties analysis simplifies the introduction of the effects of droplet sprays into the combustion model.

Typical species compositions of RP-1 have been identified, surrogate fuels have been established for analyses, and combustion and sooting reaction kinetics models have been developed. Methods for predicting the necessary real fluid properties have been developed and essential experiments have been designed. Verification studies are in progress, and preliminary results from these studies will be presented. The approach has been determined to be feasible, and upon its completion the required methodology for accurate performance and heat transfer CFD analyses for high pressure, tripropellant propulsion systems will be available.

**1995 CFD Workshop  
NASA/MSFC**

**PROPELLANT CHEMISTRY FOR CFD APPLICATIONS**

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# RP-1 COMBUSTION CHEMISTRY

- **RP-1 combustion model w/soot formation**
- **Verify model w/data from literature**
- **Verify model w/new test data**
- **Describe real fluid thermodynamic properties**
- **Add real fluid HC properties to CICM**
- **Real fluid single element model**
  - Real fluid HC, H<sub>2</sub>, and O<sub>2</sub>**
  - Real fluid tri-propellant**
  - Additional turbulence models**
- **Account for radiation**
- **Assemble elements to make injector model**

## RP-1

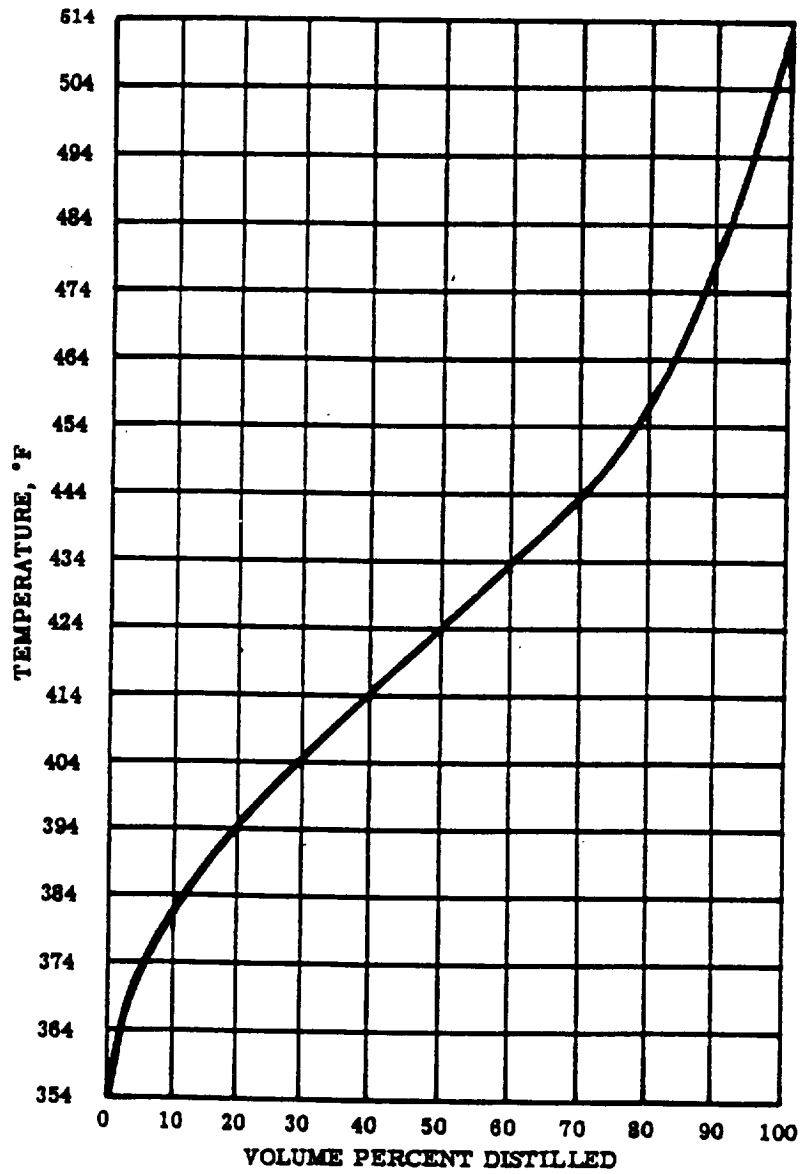
RP-1 is a straight run kerosene fraction which is subjected to acid washing and sulfur dioxide extraction. The mean molecular weight is about 174, and the H/C ratio is about 1.9. This implies that RP-1 is a multicomponent hydrocarbon fuel without a specified species distribution.

Composition by Hydrocarbon Type	
Composition	Volume %
dinuclear aromatics	2.3
mononuclear aromatics	15.1
dicyclo-paraffins	11.6
monocyclo-paraffins	33.8
branched-paraffins	15.1
normal paraffins	<u>22.1</u>
	100.0

or

Composition	Volume %
aromatics	17.4
cyclo-paraffins	45.4
paraffins	<u>37.2</u>
	100.0

Distillation Curve for RP-1



HYDROCARBONS ISOLATED FROM ONE REFERENCE PETROLEUM			
Molecular Formula	Name	Type	Normal Boiling Point
C <sub>10</sub> H <sub>14</sub>	1,3-Diethylbenzene	Benzene	181.10
C <sub>10</sub> H <sub>14</sub>	1-Methyl-3-propylbenzene	Benzene	181.80
C <sub>10</sub> H <sub>14</sub>	n-Bulylbenzene	Benzene	183.27
C <sub>10</sub> H <sub>18</sub>	Bicycloparaffin	Bicycloparaffin	183.4
C <sub>10</sub> H <sub>18</sub>	Bicycloparaffin	Bicycloparaffin	183.7
C <sub>10</sub> H <sub>14</sub>	1-Methyl-4-propylbenzene	Benzene	183.30
C <sub>10</sub> H <sub>14</sub>	1, 2-Diethylbenzene	Benzene	183.42
C <sub>10</sub> H <sub>14</sub>	1,3-Dimethyl-5-ethylbenzene	Benzene	183.58
C <sub>10</sub> H <sub>14</sub>	1, 4-Diethylbenzene	Benzene	183.78
C <sub>10</sub> H <sub>14</sub>	1, Methyl-2-propylbenzene	Benzene	184.80
C <sub>10</sub> H <sub>14</sub>	1, 4-Dimethyl-2-ethylbenzene	Benzene	186.83
C <sub>10</sub> H <sub>18</sub>	trans-Decahydro-naphthalene	Bicycloparaffin	187.25
C <sub>10</sub> H <sub>14</sub>	1, 3-Dimethyl-4-ethylbenzene	Benzene	188.20
C <sub>10</sub> H <sub>14</sub>	1, 2-Dimethyl-4-ethylbenzene	Benzene	189.48
C <sub>10</sub> H <sub>16</sub>	Tricyclo (3.3.1.1)- decane	Tricycloparaffin	190
C <sub>10</sub> H <sub>14</sub>	1, 3-Dimethyl-2-ethylbenzene	Benzene	190.01
C <sub>10</sub> H <sub>12</sub>	1-Methylindan	Aromatic-cycloparaffin	190.6
C <sub>10</sub> H <sub>12</sub>	2-Methylindan	Aromatic-cycloparaffin	191.4
C <sub>10</sub> H <sub>14</sub>	1, 2-Dimethyl-3 ethylbenzene	Benzene	193.91
C <sub>10</sub> H <sub>18</sub>	cis-Decahydro-naphthalene	Bicycloparaffin	195.69
C <sub>11</sub> H <sub>24</sub>	n-Undecane	Normal paraffin	195.89
C <sub>10</sub> H <sub>14</sub>	1,2,4,5-Tetramethyl-benzene	Benzene	196.80
C <sub>10</sub> H <sub>14</sub>	1,2,3,5-Tetramethyl-benzene	Benzene	198.00
C <sub>11</sub> H <sub>20</sub>	Bicycloparaffin	Bicycloparaffin	202.5
C <sub>11</sub> H <sub>16</sub>	1-Methyl-3-n-butylbenzene	Benzene	204.1
C <sub>10</sub> H <sub>14</sub>	1,2,3,4-Tetramethyl-benzene	Benzene	205.04
C <sub>10</sub> H <sub>12</sub>	4-Methylindan	Aromatic-cycloparaffin	205.5

**HYDROCARBONS ISOLATED FROM ONE REFERENCE PETROLEUM (Continued)**

Molecular Formula	Name	Type	Normal Boiling Point
C <sub>11</sub> H <sub>16</sub>	1,3-Dimethyl-4-n propylbenzene	Benzene	206.6
C <sub>10</sub> H <sub>12</sub>	1,2,3,4-Tetra-hydronaphthalene	Aromatic-cycloparaffin	207.57
C <sub>11</sub> H <sub>16</sub>	1,2-Dimethyl-4-n-propylbenzene	Benzene	208.5
C <sub>11</sub> H <sub>16</sub>	Trimethylethylbenzene	Benzene	212.3
C <sub>12</sub> H <sub>26</sub>	n-Dodecane	Normal paraffin	216.28
C <sub>10</sub> H <sub>8</sub>	Naphthalene	Dinuclear aromatic	217.96
C <sub>11</sub> H <sub>14</sub>	2-Methyl-(1,2,3,4-tetra-hydronaphthalene)	Aromatic-cycloparaffin	220.7
C <sub>11</sub> H <sub>14</sub>	6-Methyl-(1,2,3,4-tetra-hydronaphthalene)	Aromatic-cycloparaffin	229.03
C <sub>14</sub> H <sub>30</sub>	2,6,10-Trimethylundecane	Branched paraffin	231
C <sub>11</sub> H <sub>14</sub>	5-Methyl-(1,2,3,4-tetra-hydronaphthalene)	Aromatic-cycloparaffin	234.35
C <sub>13</sub> H <sub>28</sub>	n-Tridecane	Normal paraffin	235.43
C <sub>11</sub> H <sub>10</sub>	2-Methylnaphthalene	Dinuclear aromatic	241.05
C <sub>11</sub> H <sub>10</sub>	1-Methylnaphthalene	Dinuclear aromatic	244.64
C <sub>15</sub> H <sub>32</sub>	2,6,10-Trimethyldodecane	Branched paraffin	249
C <sub>14</sub> H <sub>30</sub>	n-Tetradecane	Normal paraffin	253.52
C <sub>12</sub> H <sub>10</sub>	Biphenyl	Dinuclear aromatic	255.0
C <sub>13</sub> H <sub>12</sub>	2-Methylbiphenyl	Dinuclear aromatic	255.3
C <sub>12</sub> H <sub>12</sub>	2-Ethylnaphthalene	Dinuclear aromatic	257.9
C <sub>12</sub> H <sub>12</sub>	1-Ethylnaphthalene	Dinuclear aromatic	258.7
C <sub>12</sub> H <sub>12</sub>	2,6-Dimethylnaphthalene	Dinuclear aromatic	262
C <sub>12</sub> H <sub>12</sub>	2,7-Dimethylnaphthalene	Dinuclear aromatic	263
C <sub>12</sub> H <sub>12</sub>	1,7-Dimethylnaphthalene	Dinuclear aromatic	263
C <sub>12</sub> H <sub>12</sub>	1,6-Dimethylnaphthalene	Dinuclear aromatic	263
C <sub>12</sub> H <sub>12</sub>	1,3-Dimethylnaphthalene	Dinuclear aromatic	265
C <sub>12</sub> H <sub>12</sub>	1,5-Dimethylnaphthalene	Dinuclear aromatic	265
C <sub>14</sub> H <sub>14</sub>	2,5-Dimethylbiphenyl	Dinuclear aromatic	267
C <sub>15</sub> H <sub>16</sub>	Trimethylbiphenyl	Dinuclear aromatic	267
C <sub>16</sub> H <sub>18</sub>	Tetramethylbiphenyl	Dinuclear aromatic	267

RP-1 SURROGATE FUELS			
Formula	Species	Mol %	NBP(°C)
C <sub>13</sub> H <sub>12</sub>	methylbiphenyl	17.4	255
C <sub>12</sub> H <sub>24</sub>	n-heptylcyclopentane	45.4	224
C <sub>12</sub> H <sub>28</sub>	n-tridecane	<u>37.2</u>	235
		100.0	

$$M_{wt} = 173.9$$

$$H/C = 1.922$$

**Note:** Critical pressure for RP-1 is 340 psia,  
and critical temperature is 679°K.



# RP-1 COMBUSTION PROPERTIES

## HEAT OF COMBUSTION

$$\text{HOC} = -18640 \text{ (Btu/lbm)} = -10.346 \text{ (kcal/gm)}$$

## HEAT OF VAPORIZATION

$$\text{HOV} = 106 \text{ (Btu/lbm)}$$

## HEAT OF FORMATION (HOF)

To determine a HOF for mixtures, an effective molecular formula must be specified **and** used to evaluate the HOF. Frequently, an arbitrary molecular weight of 100 gms is assumed for a basis for thermodynamic calculations.

H/C	HOF(kcal/100gm)	Source	Implied HOC (kcal/gm)
1.8624	-36.01	Lockheed	-10.287
1.90	-41.6	SAIC	-10.305
2.0	-44.36	Aerojet '78	-10.403
1.9063	-42.0	TMX - 1783	-10.305
1.9423	-33.068(v)	SP-273	-10.441(v)
1.9423	-38.946(l)	SP-273	-10.382(l)
1.922	-39.915	Surrogate Fuel	-10.346

**SPECTROSCOPIC ANALYSIS  
OF H-1 GAS GENERATOR EXHAUST GASES**

Compound	Sample #1	Sample #3	Sample #4
CO	26.15*	36.82	37.93
CO <sub>2</sub>	8.44	8.86	9.96
H <sub>2</sub> O	2.66	1.14	0.85
H <sub>2</sub>	1.97	2.22	2.34
CH <sub>4</sub>	2.92	4.20	4.40
C <sub>2</sub> H <sub>2</sub>	4.16	5.62	4.27
C <sub>2</sub> H <sub>4</sub>	5.93	6.93	7.70
C <sub>2</sub> H <sub>6</sub>	0.72	...	...
Propyne	0.69	0.30	0.41
Propene	2.84	3.15	3.95
Diacetylene	0.12	0.08	0.21
1,3 Butadiene	1.30	1.32	1.52
2 Butene	1.57	0.80	1.16
- Butene	...	1.76	0.54
1.5 Hexadyne	1.98	1.58	1.73
3 Methyl Pentene -1	...	0.71	0.57
Cyclopentene	...	0.74	0.99
1,2,3 trimethylcyclopantane	...	1.14	0.97
Benzene	...	1.05	1.20
Ethyl Benzene	...	0.99	0.36
Carbon	...	5.22	2.06
RP-1	38.51	17.58	17.14

\* Weight percentage composition of combustion products

# Generalized Combustion Kinetics Model

<b>I.</b> PURE PYROLYSIS	$\left[ \begin{array}{c} \text{ALIPHATICS} \\ \text{AROMATICS} \end{array} \right] \rightarrow \left[ \begin{array}{c} \text{C}_2\text{H}_2 \\ \text{CH}_4 \\ \text{C}_2\text{H}_4 \\ \text{H}_2 \end{array} \right] \equiv \text{INTERMEDIATES}$	<b>V.</b> SOOT FORMATION	$\left[ \begin{array}{c} \text{ALIPHATICS} \\ \text{AROMATICS} \\ \text{INTERMEDIATES} \end{array} \right] \rightarrow \text{SOOT}$
<b>II.</b> OXIDATIVE PYROLYSIS	$\left[ \begin{array}{c} \text{ALIPHATICS} \\ \text{AROMATICS} \end{array} \right] + \left[ \begin{array}{c} \text{OH} \\ \text{O}_2 \end{array} \right] \rightarrow \left[ \begin{array}{c} \text{CH}_4 \\ \text{C}_2\text{H}_2 \\ \text{C}_2\text{H}_4 \end{array} \right] + \left[ \begin{array}{c} \text{H}_2 \\ \text{C}_x\text{H}_y\text{O}_z \end{array} \right]$	<b>VI.</b> SOOT GASIFICATION	$\text{SOOT} + \left[ \begin{array}{c} \text{O}_2 \\ \text{CO} \\ \text{CO}_2 \\ \text{H}_2\text{O} \\ \text{H}_2 \\ \text{OH} \end{array} \right] \rightarrow \left[ \begin{array}{c} \text{CO} \\ \text{CO}_2 \\ \text{CH}_4 \end{array} \right]$
<b>III.</b> PARTIAL OXIDATION	$\left[ \begin{array}{c} \text{ALIPHATICS} \\ \text{AROMATICS} \\ \text{CH}_4 \\ \text{C}_2\text{H}_2 \\ \text{C}_2\text{H}_4 \end{array} \right] + \left[ \begin{array}{c} \text{O}_2 \\ \text{OH} \end{array} \right] \rightarrow \left[ \begin{array}{c} \text{H}_2 \\ \text{CO} \\ \text{C}_x\text{H}_y\text{O}_z \\ \text{CO}_2 \\ \text{H}_2\text{O} \end{array} \right]$	<b>VII.</b> NO <sub>x</sub> FORMATION	$\text{FUEL} + \left[ \begin{array}{c} \text{FBN} \\ \text{N}_2 \end{array} \right] \rightarrow \left[ \begin{array}{c} \text{HCN} \\ \text{NH}_i \end{array} \right]$ $\left[ \begin{array}{c} \text{HCN} \\ \text{NH}_i \end{array} \right] + \left[ \begin{array}{c} \text{O}_2 \\ \text{OH} \end{array} \right] \rightleftharpoons \left[ \begin{array}{c} \text{NO} \\ \text{NO}_2 \end{array} \right]$
<b>IV.</b> ELEMENTARY STEPS TO COMPLETION	$\left[ \begin{array}{c} \text{CO} \\ \text{H}_2 \\ \text{C}_x\text{H}_y\text{O}_z \\ \text{H}_2\text{O}_2 \end{array} \right] + \left[ \begin{array}{c} \text{O} \\ \text{H} \\ \text{OH} \\ \text{CHO} \\ \text{HO}_2 \end{array} \right] \rightleftharpoons \left[ \begin{array}{c} \text{H}_2\text{O} \\ \text{CO}_2 \end{array} \right]$		$\left[ \begin{array}{c} \text{N}_2 \\ \text{O}_2 \\ \text{N} \end{array} \right] + \left[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{OH} \end{array} \right] \rightarrow \text{NO} + \left[ \begin{array}{c} \text{N} \\ \text{O} \\ \text{H} \end{array} \right]$ THERMAL FIXATION

## Soot Model

### Initial Polycyclic Aromatic Hydrocarbon (PAH) Formation

- Pyrolysis and combustion of fuel to form benzene and acetylene
- Implicit finite-rate chemistry

### Planar PAH Growth

- HACA
- Hydrogen abstraction, carbon addition (through reactions with acetylene)
- Oxidation
- Implicit finite-rate chemistry using reactions from Frenklach, et al
- Properties for PAH compounds
- Benson's group contribution method to obtain  $C_p$  for ideal gases
- Benson data in tabular form for  $300\text{K} < T < 1500\text{K}$
- Used CEC data for selected species to generate group contributions as functions of temperature for  $300\text{K} < T < 5000\text{K}$
- Generated needed  $C_p$  data in CEC format
- $S^\circ_{298}$  corrected for symmetry and optical isomers using Benson's data.

## Soot Model (Cont.)

### Aerosol Dynamics Based on Frenklach and Harris's "Method II"

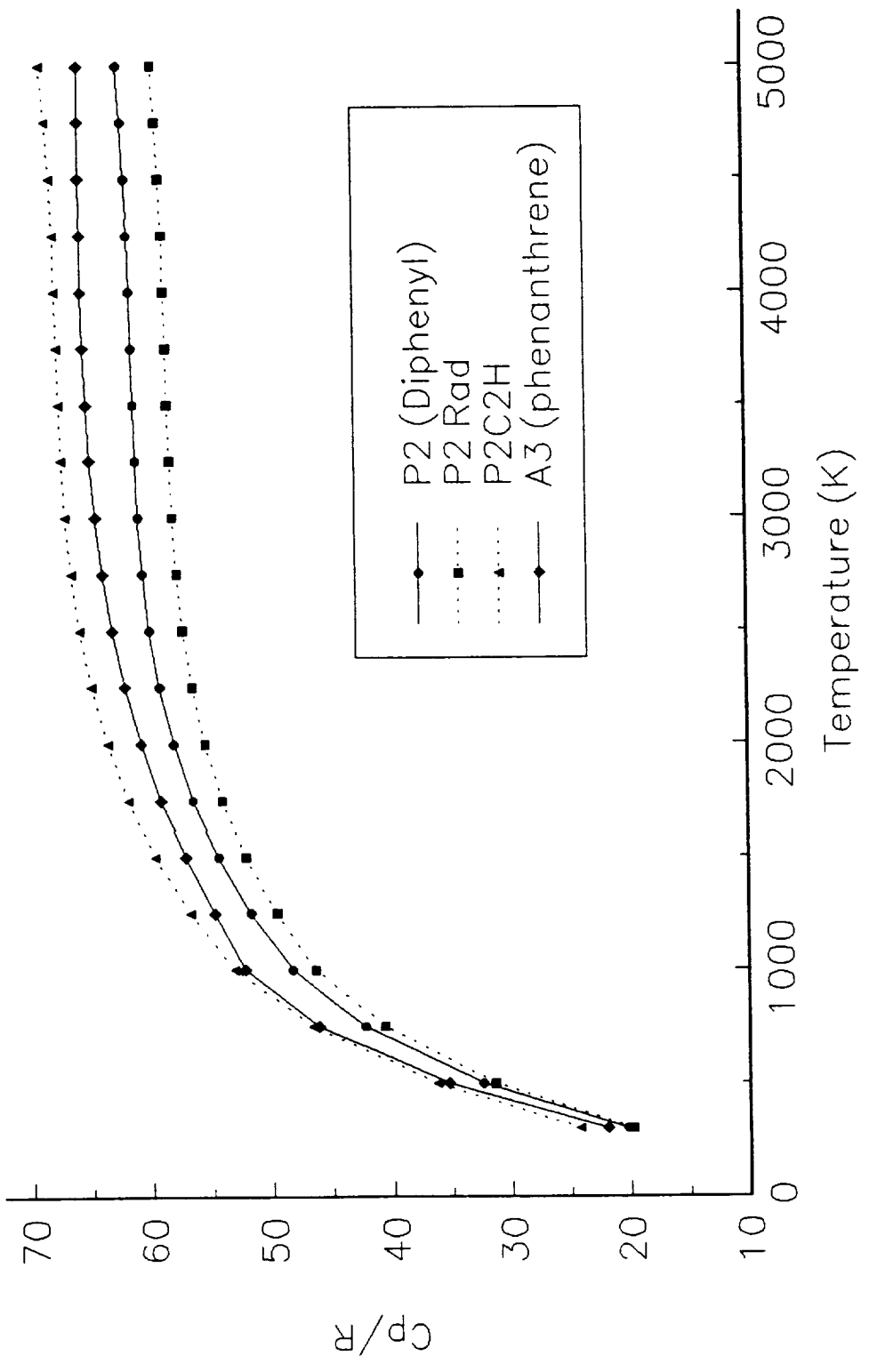
- Method of moments
- Nucleation
  - Collisions of planar PAH's to form 3-D particles
- Coagulation
  - Collisions of 3-D particles to form larger particles

### Surface Growth on 3-D Particles

- Collisions with planar PAH's
- HACA
- Oxidation by reactions with O<sub>2</sub> and OH

**Model provides soot formation and oxidation rates to be used to develop a quasiglobal reaction rate for soot production.**

Cp's for Diphenyl Compounds  
 Dotted lines are synthesized data



# Toluene and Iso-Octane Quasiglobal Kinetics Model

GLOBAL MECHANISM	A	B	E/R	POWER DEPENDENCIES
<p><u>Toluene (aromatic)</u></p> $C_7H_8 \rightarrow 3.5 C_2H_2 + 0.5 H_2$ $C_7H_8 + 3.5 O_2 \rightarrow 7 CO + 4 H_2$ $C_7H_8 + OH \rightarrow 3.25 C_2H_2 + 0.5 CO + 0.5 H_2O + 0.75 H_2$	<p>1.7982 E10 4.4963 E9 1.4721 E17</p>	<p>0 1 0</p>	<p>3.5000 E4 2.6785 E4 1.4510 E4</p>	<p><math>[C_7H_8]^{1.0}</math> <math>[C_7H_8]^{10.5}[O_2]^{1.0}</math> <math>[C_7H_8]^{1.0}[OH]^{1.0}</math></p>
<p><u>Iso-Octane (aliphatic)</u></p> $C_8H_{18} \rightarrow 4 C_2H_4 + H_2$ $C_8H_{18} + 4 O_2 \rightarrow 8 CO + 9 H_2$ $C_8H_{18} + OH \rightarrow 3.75 C_2H_4 + 0.5 CO + 0.5 H_2O + 1.5 H_2$	<p>1.0473 E12 1.2900 E9 2.0000 E17</p>	<p>0 1 0</p>	<p>3.5229 E3 2.5160 E4 1.4919 E4</p>	<p><math>[C_8H_{18}]^{1.0}</math> <math>[C_8H_{18}]^{10.5}[O_2]^{1.0}</math> <math>[C_8H_{18}]^{1.0}[OH]^{1.0}</math></p>
<p><u>Secondary Fuel</u></p> $C_2H_2 + 6 OH \rightarrow 4 H_2O + 2 CO$ $C_2H_2 + 2 OH \rightarrow 2 CO + 2 H_2$ $C_2H_4 + 4 OH \rightarrow 2 CO + 2 H_2O + 2 H_2$ $C_2H_4 + 2 OH \rightarrow 2 CO + 3 H_2$ $C_2H_2 + O_2 = 2 CHO$ $C_2H_4 + M = C_2H_3 + H_2 + M$	<p>4.7850 E15 2.8000 E16 2.2020 E15 2.1129 E27 4.0000 E12 2.0893 E17</p>	<p>0 0 0 -3.0 0 0</p>	<p>1.3883 E4 0 1.2079 E4 6.3062 E3 1.4092 E4 3.9810 E4</p>	<p><math>[C_2H_2]^{1.0}[OH]^{1.0}</math> <math>[C_2H_2]^{1.0}[OH]^{1.5}</math> <math>[C_2H_4]^{1.0}[OH]^{1.0}</math> <math>[C_2H_4]^{1.0}[OH]^{1.5}</math> <math>[C_2H_2]^{1.0}[O_2]^{1.0}</math> <math>[C_2H_4]^{1.0}[M]^{1.0}</math></p>
<p><u>Soot Parameters</u></p> $C_7H_8 = HC \rightarrow soot$ <p>i = A B T Z</p>	<p>4.0465 E14  2.000 E1 4.4600 E-3 1.5100 E5 2.1300 E1</p>	<p>-2.0  C 0 0 0</p>	<p>1.6110 E4  1.5090 E4 7.6490 E3 4.8820 E4 -2.0630 E3</p>	<p><math>[HC]^{1.43}[O_2]^{0.3}</math>  As indicated by the equation for [soot]</p>

## SOOT PARAMETERS

$$\text{soot} + O_2 \rightarrow CO_2 \quad 12 P_{O_2} A_t \left[ \frac{K_A X}{1 + K_Z P_{O_2}} + K_B(1-X) \right]$$

$$X = \left[ 1 + K_T / (K_B P_{O_2}) \right]^{-1}$$

$$K_i = A_i \exp \{ -E_i / RT \}, \quad i = A, B, T, Z$$

where  $A_t = 6 [C_s / (\rho_s \bullet D_s)]$  (cm<sup>2</sup> surface/cm<sup>3</sup>),

$P_{O_2}$  = partial pressure of O<sub>2</sub> (atm),

$C_s$  = (g • soot/cm<sup>3</sup> of gas),  $\rho_s$  = (g • soot/cm<sup>3</sup> of soot),

$D_s$  = diameter of soot (cm),

[soot] = mass of soot/volume of gas (g/cm<sup>3</sup>).



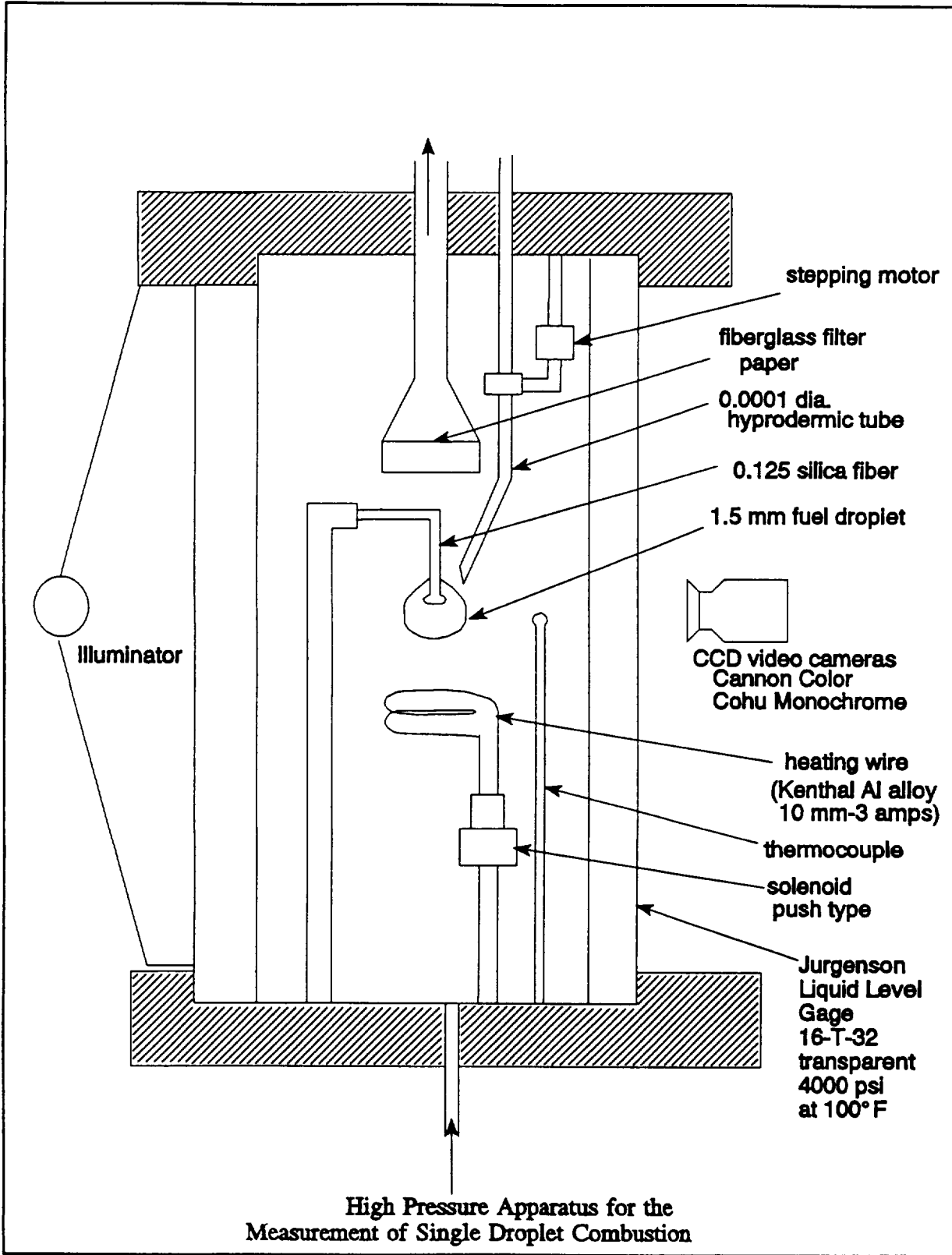
## Elementary Reactions

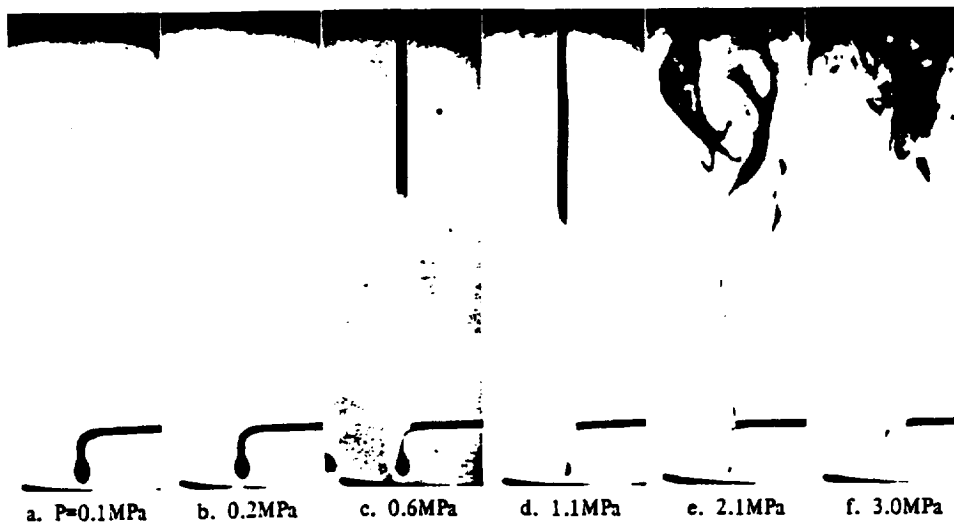
ELEMENTARY MECHANISM	A	B	E/R
<u>Wet CO Mechanism</u> $H_2 + O_2 = OH + OH$ $OH + H_2 = H_2O + H$ $OH + OH = O + H_2O$ $O + H_2 = H + OH$ $H + O_2 = O + OH$ $M + O + H = OH + M$ $M + O + O = O_2 + M$ $M + H + H = H_2 + M$ $M + H + OH = H_2O + M$ $CO + OH = H + CO_2$ $CO + O_2 = CO_2 + O$ $CO + O + M = CO_2 + M$	1.7000 E13 2.1900 E13 6.0230 E12 1.8000 E10 1.2200 E17 1.0000 E16 2.5500 E18 5.0000 E15 8.4000 E21 4.0000 E12 3.0000 E12 6.0000 E13	0 0 0 1.0 -0.91 0 -1.0 0 -2.0 0 0 0	2.4070 E4 2.5900 E3 5.5000 E2 4.4800 E3 8.3690 E3 0 5.9390 E4 0 0 4.0300 E3 2.5000 E4 0

# RP-1 COMBUSTION VERIFICATION EXPERIMENTS

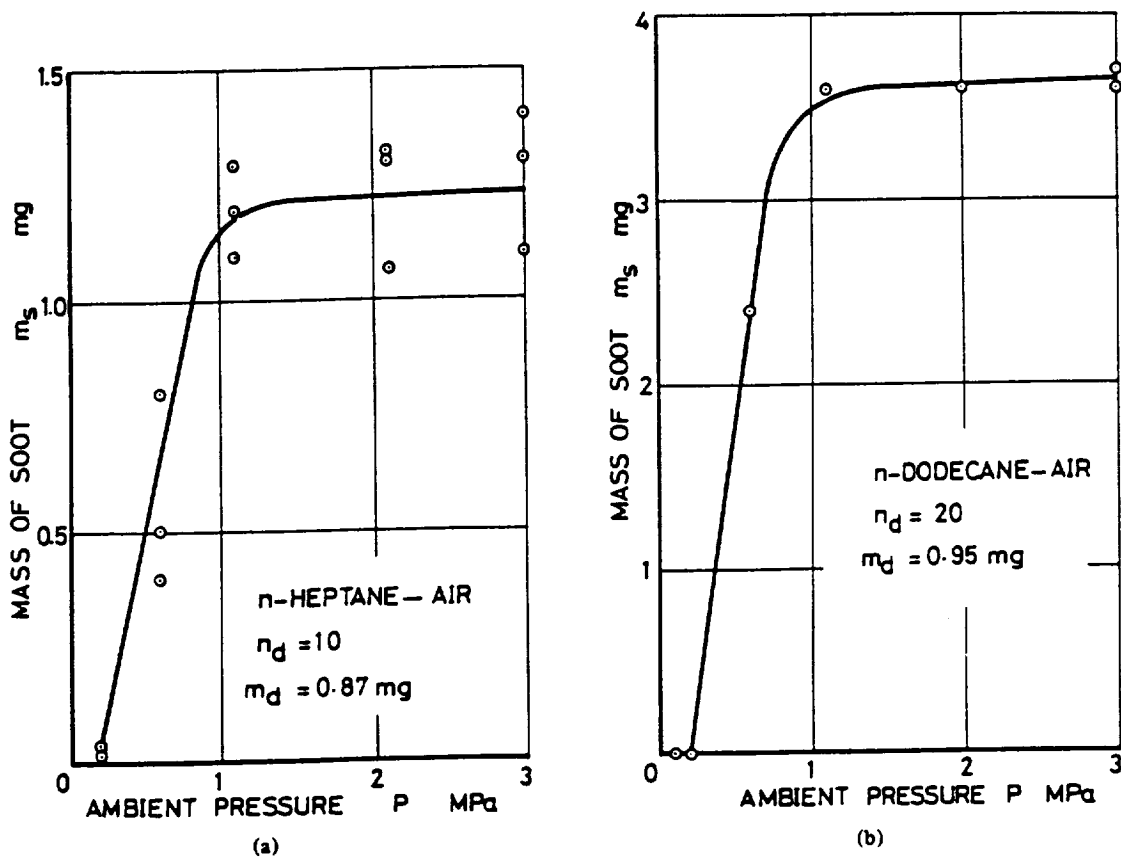
Criteria: Minimize Effect of Turbulent Mixing

- Single Drop Combustion - LSU
- Well Stirred Reactor - Exxon
- Rocket Test Motor - General Dynamics Corporation (GDC)

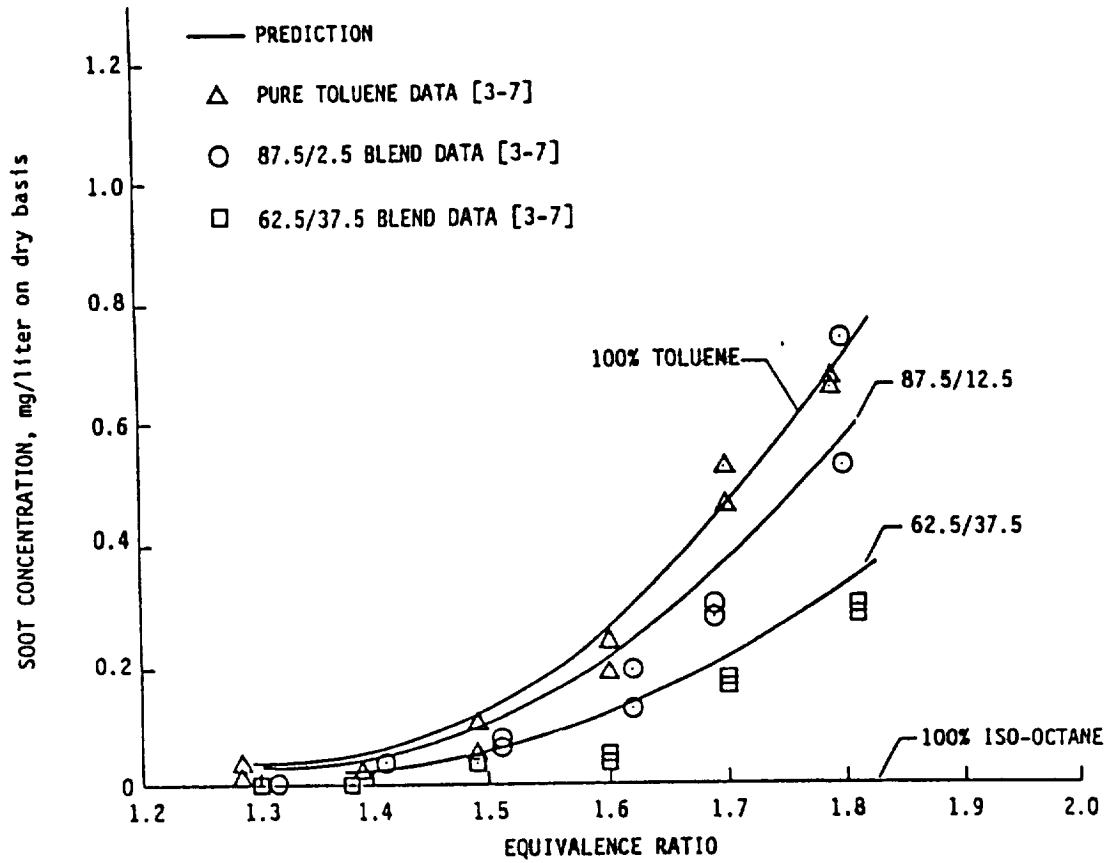




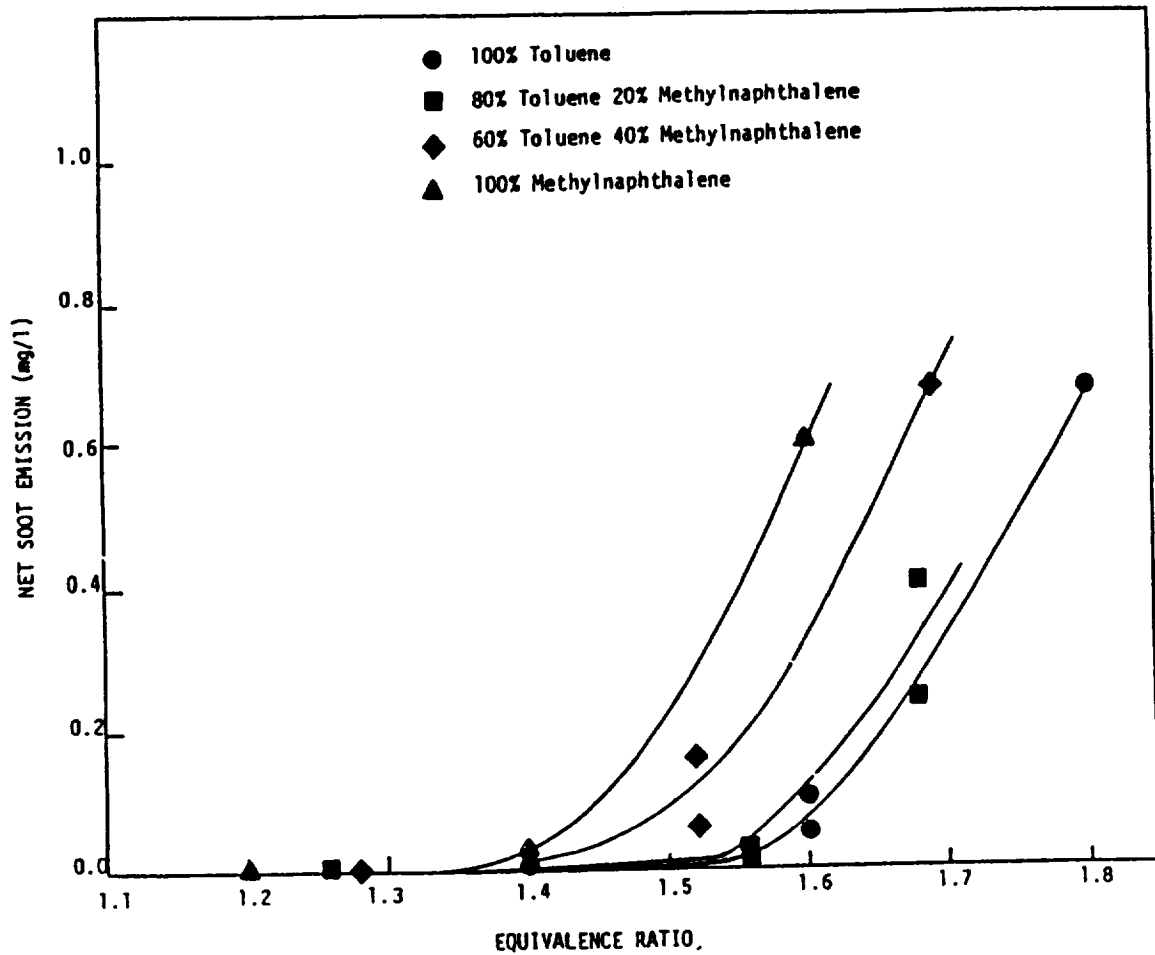
Photograph of Burning Droplets (n-heptane in air).



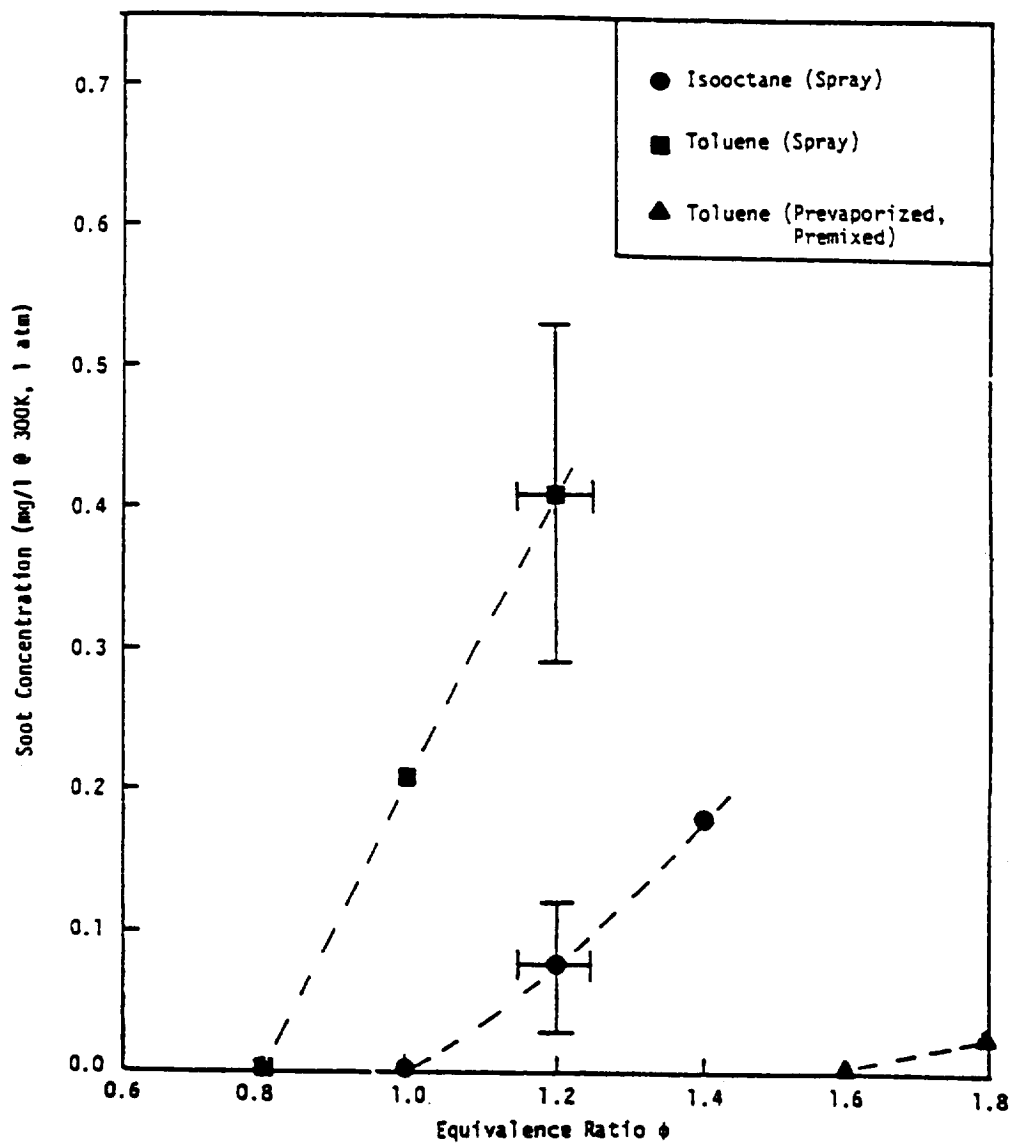
Effect of Pressure: (a) n-heptane; (b) n-dodecane.



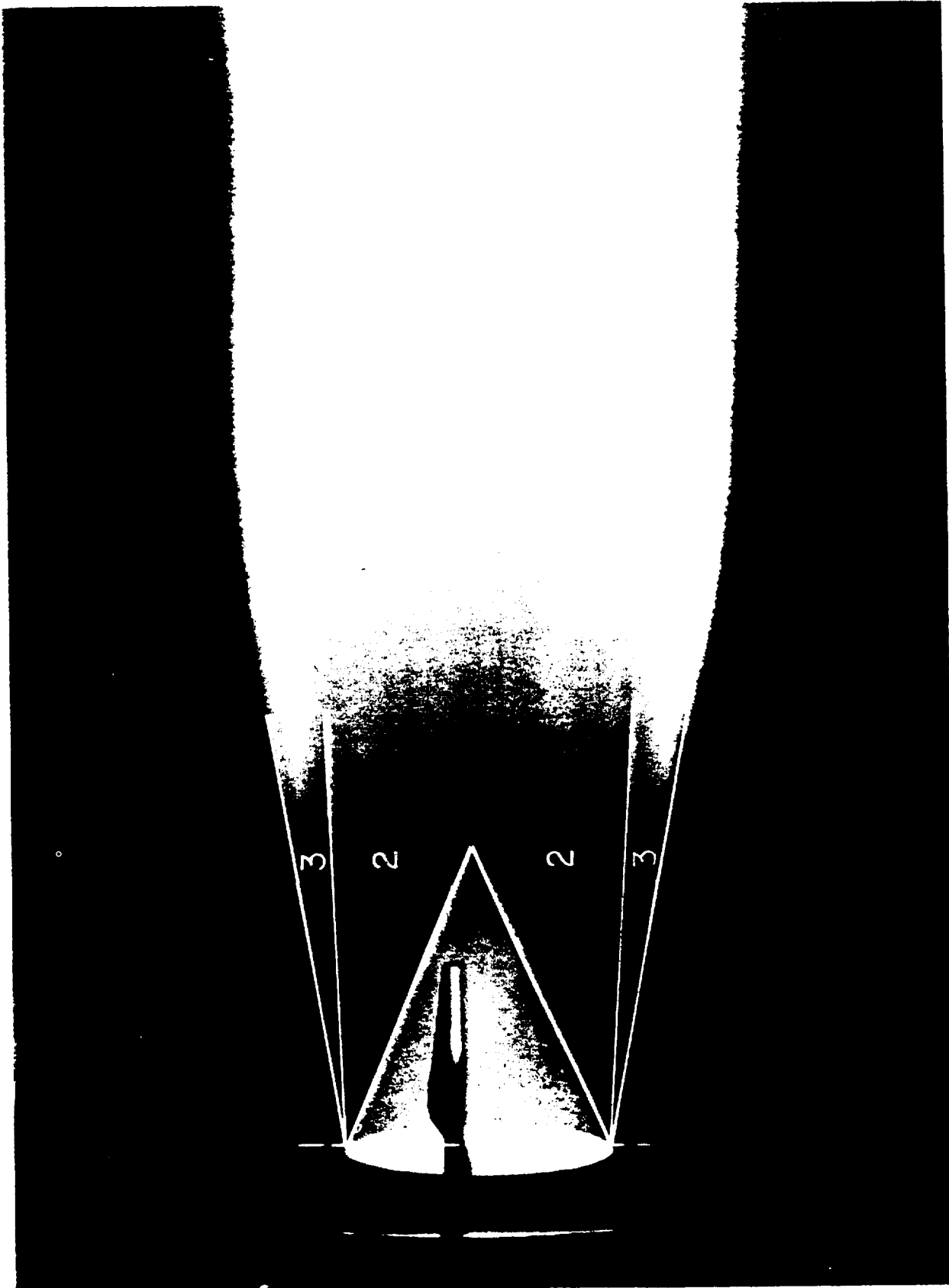
Comparison Of Quasiglobal Model Prediction Of Soot Emissions With Experimental Data For Toluene And Toluene/Iso-Octane Blends. Computation: Well-Stirred Reactor; Experiment: Jet-Stired Combustor.



JSC Soot Emissions For Toluene/Methylnaphthalene Blends;  
 $T = 1900 \text{ K}$ ;  $\tau = 3 \text{ ms}$ .

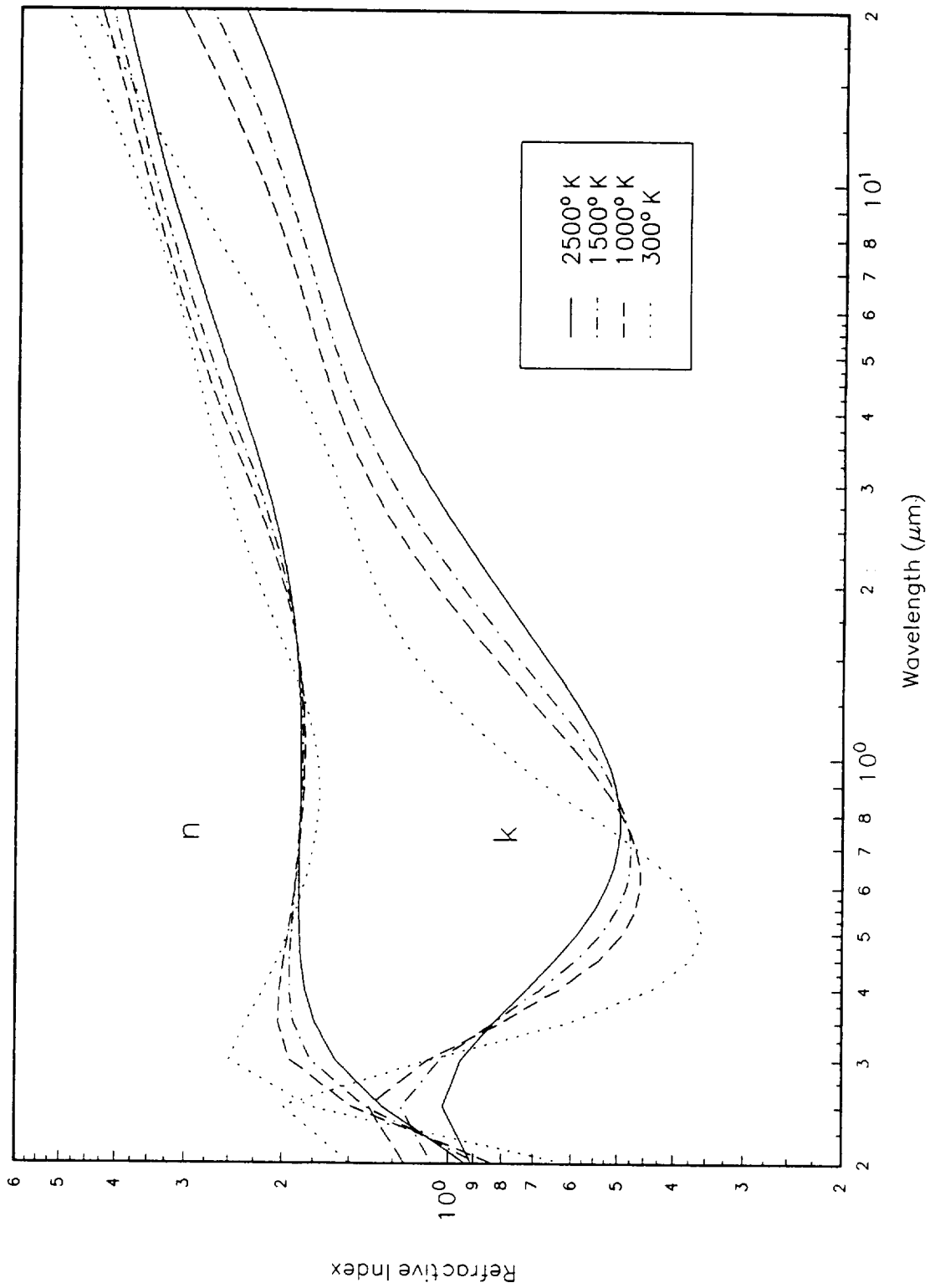


Dependence Of Soot Concentration On Equivalence Ratio;  
 Ratio; Atomization Air = 15 g/min/nozzle; Indicated  
 Temperature =  $1900 \pm 35K$ .

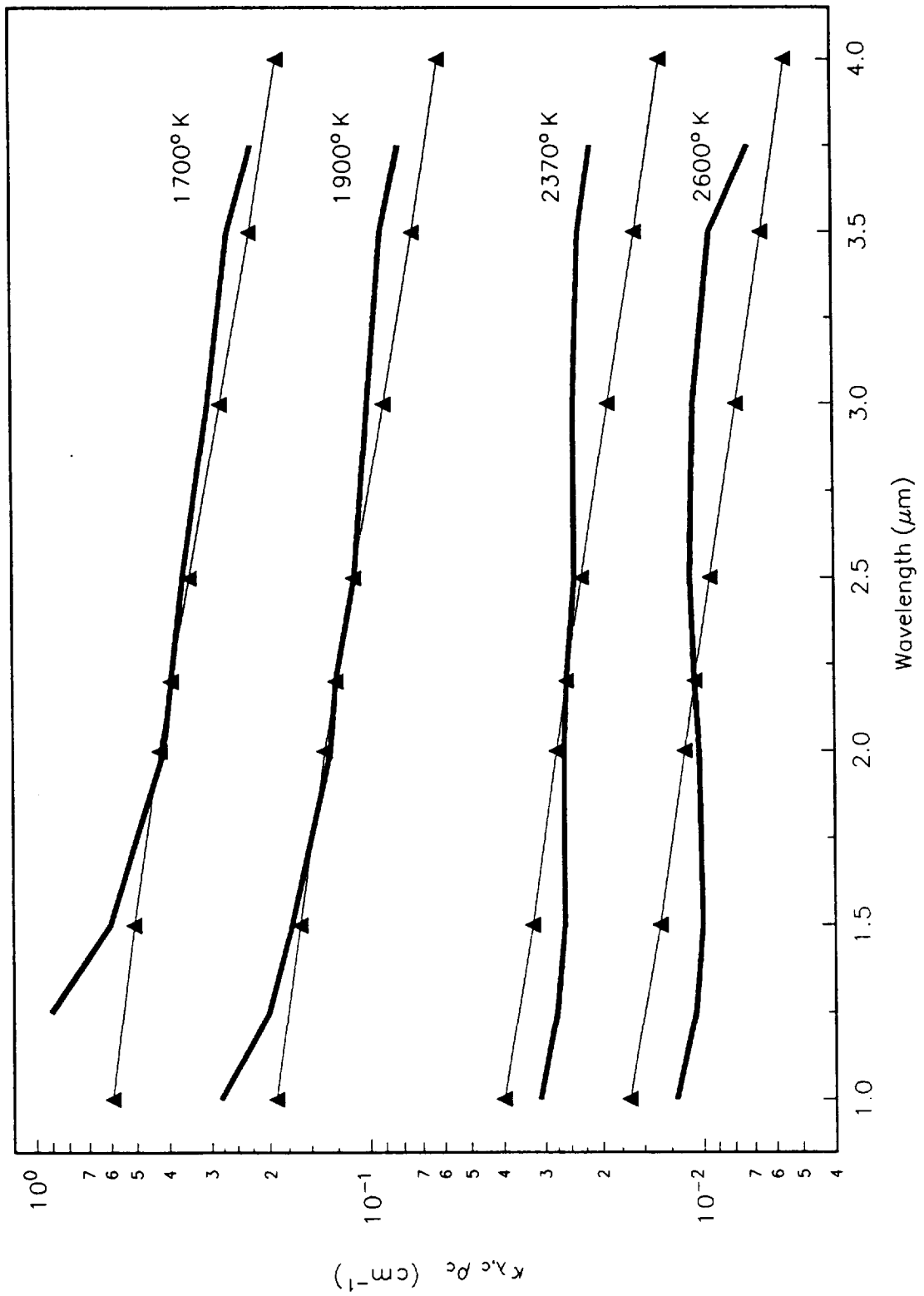


Photograph of the exit flow at an exit pressure of 2 atm. Region 1 is the undisturbed cone, region 2 is the Prandtl-Meyer expansion zone, and region 3 is the mixing zone. The spectrometer line of sight is indicated by a dotted line.

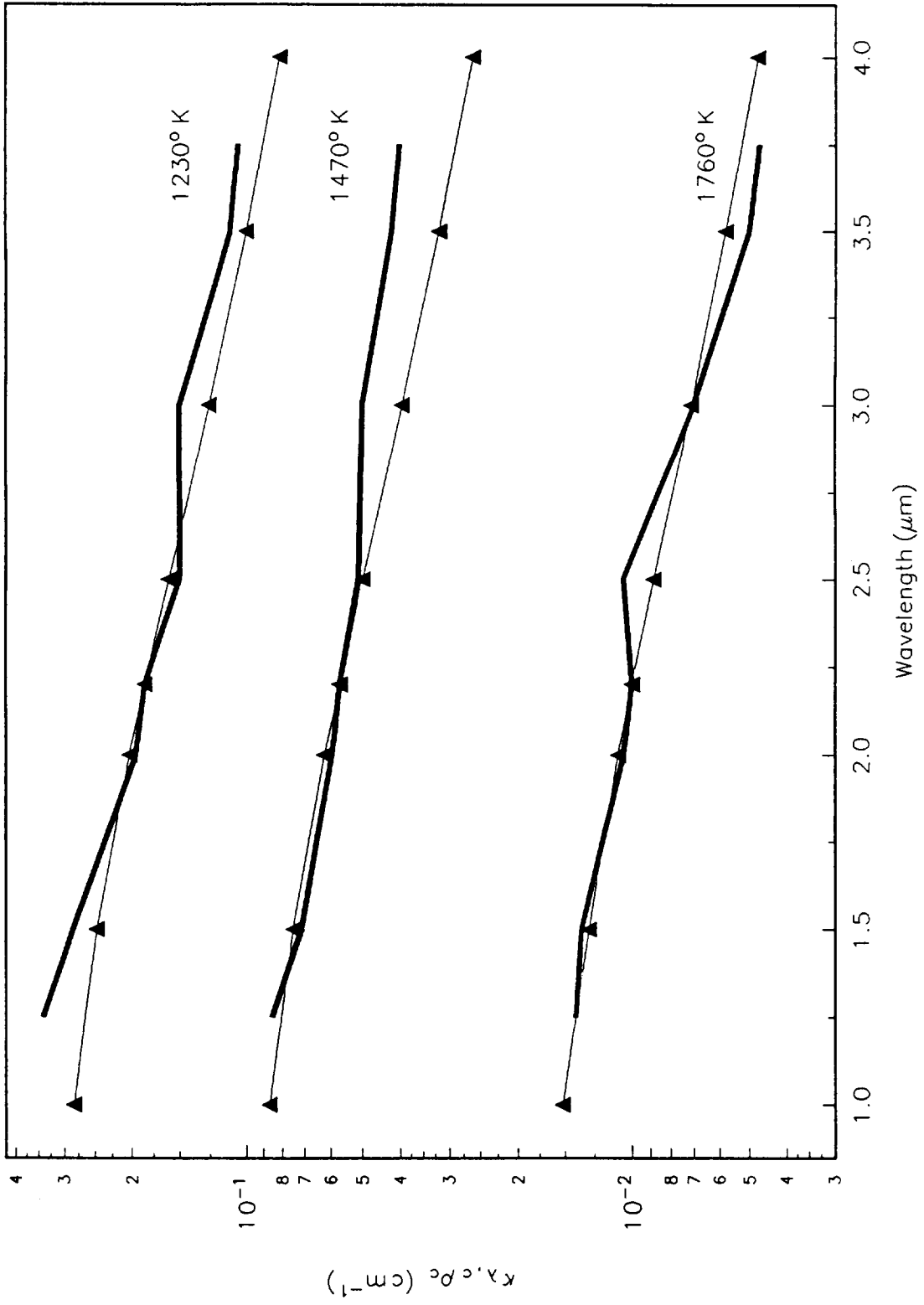




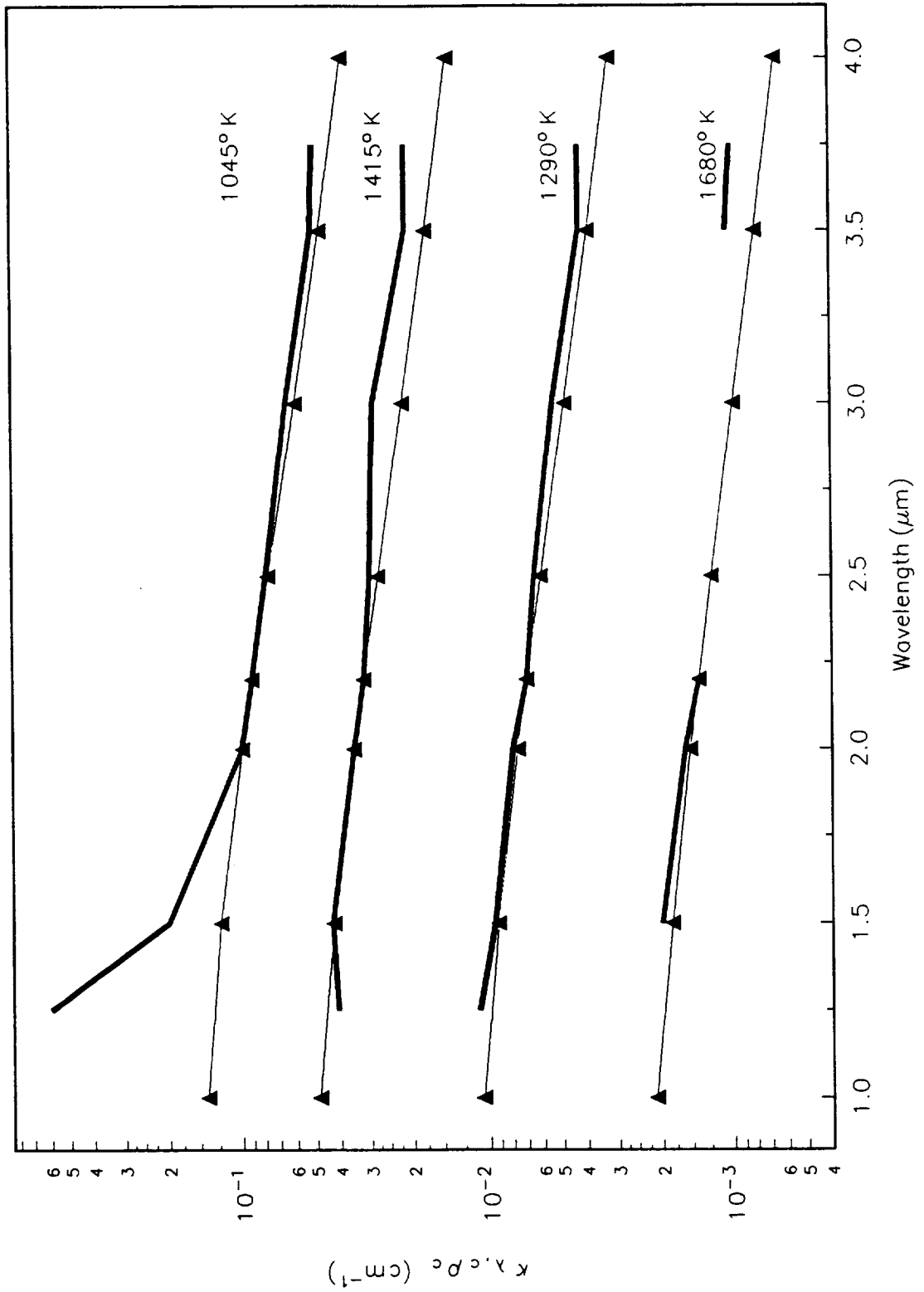
AREA RATIO = 1.50



AREA RATIO = 3.0



AREA RATIO = 5.25



Soot Density from GDC Experiments				
$\kappa_{\lambda}\rho_c$ (cm <sup>-1</sup> )	T(°K)	O/F	$\rho_c$ (gm/cc)	$\kappa_{\lambda}$ (cm <sup>2</sup> /gm)
0.1400E-02	1680.0000	1.8500	0.1087E-06	0.1288E+05
0.7000E-02	1415.0000	1.6000	0.5200E-06	0.1346E+05
0.3200E-01	1290.0000	1.5000	0.2343E-05	0.1366E+05
0.9000E-01	1045.0000	1.3300	0.6531E-05	0.1378E+05
0.1000E-01	1760.0000	1.6000	0.7886E-06	0.1268E+05
0.5700E-01	1470.0000	1.4500	0.4268E-05	0.1335E+05
0.1850E+00	1230.0000	1.2500	0.1348E-04	0.1373E+05
0.1050E-01	2600.0000	2.1000	0.9944E-06	0.1056E+05
0.2550E-01	2370.0000	1.8500	0.2295E-05	0.1111E+05
0.1250E+00	1900.0000	1.5000	0.1015E-04	0.1232E+05
0.3900E+00	1700.0000	1.4000	0.3040E-04	0.1283E+05

### Rayleigh Theory for Small Particles

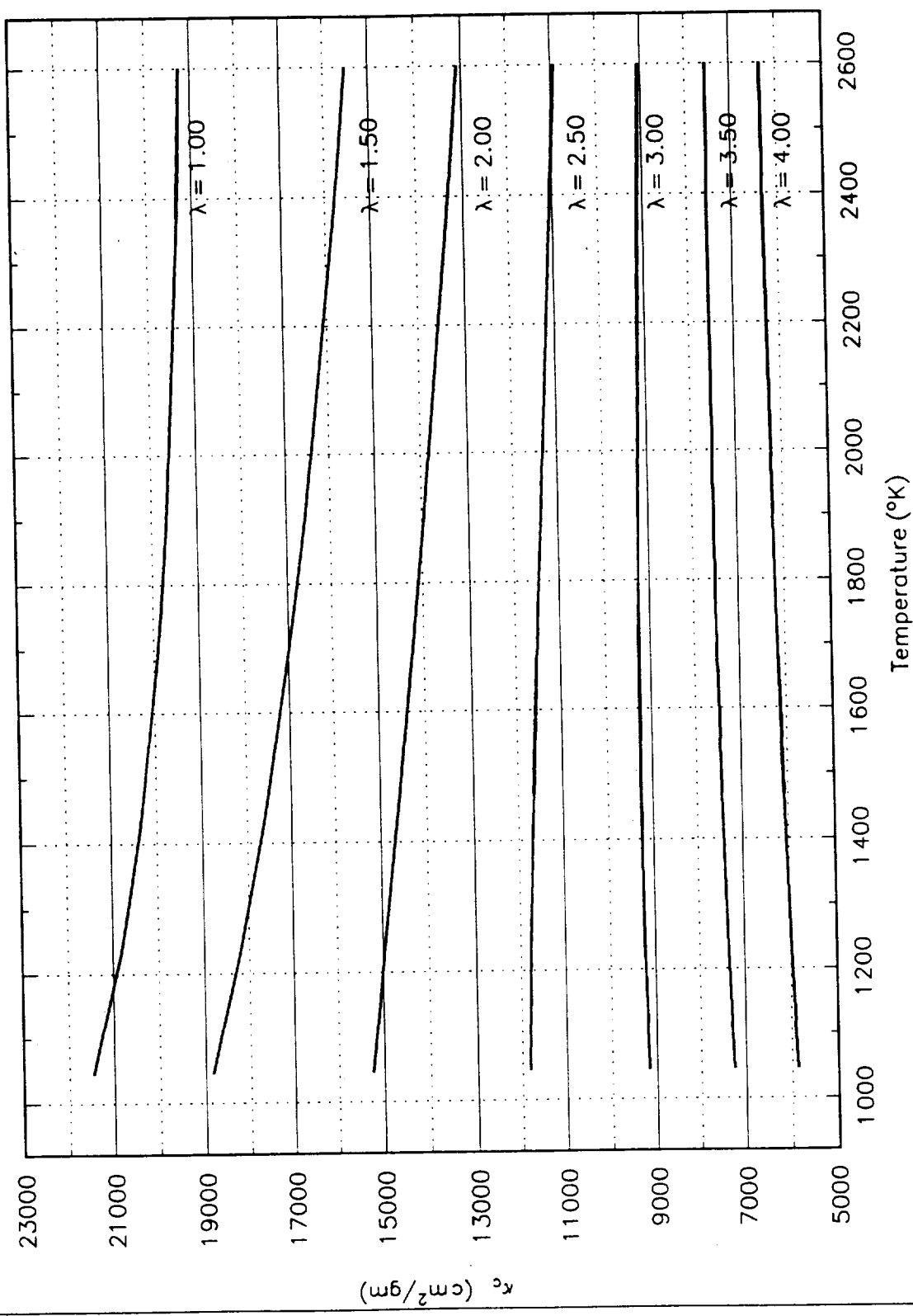
$$K_{\lambda} = \left( \frac{36\pi nk}{(n^2 - k^2 + 2)^2 + 4n^2k^2} \right) \left( \frac{\rho_c}{\rho_o} \right) \left( \frac{1}{\lambda} \right)$$

$K_{\lambda}$ (cm<sup>-1</sup>) =  $\kappa_{\lambda} \rho_c$  = linear absorption coefficient

$\kappa_{\lambda}$ (cm<sup>2</sup>/gm) = mass absorption coefficient

$\rho_c$  (gm/cc of volume) = soot density

$\rho_o$  (gm/cc of soot) = bulk soot density



## **CONCLUSIONS:**

Real fluid RP-1 and H<sub>2</sub> combustion kinetics models will be incorporated into several element models and evaluated.

The element models will be assembled into an entire injector model and the motor performance evaluated.

