135
600
5/20/79

16. 2663

COO-4272-3

MASTER

FUNDAMENTAL AND SEMI-GLOBAL KINETIC MECHANISMS OF HYDROCARBON COMBUSTION

Annual Report for October 1, 1977–September 30, 1978

By
F. L. Dryer
I. Glassman

December 1, 1978

Work Performed Under Contract No. EC-77-S-02-4272

Princeton University
School of Engineering and Applied Sciences
Guggenheim Aerospace Propulsion Laboratories
Princeton, New Jersey

U. S. DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

This report has been reproduced directly from the best available copy.

Available from the National Technical Information Service, U. S. Department of Commerce, Springfield, Virginia 22161.

Price: Paper Copy \$4.50
Microfiche \$3.00

FUNDAMENTAL AND SEMI-GLOBAL KINETIC
MECHANISMS OF HYDROCARBON COMBUSTION

Annual Report

For the period Oct. 1, 1977 to Sept. 30, 1978

F.L. Dryer and I. Glassman
Principal Investigators

Prepared by
Robert J. Santoro

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Prepared for
The U.S. Department of Energy under
Contract EC-77-S-02-4272.A00

1 December 1978

School of Engineering and Applied Sciences
Department of Mechanical and Aerospace Engineering
Guggenheim Aerospace Propulsion Laboratories
Princeton University
Princeton, New Jersey 08540

Abstract

Concern for availability of future supplies of petroleum and natural gas has generated substantial research in the areas of energy utilization and alternative fuel sources. From these efforts the development of technologies which make more efficient use of presently available resources consistent with high quality environmental standards is envisioned. Additionally programs examining the utilization of alternative fuels are aimed at the timely development of coal and oil shale derived fuels.

An extremely promising approach to the achievement of the above goals lies in the utilization of combustion modeling. Aimed at understanding practical combustion environments, present modeling efforts have been hampered by difficulties related to coupling combustion chemistry to the complex fluid mechanics present. In an attempt to circumvent such difficulties the present research program is aimed at the development of simplified chemical kinetic models (usually termed "global" models) to represent the combustion chemistry. Initially aimed at simple hydrocarbon fuels the program is progressing to studies of more complex aliphatics as well as important alternative fuels.

The objective of this research is multifold: a) to determine mechanistic oxidation routes of hydrocarbons derived from crudes and alternate sources, so that efficient and environmentally clean power plants based on internal and external combustion processes can be designed; b) to develop and validate actual simplified (global) reaction rates for these hydrocarbons so that these power plants can be modelled; and c) to develop an understanding of particulate (soot) formation to permit the rapid and successful introduction of the inexpensive, heavy, highly aromatic fuels.

In this annual report progress to date on studies of paraffin, olefin and alcohol hydrocarbons is reviewed. Appropriate global models are presented and compared with experimental data.

The results presented in this report clearly demonstrate that the turbulent flow reactor facility can be used to develop accurate global models for a variety of important fuels. Progress to date has shown the accuracy and reproducibility of detail species prediction for experimental data taken under the turbulent flow reactor conditions. Extension of these results to other combustion conditions appears to be promising.

Table of Contents

	<u>Page</u>
Abstract	ii
Table of Contents	iv
I. Introduction	1
II. Program Approach, Status and Results	4
A. Turbulent Flow Reactor	4
B. Paraffin Hydrocarbon Oxidation	5
C. Methanol Oxidation	7
D. Semi-Global Modeling	8
E. Computer Modeling	12
III. Future Work	13
References	14
Table	16
Figures	17

I. Introduction

Concern for availability of future supplies of petroleum and natural gas has generated substantial research in the areas of energy utilization and alternative fuel sources. The primary goal of such research is oriented towards the more efficient use of presently available energy sources while pursuing the timely development of alternative sources. Although assuring sufficient supplies of energy for the future is of highest priority provision of an energy technology which is environmentally consistent with present efforts directed towards pollutant control is also essential.

One approach addressing the need to develop such an energy technology involves efforts to accurately model combustion processes in real systems. Since combustion environments are typically widely spatially variant, temporally unsteady and fluid mechanically complex, attempts to couple the chemical and fluid mechanical aspects of the problem have not been wholly successful. In developing models for combustion systems, a numerical submodel must be constructed for each of the physical and chemical processes (e.g. atomization, vaporization, turbulence, chemical kinetics etc.) which contribute to the overall system behavior. Specifically in the chemical kinetics submodel, even for simple flow situations, the computer code size required for handling a detailed chemical kinetic model for hydrocarbon oxidation makes computation costs prohibitive. Nevertheless modeling efforts represent a viable and significant approach to providing understanding and insight into combustion oriented problems and can lead to developments resulting in significant energy savings.

If one considers hydrocarbon oxidation as expressible as a series of elementary chemical reactions described by rate constants and species concentrations, a typical model could involve upwards of a hundred individual reactions. As stated

above computation capabilities to handle such models in conjunction with other physical processes in typical combustion environments is not yet realizable. In an attempt to circumvent this problem, efforts have been directed towards the development of simplified (generally termed "global") expressions to describe hydrocarbon oxidation (1,2,3,4). The utility of such expressions lies in the significant reduction in the number of kinetic-like reaction steps required to describe the oxidation process.

The general approach of global modeling can be represented as an overall reaction,

in which the rate of reaction of C_1 , for example, is represented as

$$-\frac{dC_1}{dt} = k_{ov} \prod_i [C_i]^{n_i}$$

In this expression the k_{ov} is typically chosen to have an Arrhenius form,

$$k_{ov} = 10^A \exp(-E/RT)$$

where n_i is the order of the reaction with respect to C_i .

For a particular reaction the n_i 's, A and E are determined to best represent the rate data over as wide a set of conditions as possible. As an example, Dryer (3) has derived the following expression for the oxidation of methane

$$\frac{d[CH_4]}{dt} = 10^{13.2} \exp[48400/RT] [CH_4]^{0.7} [O_2]^{0.8}$$

When coupled with a suitable global mechanism to yield CO_2 and water along with an energy release value, this expression can be used to represent the overall oxidation chemistry of methane.

Thus the chemical kinetic mechanism originally constituting possibly one hundred steps can be approximated by one or two steps. Of course, a great deal of detail information is lost, especially concerning radical species. Nonetheless, the great simplification of the kinetic mechanism afforded by the global approach makes it particularly advantageous for combustion modeling efforts.

The objective of the combustion studies presently underway involves the development of semi-global models to represent overall chemical kinetic mechanisms for simple hydrocarbon fuels. Fuels of present interest include the alkanes: ethane, propane, butane, hexane and octane as well as the important alkenes: ethene, propene and butene. As an extension to this work the study of the detailed characteristic of combustion systems forms a second major aspect of the present program with particular emphasis on the role of OH radicals. Finally, studies of important alternative fuel problems link the program to potential non-petroleum fuel developments. Studies of alternative fuels such as methanol and coal-derived fuel constituents, such as aromatic compounds, compose the major elements of this area of the program.

In the following sections of this report progress made during the past year on the above described effort will be given. Since some of this material was presented in a previous progress report (5), an attempt will be made to summarize material which was already reported and stress newer developments.

II. Program Approach, Status and Results

A. Turbulent Flow Reactor

The studies to be described in detail later in this section have all been undertaken using the Princeton adiabatic flow reactor. This facility has been described in detail elsewhere (3,5) and will only be briefly described here.

Figure 1 shows a schematic of the flow reactor quartz duct and serves to guide the description of the reactor facility. The apparatus employs a hot nitrogen carrier stream produced using an arc plasma torch technique. The nitrogen can be heated to between 900 and 1500 K with all experiments conducted under atmospheric conditions. For oxidation experiments, oxygen is introduced about midway along the inlet section of the reactor. Small amounts of prevaporized fuel are rapidly mixed with the carrier at the throat of the quartz duct via four high velocity mixing inlet nozzles. Following the conically expanding mixing section, is a 10 cm diameter cylindrical section about one meter in length. The entire duct is heated using electrical resistance heaters to the inlet temperature of the gas to approximate adiabatic conditions.

Proper adjustment of the carrier temperature, flow velocity and reactant concentrations results in a steady, one dimensional, adiabatic reaction extending over approximately 85 cm of the cylindrical portion of the reactor duct. Simultaneous thermal and chemical data at discrete longitudinal locations in the reaction zone are obtained by extension of an instrumented probe along the centerline of the reactor duct. Temperature measurements are made with a silica coated Pt/Pt-Rh thermocouple and gas samples are removed through a water-cooled stainless steel sampling probe. Samples are stored at low pressure in an all glass/teflon sampling assembly. Samples are analyzed by gas chromatography for stable products. Hewlett-Packard 7624 and 5840 Research Gas Chromatograph Systems equipped with electronic integrators, thermal conducting and flame ionization detectors are utilized in this analysis.

B. Paraffin Hydrocarbon Oxidation

Current work in this laboratory on the oxidation of paraffin hydrocarbons has been concerned with the lean oxidation of propane and ethene. Previous work on the oxidation of ethane had been completed prior to the current contract year (6), and established that alkane oxidation proceeds through three distinct regions (see Fig. 2). These involve the conversion of the alkane fuel to alkenes nearly isothermally, the conversion of the alkene to carbon monoxide and conversion of carbon monoxide to carbon dioxide. Work to extend and better characterize this sequential process has continued during this contract year.

Studies of the oxidation of propane have further verified the sequential nature of the overall oxidation process. Figure 3 shows the product distribution observed for the oxidation of propane. Again the alkane fuel is converted to olefin species, in this case propene and ethene are produced. The succeeding steps then involve the olefin conversion to CO and finally CO oxidation to CO₂. Thus, for alkane oxidation more than a single global step is required to adequately represent the oxidation process. In semi-global modeling of such a system we have chosen a three step sequence to represent the oxidation process for alkane species more complex than methane:

Studies of the oxidation of propane have been directed towards obtaining the necessary parameters from the experimental data which are required for the overall global expression. Following the same approach as for ethane oxidation, the lean propane oxidation has been assumed to have a region where fuel disappearance is proportional to the extent of the reaction followed

by a region in which only the fuel and oxidizer concentrations are important. Utilizing this approach preliminary expressions for the experiments completed to date yields for the first region:

$$-\frac{d[C_3H_8]}{dt} = 10^{14.7 \pm 2.3} \exp(-46.87 \pm 5.3/RT) [C_3H_8]^{0.42 \pm 0.05}$$

$$[O_2]^{0.70 \pm 0.16} ([C_3H_8]_0 - [C_3H_8])^{0.49 \pm 0.03}$$

$$994 \leq T \leq 1052K$$

and for the second region:

$$\frac{d[C_3H_8]}{dt} = 10^{11.8 \pm 3.2} \exp(-44.2 \pm 5.3/RT) [C_3H_8]^{0.77 \pm 0.04}$$

$$[O_2]^{0.47 \pm 0.36}$$

$$1000 \leq T \leq 1100$$

It should be reemphasized that these expressions describe the oxidation of the alkane to alkenes and production of carbon monoxide and carbon dioxide follow.

Since alkene oxidation to carbon monoxide is one of the sequential steps in the oxidation process, a study of ethene oxidation has been undertaken and completed during this year (7). The product distribution for a typical ethene oxidation is shown in Figure 4. Semi-global analysis has been applied to describe the experimentally observed ethene oxidation rate and the resulting expression for the lean region is

$$-\frac{d[C_2H_4]}{dt} = 10^{10.9} \exp(-51,000/RT) [C_2H_4]^{0.8}$$

As will be described later this expression has been incorporated into work describing the overall oxidation of ethane to predict the ethene conversion to CO.

Tables I and II summarized the semi global models resulting to date in the lean region. As is evident some trends in the semi-global parameters in Table I are evident for the alkane, alkene and alcohol species studied. Typically, the fuel order is 0.8 with no oxygen dependency observed (methane is an exception in this trend and the propane case is not yet complete). Activation energies are generally of the order of 45 to 55 kcal/mole with the major differentiating parameter being the pre-exponential factor. For the extent of reaction case no clear trends are yet evident.

C. Methanol Oxidation

Studies of the oxidation of methanol have also been initiated since the contract began. A number of experiments have been conducted spanning a range of equivalence ratios between 0.05 and 3.15 and temperatures between 940 and 1030 K. Analysis of the results has initially involved extending the kinetic mechanism previously derived for pyrolysis of methanol (8).

The results of a typical oxidation experiment for methanol are given in Figure 5. Of particular note is the absence of

methane and C_2 species which indicates that methyl radicals are not of major significance to the reaction mechanism. In addition it is interesting to note that appreciable CO_2 production does not occur until nearly all the methanol fuel has disappeared. This implies that either OH radicals are absent during the oxidation of the fuel or that reactions with OH and methanol or one of its primary products is much faster than the $CO + OH$ reaction. This conclusion can be drawn from early work done on the moist oxidation of CO. (3)

Semi-global modeling has resulted in the development of two global expressions. One describing the lean region ($\phi < 1$)

$$-\frac{d[CH_3OH]}{dt} = 10^{11.53 \pm 0.76} \exp(-54800 \pm 2900/RT) [CH_3OH]^{0.65 \pm 0.03}$$

$$1000 \leq T \leq 1120 \text{ K}$$

and second for the rich region ($\phi > 1$)

$$-\frac{d[CH_3OH]}{dt} = 10^{31.54 \pm 0.96} \exp(-123000 \pm 4500/RT) [CH_3OH]^{1.55 \pm 0.11}$$

$$1000 \leq T \leq 1075 \text{ K}$$

These expressions have been utilized to model the flow reactor results with good success. This aspect of the work will be discussed in Section D of this part of the report. Further discussion of the results of the methanol oxidation study is given in Ref. 9.

D. Semi-Global Modeling

Global modeling offers the opportunity of utilizing a small number of elementary-like reaction steps to describe complex hydrocarbon oxidation processes. A comprehensive review of global modeling efforts for combustion applications has been given by Dryer (4).

As mentioned above, extensive efforts have been underway in this laboratory to develop global expressions for a number of fuel species. To date expressions for methane, ethane, ethene, propane, methanol and carbon monoxide have been derived. With the completion of the work on ethene, modelling of the three step sequence described above for hydrocarbon oxidation is feasible.

Since the methanol system has proved to be a simpler system to treat, approaches to validate the derived semi-global expressions have been applied first to this system. Using the semi-global expressions for the oxidation of methanol and the oxidation of CO individual flow reactor experiments were predicted in the form of the species profiles. The global model used was a two step process:

$$\Delta H = 93900 \text{ cal/mole}$$

$$\Delta H = 67550 \text{ cal/mole}$$

The approach taken has been to use the derived semi-global expression to predict the fuel and product species curves observed in the flow reactor experiments. A Runge-Kutta integration has been used to integrate the semi-global expressions with respect to time. The energy release for each step of the global model has been used to calculate the temperature (the ethane results reported later in this section use only the experimentally measured temperature). Conversion of CO to CO₂ has been treated using the correlation derived by Dryer (3).

The results of the comparison between the flow reactor data and the semi-global model is shown in Figure 6. Since the semi-global expressions were derived from such data one would expect reasonable agreement between the fuel disappearance prediction

and the data. Nonetheless it is gratifying to obtain such good agreement since it is possible to derive correlation expressions which represent the data of several runs to some degree, but fail to predict any single experiment.

In the case of the CO to CO₂ conversion, two points are worth making. First, the CO to CO₂ step has been represented by the expression derived by Dryer for the pure CO/H₂O/O₂ system (3). Thus, these results verify the applicability of this expression in other oxidation systems. Additionally, in the early stages of the reaction to CO to CO₂ conversion has been moderated to take into account the competition for OH radicals. As was mentioned above, CO₂ is formed mainly by the reaction

Early in the reaction where fuel and fuel radicals are still present

competes successfully with the CO attack. In fact, CO₂ formation is largely precluded as is evident from the product profiles in Figure 5. To account for this effect, the CO correlation has been moderated by the ratio of the rate of Reaction 4 and 5

$$R = \frac{k_4 [\text{CO}]}{k_5 [\text{CH}_3\text{OH}]} \quad R < 1$$

$$R = 1 \quad \text{for} \quad \frac{k_4 [\text{CO}]}{k_5 [\text{CH}_3\text{OH}]} > 1$$

Thus, for CO to CO₂, the correlation has the form

$$\frac{d[\text{CO}_2]}{dt} = R 10^{14.6} \exp[-40000/RT] [\text{CO}]^{1.0} [\text{H}_2\text{O}]^{0.5} [\text{O}_2]^{0.25}$$

As can be seen in Figure 6, this results in good agreement between the early CO_2 prediction and the observed data.

In the ethene case a two step process has also been used to represent the oxidation process.

$$\Delta H = 181000 \text{ cal/mole}$$

$$\Delta H = 67550 \text{ cal/mole}$$

and a similar comparison has been made between the flow reactor data and the semi global model results. As can be seen in Figure 7, the agreement between the semi global model and the data is very good. In this example the same approach was taken into account for the CO oxidation to CO_2 early in the reaction as was described above except that

was substituted for reaction 5.

With the completion of the ethene studies and the validation of the applicability of the previously derived CO correlation for application in hydrocarbon oxidation systems, it is now feasible to attempt to model an alkane system. The ethane system has been initially addressed. Figure 8 shows the results of applying the previously described three sequential step mechanism to the ethane system:

Although the comparison in Figure 8 shows agreement is not quite as good as in the ethene case, the predictions do show good agreement with respect to peak concentrations and reaction times. Additionally, these results do support the three step sequential model as an approach to adequately describing the alkane oxidation process.

E. Computer Modeling Efforts

We have established working relations with and received considerable cooperation from the Lawrence Livermore Laboratory, Livermore, California (T Division). This group has been specifically interested in developing chemical kinetic modeling capabilities suitable for analytical experiments on combustion systems. A one-dimensional analytical model of the Princeton turbulent flow reactor and a thermodynamic chemical kinetic program have been developed and exercised.

The flow reactor model contains turbulent diffusion effects in the longitudinal direction but no turbulent chemical kinetic coupling.

To date detailed carbon monoxide and methane oxidation mechanisms have been assembled and used to test analytical programs. Results have confirmed that reactor turbulence has little effect on observed combustion chemistry and several interesting features regarding elementary kinetics have also been discovered. Of particular note, modeling efforts for the carbon monoxide oxidation demonstrated reactions involving HO_2 and H_2O_2 were extremely important in reproducing the experimental results. For this reaction HO_2 reactions moderate OH concentration and thus slow down the oxidation of CO.

In the methane oxidation case, modeling efforts (10) indicate that up to half the methane is oxidized via an ethane route due to recombination of radicals and finally to CO. As fuel to air ratio increases, this route plays an increasing role and under certain conditions, can dominate the oxidation mechanisms.

Comparisons of the semi-global expressions with the detailed kinetics model show general agreement between the predicted

results (11). Thus, for the methane case, the applicability of the semi-global approach has been validated. Extension of this approach to other fuels under study in this program is currently underway in the laboratory. Additionally, Dryer and Westbrook are independently considering the cases for methanol and ethane for which the flow reactor data will represent one of the data base inputs to validate the kinetic models.

The utility of the measurement of detailed product profiles made with the Princeton turbulent flow reactor is especially evident in studies of the type discussed above. The accuracy and detail of these measurements provides for extension verification of the computer model under consideration. In fact, the present flow reactor represents a unique capability in this respect and thus is a substantial resource in terms of combustion modeling.

III. Future Work

Research efforts during the next year will concentrate in four areas:

- (1) Work on the oxidation of the alkane species will continue with more complex fuels (e.g. butane, hexane and octane) to be considered. These studies will utilize the insights gained in the ethane and propane studies to aid in the rapid development of semi-global expressions to characterize these fuels. As was pointed out above, results to date have lent encouragement to this approach since certain common features are emerging from the previous semi-global studies.
- (2) The detailed studies of OH radical concentrations in the flow reactor experiments will be initiated. The experimental facility is presently under construction and the dye laser system has been installed. The initial experiments will be done in the $\text{CO/O}_2/\text{H}_2\text{O}$ system with sensitized

reaction studies to commence at the end of the next contract year.

- (3) Semi-global modeling validation will also continue with emphasis on predicting data which lies outside the flow reactor conditions. Such considerations will better establish the useful range of the semi-global expressions.
- (4) Studies of the oxidation of aromatic fuels will also commence. The first studies will involve toluene, xylene and other alkylated benzenes. Emphasis will be on the reaction mechanism and product distribution observed over a wide range of operating conditions. These studies will involve the use of the gas chromatography and mass spectrometry capabilities of the laboratory.

Work in conjunction with Westbrook at Lawrence Livermore involving detailed modeling will continue on the basis of mutual interest with the ethene and propane oxidation systems being of primary interest.

References

1. A Quasi-Global Chemical Kinetic Model for the Finite Rate Combustion of Hydrocarbon Fuels, R.N. Edelman and O. Fortune, AIAA Paper 69-86, (1969).
2. Experimental and Theoretical Studies of NO_x Formation in a Jet-Stirred Combustor, V.S. Engleman, R.B. Edelman, W. Bartok, and J.P. Longwell, 14th Symposium (International) on Combustion, The Combustion Institute, 755 (1973).
3. The High Temperature Oxidation of CO and CH_4 , F.L. Dryer and I. Glassman, 14th Symposium (International) on Combustion, The Combustion Institute, 987, (1973).

4. Combustion Chemistry of Chain Hydrocarbons, F.L. Dryer and I. Glassman.
5. Fundamental and Semi-Global Kinetic Mechanisms of Hydrocarbon Combustion, I. Glassman, F.L. Dryer and R.J. Santoro, Progress Report Oct. 1, 1977 to June 30, 1978, DOE Document Number COO-4272-2 (1978).
6. The High Temperature Oxidation and Pyrolysis of Ethane, R. Cohen, Princeton University AMS Department Ph.D. Thesis Report No. 1338T (1977).
7. An Investigation of the Pyrolysis and Oxidation of Ethylene in a Turbulent Flow Reactor, K.P. Schug, R.J. Santoro, F.L. Dryer and I. Glassman, presented at the Spring Western States Section/Combustion Institute Meeting (1978).
8. Kinetics of the Pyrolysis of Methanol, D. Aronowitz, D.W. Naegeli and I. Glassman, J. Phys. Chem. 81, 2555 (1977).
9. Kinetics of the Oxidation of Methanol: Experimental Results, Semi-Global Modeling and Mechanistic Concepts, D. Aronowitz, R.J. Santoro, F.L. Dryer and I. Glassman, presented at the 17th Symposium (International) on Combustion, University of Leeds, England (1978).
10. A Numerical Model of Chemical Kinetics of Combustion in a Turbulent Flow Reactor, C.K. Westbrook, J. Creighton, C. Lund and F.L. Dryer, J. Phys. Chem. 81, 2542 (1977).
11. Detailed Models of Hydrocarbon Combustion, F.L. Dryer and C.K. Westbrook, Proceedings of the DOE, Division of Power Systems Workshop on Modeling of Combustion in Practical Systems, Los Angeles, Ca. (1978).

TABLE 1

SEMI-GLOBAL EXPRESSIONS FOR LEAN OXIDATION CONDITIONS-

$$-\dot{F} = k_{OV} (F)^A (O_2)^B (H_2O)^C$$

$$k_{OV} = 10^A \exp(-E/RT), 950 \leq T \leq 1200K$$

FUEL		A	E	A	B	C	NOTE
C ₂ H ₄		10.9	51,000	0.8	0.0	N.A.	
CH ₃ OH		11.53	54,800	0.81	0.0	N.A.	
C ₃ H ₈		11.8	44,200	0.77	?	N.A.	(1)
C ₂ H ₆		9.9	45,900	0.80	0.0	N.A.	(2)
CH ₄		13.2	48,400	0.70	0.8	N.A.	(2)(3)
CO		14.6	40,000	1.0	0.25	0.50	(2)(3)
CO		14.8	42,900	1.0	0.25	0.50	(2)(4)

(1) PRELIMINARY EXPRESSIONS

(2) PREVIOUSLY REPORTED

(3) IN CO/H₂O/O₂ SYSTEM(4) IN CH₄/O₂ SYSTEM

SEMI-GLOBAL EXPRESSIONS FOR EXTENT REGION

$$-\dot{F} = k_{OV} (F_0 - F)^A (F)^B (O_2)^C$$

FUEL	A	E	A	B	C
C_3H_8	14.7	46900	0.49	0.42	0.70
C_2H_6	14.4	55300	0.80	0.4	0.0

FIGURE 1

CHEMICAL COMPOSITION OF SPREAD ETHANE-AIR REACTION

FIGURE 2

FIGURE 3

FIGURE 4

FIGURE 5

METHANOL OXIDATION

CH₃OH OXIDATION

FIGURE 6

FIGURE 7

ETHANE OXIDATION

FIGURE 8