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NO_x DESTRUCTION IN DIFFUSION FLAME ENVIRONMENTS
Final Report

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July 31, 1991

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ABSTRACT

This research is concerned with reburning, which is an NO_x abatement technique involving the injection of secondary fuel into the post flame of a furnace. The specific objectives of this research are to determine whether heterogeneities inherent in diffusion flame environments can be exploited to achieve greater reductions in NO than can be achieved in premixed systems. The research project described here is but a first step to explore this question, and should be viewed more as a screening study rather than as completed research, the results of which are completely understood.

The problem was attacked through both experimentation and theoretical modeling. Experiments employed a bench scale, laminar, counter-flow, diffusion flame, which was designed to simulate the stretched diffusion flamelets that arise at the interface between turbulent fuel and oxidant jets. Data gathered were of two types. First, NO destruction from the integral system was investigated through parametric studies in which only inlet and outlet species and flows were measured. Three different experimental configurations were examined, under a wide range of operating conditions, with emphasis on reburning under overall fuel lean conditions. Second, in order to gain insight into the observed phenomena, detailed axial profiles of major and minor species were measured for one configuration.

Theoretical modeling consisted of computer simulations which attempt to describe the experimental configuration as an infinitely wide flat flame. This yielded predictions of axial profiles but was not readily adaptable for (integral) predictions of total NO destroyed in our flame. The model employed detailed chemical reactions, and was also used to determine regimes in which ignition occurs under diffusion flame conditions.

Experimental results are new, and suggest that, under diffusion flame conditions, significant NO destruction occurs, even when the overall conditions are fuel lean. Furthermore, destruction is extremely efficient for NO molecules that contact the (diffusion) flame zone, and, in our system, the exhaust NO concentrations are roughly independent of the primary NO level, when that is above 450 ppm. Mathematical modeling results were consistent with the (differential) experimental observations of species profiles, but more work is required to connect it to the integral experimental measurements, and to practical systems.

Overall, results from this research support the idea that reburning through large scale eddies in full scale furnaces, may be able to: 1) allow retrofit reburning under overall fuel lean conditions, and 2) achieve greater reburning efficiencies than are possible under more premixed conditions. The work reported here provides a basis for additional research which is required to understand how the concept of reburning through large reducing eddies can be optimized and subsequently applied to practical systems.

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RESEARCH OBJECTIVES

This report presents research results of a project that was designed to address two questions: First, can large reductions in NO be achieved by exploiting non-equilibrium aspects and heterogeneities present in diffusion flames? Second, what are the mechanisms governing the destruction of NO during reburning in diffusion flame environments? Emphasis was on *overall* fuel lean environments, since these constitute more benign environments for the retrofit application of reburning in the field.

SIGNIFICANCE

Available understanding of the parameters which limit and control reduction of NO by reburning in full scale boilers is limited. Much of previous research on reburning has been directed at premixed or almost premixed systems (Chen et al.1986, Mereb and Wendt, 1990, Wendt and Mereb, 1990). That research has provided useful insight into kinetic mechanisms in downflow laboratory combustors, where mixing is rapid, but has overlooked potentially important phenomena which can occur in large turbulent diffusion flames or in transient reducing eddies, which may occur in large scale units. It is hypothesized that heterogeneities or unmixedness, as exemplified by a diffusion flame front sweeping through a NO containing mixture, can produce free radicals that allow NO destruction kinetics to destroy NO to values approaching equilibrium. Of course, the flue gas temperatures and oxygen contents that support a diffusion flame (front) before micro-mixing occurs are not known, and so a secondary issue that must be addressed is the determination of diffusion flame stability limits as a function of these two parameters.

A recently developed reburning concept is a process denoted as "Reducing Eddy After-Burn (REAB)" (Breen, Gabrielson, and Lange, 1988), in which puffs of natural gas sweep through the primary flue gas of a boiler. The hypothesis is that the diffusion flame attributes at the boundaries of each puff are sufficient to destroy NO efficiently, without ever having to operate the upper half of the furnace under overall fuel rich conditions, i.e., without having to add additional burnout air, as is required for conventional reburning processes. The screening study conducted here was designed to determine whether this idea had merit, and whether, in fact, NO could be destroyed in diffusion flames more efficiently than is possible in premixed systems, and under more benign overall environments. Therefore, emphasis in this work is on reburning in diffusion flames under overall fuel lean conditions, although it should be noted that as far as a diffusion flame front (which is always located at a point where the local stoichiometry is close to unity) is concerned, the overall stoichiometry is irrelevant.

BACKGROUND

Reburning Mechanisms

NO is not favored by equilibrium at low temperatures. Therefore, its destruction is kinetically limited. Free radicals can form a path to allow NO destruction, but they have very short lifetimes at significant concentrations in the cooler portions of the flue gas. Most of the available literature on reburning mechanisms has focussed on homogeneous, premixed systems. Detailed kinetic mechanisms have been developed by Glarborg, Miller and Kee (1986) and later modified by Miller and Bowman (1989). The major paths to production of N_2 from NO are shown on Figure 1. A reaction subset, derived from these references and employing 151 reactions was used in the theoretical portion of this work and is shown on Table 17 in the Appendix.

More recently, Mereb and Wendt (1990) developed global approximations to reburning mechanisms as they occurred under premixed conditions in the reburning zone. This approach provides insight into rate controlling mechanisms under premixed conditions, and therefore is presented here. Following Bose and Wendt (1988), they used the detailed kinetic mechanism of Glarborg, Miller and Kee (1986) as a basis for determining both, which reactions were likely to be most important, and values of kinetic rate coefficients to be employed. No adjustment of any rate constant was made and the analysis was done only in terms of known detailed kinetic mechanisms taken from the literature.

According to their data, the rate of destruction of NO can be given by:

where NH_i and CH_i concentrations were calculated from partial equilibria:

This yields the following expression for the rate of change of NO:

This yields the following expressions for the rates of change of HCN:

$$\frac{d(HCN)}{dt}_{\text{destruction}} = -(HCN)[f_3+f_4] \quad (9)$$

$$\frac{d(HCN)}{dt}_{\text{formation}} = (CH_4)[(NO)f_2+(N_2)f_5+(NH_3)f_6] \quad (10)$$

N_2 was formed by Reaction (1) and destroyed by Reaction (7), yielding:

$$\frac{d(N_2)}{dt} = (NO)(NH_3)f_7 - (CH_4)(N_2)f_5 \quad (11)$$

The rate of change of NH_3 was determined from a nitrogen balance:

$$\frac{d(NH_3)}{dt} = -\frac{d(NO)}{dt} - \frac{d(HCN)}{dt} - 2\frac{d(N_2)}{dt} \quad (12)$$

The f_i in Equations (5 and 9-11) have the form:

$$f_i = \sum_{j=1}^{1,2, \text{ or } 3} A_{ij} T^{N_{ij}} \exp\left(\frac{B_{ij}}{T}\right) \times \frac{(OH)^{m_{ij}}}{(H_2O)^{l_{ij}}} \quad (13)$$

where values for parameters in f_i are derived from fundamental equilibrium and rate constants taken from the literature, and are given by Mereb and Wendt (1990). Equations (5 and 9-12) can predict XN species profiles, *ab initio*, provided initial conditions and estimates for OH are available.

The relevance of the above discussion to the current research, which is concerned with non premixed systems, lies in the importance of hydrocarbon radicals both to destroy NO directly and to form HCN, which is then the source for additional N radicals that can further destroy NO to make N_2 . Unfortunately, that research also showed that hydrocarbon radicals can also fix nitrogen by making HCN from N_2 , and this can limit reburning

effectiveness. Under premixed conditions, CH radicals have a very short lifetime, and this also limits reburning effectiveness.

Laminar Flamelets.

The issue is how to produce free radicals (CH_i , NH_i) under conditions where they would not normally exist, namely under fuel lean conditions and at low temperatures. A diffusion flamelet, containing locally steep gradients of temperature and species concentrations and originating from large turbulent diffusion flames can exist under such overall environments. It may, in fact, sweep through the surrounding gases, and serves to produce large quantities of super-equilibrium free radicals, which, upon diffusing into the cooler neighboring regions which contain NO, react with it to form N_2 on their path to low equilibrium values. This process is hereafter denoted as the "Breen Hypothesis", after Bernard P. Breen, who first enunciated it.

Figure 2: Schematic of a Diffusion Mixed Burner

A crude schematic of a large diffusion mixed burner is shown on Figure 2. The actual burning process is an extremely complicated one, and there are many chemical and physical processes occurring simultaneously. Only in a relatively thin interface is there a combustible mixture, and this governs the formation of a (fluctuating) sheet of flame. This sheet is very much warped and wrinkled, as eddies of fuel are swept out into the air section or as eddies of oxygen containing air move into the fuel. Pockets of flame will be carried into unignited regions, which will burst into new flames; or they may be projected into zones that have already been burned out, whereupon the flame is diluted and quenched. The turbulent combustion process is, therefore, far different from one in which mixing occurs by

an "eddy viscosity" or by "eddy diffusion". Rather it occurs through engulfment and stretched laminar flamelets, which represent the burning interfaces between fuel and air.

That stretched laminar flamelets can be used to describe turbulent diffusion flames has been shown experimentally by Drake (1986) and theoretically by Peters (1986) amongst others. The discovery of coherent structures in turbulent flames (Roshko, 1974) reactivated the idea that the turbulent flame is composed of an ensemble of laminar flamelets, each of which is stretched in its own plane (Chigier and Yule, 1979). Marble and Broadwell (1977) postulated a model which involved a balance equation for flame density, where the rate at which reactants are consumed in a volume (which is small compared to the turbulent motion, but large compared to the flame thickness) is set equal to the product of the flame density (flame surface per unit volume) and the rate of reactant consumption per unit area. This is illustrated in Figure 3. On a micro-scale, laminar flame fronts are continuously stretched and deformed by turbulent motion. The straining, which increases the area of the laminar diffusion flamelet, has a definite effect on the rate of reaction per unit area, affecting in this form the rate of formation and destruction of various intermediate species.

Counterflow Diffusion Flames

A schematic of a counterflow diffusion flame is shown on Figure 4. Fuel and air streams impinge from two opposed parallel plates, to form a thin, stretched, diffusion flame sheet between them. This system can be described by the conservation equations for momentum, energy and species. If it is assumed that the plates are infinitely wide, the two dimensional conservation equations can be transformed using the following:

$$\begin{aligned}
 v_z &= v(z) \\
 v_r &= r\psi(z) \\
 \rho &= \rho(z) \\
 T &= T(z) \\
 x_i &= x_i(z) \quad i=1, \dots, N \\
 p &= p(z) - Qr^2
 \end{aligned} \tag{14}$$

where Q is a constant and an eigenvalue of the system when velocities at both burners are specified. This similarity transformation is only valid at low Mach Numbers, when changes in pressure are small compared to its absolute value.

Applying the transformations shown in Equation (14) to the conservation equations yields:

Figure 3: Schematic showing relationship between a turbulent diffusion flame and a stretched laminar flamelet.

Figure 4: The flat, laminar, opposed jet, diffusion flame.

Continuity:

$$\frac{d\rho v}{dz} + 2\rho\psi = 0 \quad (15)$$

r-Momentum:

$$\psi^2 + v_z \frac{d\psi}{dz} = -2 \frac{Q}{\rho} + \frac{1}{\rho} \frac{d}{dz} \left(\mu \frac{d\psi}{dz} \right) \quad (16)$$

Species: (i = 1, ..., N)

$$D_{im} \frac{d^2 x_i}{dz^2} + \left\{ \frac{1}{c} \frac{d(cD_{im})}{dz} - v_z \right\} \frac{dx_i}{dz} + \left\{ \frac{v_z}{M} \frac{dM}{dz} \right\} x_i = -\frac{R_i}{c} \quad (17)$$

Energy:

$$\frac{\lambda}{\rho C_p} \frac{d^2 T}{dz^2} + \left\{ \frac{1}{\rho C_p} \left[\frac{d\lambda}{dz} + \sum_{i=1}^N \rho C_{p,i} D_{im} \right] - v_z \right\} \frac{dT}{dz} = \frac{1}{\rho C_p} \sum_{i=1}^N H_i R_i \quad (18)$$

where pseudo binary diffusion has been assumed and thermal diffusion has been neglected.

The approach used to solve this system of equations is to solve the equations of r-momentum, energy and species conservation in a fully implicit manner after discretizing in the spatial domain. A time dependence was added to allow iteration to a steady state from an initial guess. In all, $N+2$ second order ODE's were solved in this way, where N is the number of species appearing in the reaction set used. Continuity was solved at each time step, using Simpson's Rule, and this updated the axial velocity field.

The momentum, energy and species conservation have the general form:

$$A_i(z) \frac{d^2 Y_i}{dz^2} + B_i(z) \frac{dY_i}{dz} + D_i(z) Y_i = F_i(z) \quad i=1, \dots, N+2 \quad (19)$$

The following problems arise when attempting a solution:

1. Stiffness through the forcing function $F_i(z)$ due to detailed reaction mechanisms.
2. Coefficient $B_i(z)$ changes sign, causing a regular first order turning point.

3. Steep spatial gradients occur, especially near the flame zone.
4. Instabilities due to numerical approximations.
5. Step-size and convergence criteria.
6. The eigenvalue nature of the problem, where Q is an eigenvalue consistent with specification of upper and lower velocities.

Stiffness was addressed by expanding $F_i(z)$, which contain the stiff kinetics, in a Taylor Series about the k 'th time step values, giving:

$$F_i^{k+1} = F_i^k + \sum_{j=1}^N \left. \frac{dF_i}{dY_j} \right|^k (Y_j^{k+1} - Y_j^k) \quad (20)$$

The problem associated with steep spatial gradients was solved by using a modified, weighted, finite difference formulation, as described by Hahn and Wendt (1985) and Corley and Wendt (1985):

$$\frac{dY}{dz} = \frac{W_{p+1,1}Y_{p+1} - W_{p-1,1}Y_{p-1}}{2h} + W_1^0 \quad (21)$$

and:

$$\frac{d^2Y}{dz^2} = \frac{W_{p+1,2}Y_{p+1} - 2Y_p + W_{p-1,2}Y_{p-1}}{h^2} + W_2^0 \quad (22)$$

where the actual expressions for the weighting functions, $W_{i,k}$, depend on whether the roots of the characteristic equation of the second order ODE are real and distinct, complex, or real and equal, and the W_{i0} arise from inclusion of the forcing function in the development.

The ensuing system of equations to be solved at each time step, defines a block, tridiagonal matrix, where the diagonal blocks are full matrices containing the Jacobian, and the off diagonal blocks are diagonal matrices. This system was solved using LU decomposition.

The eigenvalue nature of the problem is handled in a simple and straightforward manner. A value of Q is selected, based on the approximation:

$$Q = \frac{[\rho_{fuel}^{1/2} v_{fuel} + \rho_{ox}^{1/2} v_{ox}]^2}{L_{spacing}^2} \quad (23)$$

Specifying boundary conditions for T_{∞} and reactants, the fuel-side burner velocity is set. The converged solution yields the value for v_{ox} consistent with Q . If the oxidant side velocity is different than the experimental value, a new value of Q is selected and the process repeated until a match is found.

EXPERIMENTAL EQUIPMENT

Laminar Counterflow Burner

A schematic of the experimental system is shown on Figure 5. The burners were four inches in diameter, and enclosed in a chamber as shown. The oxidant to simulate flue gas that contains NO were introduced at the bottom, while fuel diluted with nitrogen was introduced at the top. The burners were made of stainless steel tubes which were filled with glass beads as shown in Figure 6 and sealed at the ends with stainless steel porous disks. The purpose of the beads is to randomize the flow pattern in the burner thus avoiding the formation of a velocity profile (Hahn,1979). All gas flows were measured using Matheson type Rotameter series 602-610 at 50 psi back pressure. The feed lines and sampling lines were made of teflon tubing connected with Swagelock fittings. No brass fittings were used.

Modification to the burner design adopted for later experiments consisted of a 1.81 inch diameter stainless steel pipe coaxially arranged in a 4 inch pipe as shown in Figure 7. NO was fed via the inner pipe while the oxidant gases went through both the inner and outer pipes. This is denoted as Configuration C-4. Both flows passed through a half inch thick bronze porous plate. A double seal arrangement was adopted to prevent edge leaks from the burner cap due to warping, which was a persistent problem when a thin stainless steel disk was used. The purpose of this modification is to increase the portion of NO that reaches the flame front. However, as shown on Figure 8, this configuration did not achieve one dimensionality until some distance away from the burner. Future work should improve precision of the experimental conditions examined and that of the ensuing data, if any comparison with the model described above is to be meaningful.

Sampling and Analysis

A schematic of the analysis train is also shown in Figure 5. The sample gas was drawn by a vacuum pump at constant rate either from the exhaust line or from the in-flame sampling probe. In the case of flame region sampling the rate of sampling was adjusted to a level where no visual disturbance on the flame due to sampling was observed.

The sample was passed to an expansion flask jacketed in ice to remove water in the sample gas. The sample train was then divided into two streams for simultaneous analysis of NO_x and other (stable) species. The NO_x analysis was done by a (TECO) Model 10A self contained chemiluminescent NO/NO_x analyzer with a (TECO) Model 300 Molybdenum $\text{NO}-\text{NO}_2$ convertor. The analysis of other species was made through an analytical Gas

Figure 5: Experimental System.

Chromatography. Specially ordered for this project was a GC completed with a digital Integrator (model SP4400, Spectra-Physics) with 4K RAM storage capacity. The GC, model 01311-SP, manufactured by Hach Carle Chromatography, consists of TCD and FID that can be operated independently and simultaneously. The highest sensitivity for the instrument can be achieved with helium as the carrier gas. In all the experiments presented in this report, helium was used.

A schematic sketch of the GC flow system is shown in Figure 9. The GC consists of 2 columns each requiring a carrier gas flow rate of 20 ml/min. It is important to maintain these flow rate as constant as practically possible. Regular check of the flow rates was carried out using a simple soap bubble meter.

Figure 6: Opposed jet diffusion flame: burner details.

The combined GC integrator arrangement gave readings of resolution of $\pm 0.001\%$ of a species in sample. The species analyzed this way were CH_4 , CO_2 , CO , O_2 , N_2 , H_2 , C_2H_2 , C_2H_4 and C_2H_6 . Trace species of NH_3 and HCN were further analyzed using standard wet chemistry electrode tests.

EXPERIMENTAL RESULTS

Parametric Studies

The objective of the parametric screening studies was to determine, through *integral* input/output measurements of NO destruction in our apparatus, whether diffusion flames might be more efficient for destroying NO than premixed flames, as hypothesized by Breen. These experiments were also necessary to determine whether NO destruction was likely under overall fuel lean conditions. Furthermore, these studies also helped define more precisely, issues requiring resolution.

Input/output measurements consist of species concentrations and flows. Unknown quantities were N_d , the *dry* molar flow rate of the exhaust, per 100 moles/min of total flow

Figure 7: Modified coaxial bottom burner.

in, and N_{H_2O} , the moles/min of water in the exhaust, per 100 moles/min of total flow in.

The carbon balance:

$$\{\%CH_4 + \%CO_2\}_{inlet} = \frac{N_d}{100} \left\{ \%CO + \%CO_2 + 2 \sum_{i=2,4,6} \%C_2H_i \right\}_{exhaust} \quad (24)$$

yields N_d , since all other quantities in Equation (24) are measured.

The oxygen and hydrogen balances:

$$2\{\%O_2 + \%CO_2\}_{inlet} = \frac{N_d}{100} \{ \%CO + 2\%CO_2 + 2\%O_2 \}_{exhaust} + N_{H_2O} \quad (25)$$

were solved simultaneously to yield values for N_d (independently of that calculated by Equation (24)) and N_{H_2O} . Everything else in Equations (25) and (26) was measured. For all runs reported here, the two values of N_d (calculated by Equation (24) and Equations (25))

Figure 8: Radial profiles of NO_x for Configuration C-4.

$$4\{\%CH_4\}_{inlet} = \frac{N_d}{100} \{2\%H_2 + 4\%CH_4 + 2\%C_2H_2 + 4\%C_2H_4 + 6\%C_2H_6\}_{exhaust} + 2N_{H_2O} \quad (26)$$

& (26) together) were within 3% of each other, indicating that all our concentration and flow measurements were consistent, and that there were no leaks diluting the exhaust sample. Details are found on the tables of results following. This is important, since our conclusions from this phase of the work hinge on our being able to close all mass balances accurately.

In the presentation of results that follows, raw data can be found in the tables in the Appendix, while data in the figures represent ppm values which, in order to account for any dilution effects, have been reduced to the inlet molar flow rate, thus:

$$\{NO_x\}_{ppm, reduced} = \frac{N_d}{100} \{NO_x\}_{ppm, measured} \quad (27)$$

Integrated input/output results from four burner configurations (C-1 through C-4) are presented. It was not easy to stabilize a steady stretched diffusion flame at perceived optimum values of overall stoichiometric ratio, flue gas oxidant concentrations, diluent concentrations, and flame stretching rates (as determined from burner velocities).

Figure 9: Schematic of flow system in Model AGC 01311 chromatograph.

Therefore, in this preliminary effort, we focussed on overall fuel lean flames, and on high levels of O_2 in the "flue" gas. It will be shown later, through theoretical analysis, that at lower oxygen concentrations, stable diffusion flames can only be established at high inlet temperatures.

The first set of results was obtained with the burner configuration shown on Figure 6. Here, NO was distributed uniformly across the bottom burner exit, and so a large fraction of the inlet NO failed to ever reach the (finite width) flame. Experimental results are shown on Tables 1 and 1a¹, and the NO ppm in the exhaust, shown by filled circles, is compared to that in the total inlet on Figure 10. The solid line depicts what the results would be were zero NO destroyed. It is evident that at higher inlet NO values, a significant portion of the NO is destroyed, even though the overall stoichiometric ratio was fuel lean and even though only a fraction of NO actually enters the diffusion flame front.

In order to force more NO to enter the flame front, tests in which pure NO was injected through a very small diameter tube into the oxidant stream, were conducted. In configuration C2, the pure NO was introduced horizontally, with the results shown on Tables 2 and 2a. Exhaust levels of NO were extremely low, until, at a high inlet flow rate, the NO

¹Tables are located in the Appendix.

Figure 10: NO destruction in diffusion flames 1C-1 and 1C-3.

stream broke through the combustion zone and NO exhaust levels rose steeply. In configuration C3, pure NO was introduced through a narrow tube oriented along the burner axis, and located at the center streamline. Experimental data are shown on Tables 3 and 3a, and by the open symbols on Figure 10. The results are very encouraging, since they indicate that extremely high destructions of NO are possible, (in excess of 95% for the high NO case). Here all the NO, which was injected axially along the center stagnation streamline, came into contact with the flame, and was essentially completely destroyed.

It can be argued that in this experiment, the actual concentration of NO reaching the flame may be very high, because pure NO was injected down the center. Therefore we proceeded to configuration C4, consisting of two coaxial pipes in the bottom burner, as shown on Figure 7. Known quantities of NO were introduced into the center pipe, while the remaining oxidant mixture was the same in both inner and outer pipes. Here, there was more control over the concentration of NO seeing the flame. However, our radial NO profiles (Figure 8) indicated that our method of NO introduction into the burner could be improved, and there were some radial variations upon exiting from the lower burner. Therefore, these data are not as well defined as they might be. The actual overall stoichiometries of Flames 1C-4 through 6C-4 were not equal to those calculated from the entering flows because a leak on the upper (fuel side) burner allowed substantial, but undetermined, quantities of methane to leak out into the container vessel, without being oxidized in the flame. Therefore, all true overall stoichiometries investigated, are very much more fuel lean than denoted on Tables 4 through 9a. The NO destruction results, however,

Figure 11: NO destruction in (overall) fuel lean diffusion flames (1C-4 through 6C-4).

are quite valid (since the atom balance calculations for exhaust flow rates still held), and are grouped together on Figure 11. In this, and subsequent, figures, the thermal NO, corresponding to the exhaust NO measured with zero NO addition to the oxidant was subtracted from the exhaust values.

The leak in the upper burner was fixed, and Flames 8C-4 through 12C-4 were investigated. Results are shown on Tables 10 through 13a, and are depicted on Figure 12. It appears that, in general, a most important variable is the location of the flame. As the flame was stabilized closer to the bottom burner, greater destructions of NO were observed. One might speculate that the key variable is the fraction of NO that "sees" the flame front. Again, it should be emphasized that these high values of NO destruction, shown on Figure 12, were obtained under *overall fuel lean conditions*, indicating that phenomena in diffusion flames are very different than those in premixed systems.

Flame 11C-4 was chosen for more detailed studies. Results for four replicate runs are shown on Figure 13. HCN and NH_3 values in the exhaust are shown on Figure 14. Clearly, NO is being destroyed, and is *not* leaving the system as NO_2 , HCN or NH_3 .

Detailed Profiles.

Flame 11-C4 was chosen as the prototype for measuring detailed axial species profiles. The purpose of this phase of the work was to provide a basis of comparison

between the experiment and the model, which was capable only of predicting profiles, but not capable, at this time, of predicting integral input/ output results. The model would be essential in relating the steady state experimental findings to a transient practical application. Axial profiles for the case with zero NO added are shown on Figure 15. Note how appreciable thermal NO is formed in the fuel rich part of the flame. Axial species profiles for the case with 250 ppm (based on total bottom flow) NO added are shown on Figure 16. HCN and NH₃ axial profiles are shown on Figure 17. It is noteworthy that appreciable quantities of NO are seen on the fuel rich side of the flame. This may be due to the fact that the fuel stream was heavily diluted with nitrogen, and may account for the very high destruction of NO entering the flame zone, that was observed. Although *radial* gradients had essentially disappeared at a distance of 16.5mm from the bottom burner, their presence at lower axial positions may have influenced the axial profiles higher up.

THEORETICAL MODEL

The purpose of the theoretical modelling was to gain insight into the experimental results obtained, and to determine whether they could be modeled using a known kinetic mechanism.

Kinetic Mechanism

The reaction mechanism listed in Table 17² involves 193 reactions and 40 chemical species. The first 50 reactions were taken from the existing reaction set for CO/H₂/O₂/He flames (Corley, 1988) with Helium replaced by N₂, the rate constants of which were taken from NIST (National Institute of Standards and Technology) Chemical Gas Kinetics Database (1989). The remaining reactions were selected from Glarborg, Miller and Kee's (GMK) mechanism developed for well-stirred reactors (1986), with the omission of reactions involving three reacting species, due to limitations in the current simulation code. This selection of combined mechanisms appeared to give superior flame stability to that using GMK mechanism alone. The subset used here contains only the first 151 reactions shown in Table 17, i.e., omitting the C₂ chemistry. It was, however, confirmed that the exclusion of C₂X reactions did not make a significant difference in this investigation.

Thermochemical Data

NASA polynomials (i.e. expressions consistent with the NASA chemical equilibrium program, and also with CHEMKIN) were adopted for the expressions of thermochemical properties, C_p (heat capacity), S (entropy) and H (enthalpy). The coefficients of NASA polynomials are tabulated in Table 18 for each species. All the data have been updated to be consistent with the NASA polynomials of 1982 (Corley, 1988). The data for HNO and-

² See Appendix

Figure 12: NO destruction in (overall) fuel lean flames (8C-4 through 12C-4).

Figure 13: NO destruction in Flame 11C-4.

Figure 14: HCN and NH₃ concentrations in exhaust (Flame 11C-4).

Figure 15: Axial species concentration profiles (Flame 11C-4 without NO added).

Figure 16: Axial species concentration profiles (Flame 11C-4 with 250 ppm NO in oxidant).

Figure 17: Axial concentration profiles of HCN and NH₃ (Flame 11C-4).

HO₂ were those updated by Corley (1988); those for CH₃O and CH₂OH were taken from Burcat and Kudchadker (1979). Data in Sandia Reports (SAND80-8003.UC4 & SAND878215.UC4) were adopted for species C_(s), C, N₂H and N₂H₂. These data are necessary for evaluation of equilibrium constants, $K_{p,i}$, which in turn determine the reverse rate constant (k_r) of each reaction with known forward rate constant (k_f). Table 19² lists the required information for each species.

Other Parameters

In addition to the thermochemical data described above, the transport properties are necessary for the solution to the model. They were estimated using the correlations proposed by Reid and Sherwood (1958).

Diffusivities: In the combustion mixture pseudo binary diffusion has been assumed and the diffusivity of species i in the mixture was calculated as:

where D_{ij} was evaluated using the Chapman-Enskog relation:

where all symbols in Equation (29) have their usual connotations.

$$D_{im} = \frac{1-y_i}{\sum_{j=1, j \neq i}^N \frac{y_j}{D_{ij}}} \quad i=1, \dots, N \quad (28)$$

$$D_{ij} = \frac{0.001858 \ T^{3/2} \left[\frac{1}{M_i} + \frac{1}{M_j} \right]^{1/2}}{p \sigma_{ij}^2 \Omega_D} \quad (29)$$

Viscosities: The viscosity of the combustion mixture was obtained as:

$$\mu = \sum_{i=1}^N \frac{\mu_i}{1 + \sum_{j=1, j \neq i}^N \left(\frac{y_j}{y_i} \right) \phi_{ij}} \quad (30)$$

where:

$$\mu_i = 2.6693 \times 10^{-5} \times \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega_\mu} \quad (31)$$

and:

$$\phi_{ij} = \frac{\left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2}{2\sqrt{2} \left[1 + \frac{M_i}{M_j} \right]^{1/2}} \quad (32)$$

Thermal conductivities: For the combustion mixture, the conductivity is approximated by:

$$k = \sum_{i=1}^N \frac{k_i}{1 + \sum_{j=1, j \neq i}^N \left(\frac{y_j}{y_i} \right) G_{ij}} \quad (33)$$

where:

and:

$$k_i = 1.9891 \times 10^{-4} \times \frac{(T/M_i)^{1/2}}{\sigma_i^2 \Omega_\mu} \quad (34)$$

$$G_{ij} = 1.065 \frac{\left[1 + \left(\frac{k_i}{k_j} \right)^{1/2} \left(\frac{M_i}{M_j} \right)^{1/4} \right]^2}{2\sqrt{2} \left[1 + \frac{M_i}{M_j} \right]^{1/2}} \quad (35)$$

Estimates of the parameters of the 6-12 Lennard-Jones potential function for each species were facilitated by the Energy and Environmental Research Corporation Staff (1979) and Corley (1989). The data for species C_2H , C_2H_2 , C_2H_3 , C_2H_4 , C_2H_5 , C_2H_6 , N_2H , N_2H_2 , CH_2CO , C , and $HNCO$ were obtained from Sandia Report (SAND83-8209.UC-32). The parameters of transport properties are listed in Table 20.

Implementation of Computer Code

Figure 18 shows the various steps involved in solving the laminar opposed jet diffusion flame equations. Required first are the thermochemical and transport properties, the detailed reaction stoichiometry, the reaction rate coefficients, a starting initial guess for axial profiles, and a few other inputs. The thermochemical data were used to evaluate the values of $K_{p,i}$ at different temperatures. Regression was then applied to obtain the coefficients (A, N, E) of $K_{p,i}$ as expressed in modified Arrhenius form. The reaction set, with a known forward rate constant (k_f) for each reaction, would then give the reverse rate constants (k_r), through introduction of $K_{p,i}$. Transport properties for all species were included in the main simulation code. The initial starting estimate of the solution (for axial profiles of temperature, species concentration, and axial velocity) was usually taken from the converged solution of a similar problem. The initial time step, burner spacing and eigenvalue (Q) were then introduced, in order initiate the computation. A steady state solution is reached when, in the course of one iteration, with a significant time step, changes in all dependent variables are less than a set tolerance.

THEORETICAL RESULTS

Stability Domains

Strained diffusion flamelets are not stable under all conditions. Indeed, the experimental work quickly demonstrated that stable diffusion flames could only exist under

Figure 18: Implementation of laminar, opposed jet, computer code.

a restricted set of P_{O_2} , T and strain rate conditions. Therefore, this problem was investigated theoretically. A reaction subset involving neither nitrogenous nor C_2 - species was used in this investigation. In order to investigate blow off conditions, it was necessary to perform a very large number of numerical experiments. Results are shown in Figure 19. With same stretching rate, higher inlet temperature (T_o) of flue gas provides higher stability. At lower oxidant temperatures ($T_o = 298$ K), flame stability is sensitive to flame stretching rate (determined by the eigenvalue, Q), while this trend becomes less obvious as T_o increases to 1200 K. Figure 20 shows that the peak flame temperature (T_{max}) increases as T_o increases, and as stretching rate increases. Peak temperature must be minimized if thermal NO is to be avoided. Figure 21 shows the temperature profiles corresponding to the upper curve ($T_o = 1200$ K) in Figure 20. As is shown, steeper temperature gradients result at higher stretching rates.

Figure 19: Stability domain of opposed jet diffusion flames as a function of P_{O_2} , oxidant temperature, and stretching rate, the latter given by the eigenvalue, Q (see Equations 14 and 23 in text).

Axial Profiles

Flame 11C-4 was simulated using the computer code described above. Since the code solves the conservation equations for infinitely wide burners, it is difficult to compare the theoretical results to the integral input/output experiments described above. Rather, at this time, we present predicted axial profiles of temperature, velocities, and major and minor species. These predicted profiles allow comparison between theoretical predictions and data.

Figure 22 and 23 show predicted temperature and axial velocity profiles for Flame 11C-4. The predicted heat release profile is shown in Figure 24, while major species are shown in figure 25. Figure 26, 27 and 28 show axial profiles of nitrogenous species for zero NO, 250 ppm NO and 1240 ppm NO added (in oxidant stream) respectively. Figures 29, 30 and 31 depict comparisons between predictions and data for Flame 11C-4. There are severe discrepancies between predictions and data, due in part to non-uniformity in the radial profiles of NO, as shown in Figure 8. Other experimental errors relating to poor precision may also play a role in these preliminary, screening data. In the absence of more precise data, and a more precise experimental configuration, we feel that it may be

Figure 20: Predicted maximum temperatures of opposed jet flames, as a function of inlet oxidant temperature and stretching rate.

Figure 21: Predicted axial temperature profiles.

Figure 22: Predicted axial temperature profile for Flame 11C-4.

Figure 23: Predicted axial velocity profile for Flame 11C-4.

Figure 24: Predicted axial profile of the heat release rate, for Flame 11C-4.

Figure 25: Predicted axial profiles of major species mole fractions.

Figure 26: Predicted axial profiles of nitrogenous species- Flame 11C-4 without NO addition.

Figure 27: Predicted axial profiles of nitrogenous species -Flame 11C-4 with 250 ppm NO added to oxidant.

Figure 28: Predicted axial profiles of nitrogenous species- Flame 11C-4 with 1240 ppm NO added to oxidant.

Figure 29: Predictions and data- NO concentration profiles in Flame 11C-4

Figure 30: Predictions and data- HCN and NH₃ profiles for Flame 11C-4.

Figure 31: Predictions and data- major species profiles for Flame 11C-4.

premature to put too much weight on discrepancies shown on Figures 29 through 30. Future work will hopefully resolve them.

CONCLUSIONS AND FUTURE WORK

This research should be viewed as only a preliminary study to determine whether diffusion flame phenomena can be exploited to yield reburning efficiencies much greater than those obtainable in premixed systems. The experimental results are very encouraging. They show that in diffusion flames NO can be destroyed under overall very fuel lean conditions, and that destruction can be in excess of 95%.

We do not yet understand the reasons behind the phenomena uncovered. Mathematical modelling is useful to allow us to refine kinetic sets by comparing predicted and measured axial profiles. Some refinement in both experimental technique and kinetic set development is still required, and should be the subject of future work.

The key issue now is how to apply these results to practical systems. Can a diffusion flame front be made to sweep through flue gases to destroy NO via mechanisms uncovered here? Can these data, showing very large NO destructions, be exploited and implemented in practical systems? We believe that future experimental and theoretical work should be oriented towards two issues:

- 1) what are the mechanisms by which NO is destroyed in such large amounts in laminar counterflow diffusion flames?
- and
- 2) how can these mechanisms be exploited in practical systems, to allow greater reburning effectiveness under more benign furnace conditions?

REFERENCES

- Bose, A.C. and Wendt, J.O.L., 22nd Symposium (International) on Combustion, p. 1127, The Combustion Institute, 1988.
- Breen, B.P., J. Gabrielson and H. E. Lange. U. S. Patent Number 4,779,545 "*Apparatus and Method of Reducing Nitrogen Oxide Emissions*" Assignee: Consolidated Natural Gas (1988)
- Chen, S.L., McCarthy, J.M., Clark, W.D., Heap, M.P., Seeker, W.R. and Pershing, D.W., 21st Symposium (International) on Combustion, p. 1159, The Combustion Institute, 1986.
- Chigier, N.A. and A.J. Yule, "*The Structure of Eddies in Turbulent Flames-I*" Project SQUID Technical Report US-1-PU, March, 1979

Corley, T.L., and J.O.L. Wendt: "*Computational Aspects of the Numerical Analysis of Laminar Opposed Jet Diffusion Flames*", 1985 Fall Meeting, Western States Section/The Combustion Institute, Davis, CA, October 21-22, 1985.

Corley, T.L., and J.O.L. Wendt: "*Analysis of Complex Thermal Reaction Pathways In Laminar Opposed Jet Diffusion Flames*", Paper 10a, presented at 1984 Annual Meeting of the AIChE, San Francisco, CA, November 1987.

Dimotakis, P.E., R.C. Miake-Lye, and D.A. Papantoniou, *Phys.Fluids*, 26,3185-92, (1983)

Dimotakis P.E. and G.L.Brown, *J. Fluid Mech.* 78, 535-560 (1976)

Dixon Lewis, G. *et al*, 20th Symposium (International) in Combustion, pp1893-1904, The Combustion Institute, Pittsburgh, PA (1984)

Drake, M.C., 21st Symposium (International) on Combustion, p1579, The Combustion Institute, Pittsburgh, PA (1986)

Fenimore, C.P., 17th Symposium (International) on Combustion, p. 661, The Combustion Institute, 1979.

Fenimore, C.P., 13th Symposium (International) on Combustion, p. 373, The Combustion Institute, 1973.

Glarborg, P., Miller, J.A. and Kee, R.J.: *Comb. Flame*, 65, 177:202, (1986).

Hahn, W.A. and J.O.L. Wendt, "*Integration of the Stiff Boundary Valued ODE's for the Laminar Opposed Jet Diffusion Flame*" in Stiff Computation ed. Aiken, Oxford University Press (1985)

Hahn, W.A. and J.O.L. Wendt, 18th Symposium (International) on Combustion, pp121-131 The Combustion Institute, Pittsburgh, PA (1981)

Haynes, B.S., *Comb. Flame*, 28, 113 (1977).

Haynes, B.S., *Comb. Flame*, 28, 81 (1977).

Kee, R.J., Rupley, F.M., and Miller, J.A., Sandia Report, SAND83-8209.UC-32, printed March, 1983.

Kee, R.J., Warnatz, J., and Miller, J.A., Sandia Report, SAND87-8215.UC-4, printed April, 1987.

Kee, R.J., Miller, J.A., and Jefferson, T.H., Sandia Report, SAND80-8003.UC-4, reprinted July, 1987.

Marble, F.E., and J.E. Broadwell, *"The Coherent Flame Model for Turbulent Chemical Reactions"*, Project SQUID Report (1977)

Mereb, J.B. and Wendt, J.O.L., Reburning Mechanisms in a Pulverized Coal Combustor", in press, 23rd Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, Pa (1990)

NIST Chemical Gas Kinetics Database, Standard Reference Database 17, National Institute of Standards and Technology, May, 1987.

Peters, N., 21st Symposium (International) on Combustion, p1231-1250, The Combustion Institute, Pittsburgh, PA (1986)

Reid, R.C., and Sherwood, T.K., The Properties of Gases and Liquids, McGraw and Hill, New York, 1958.

Roshko, A., in Turbulent Mixing in Non-Reactive and Reactive Flows, ed. S.N.B. Murthy, p 295,(1974)

Smooke, M.D., Puri, I.K., and Seshadri, K., 21st (International) on Combustion, pp1783-1792, The Combustion Institute, Pittsburgh, PA (1986).

Smooke, M.D., Seshadri, K., and I.K. Puri, 22nd Symposium (International) on Combustion, pp1555-1563, The Combustion Institute, Pittsburgh, PA (1988)

Wendt, J.O.L., and Mereb, J.B. *"Mechanismen der Nachverbrennung bei der Kohlenstaubverbrennung"* Presented at VGB Congress "Kraftwerke 1990" Essen, W. Germany, 18-21 September 1990.

Wendt, J.O.L., Sternling, C.V. and Matovich, M.A.: 14th Symposium (International) on Combustion, p. 897, The Combustion Institute, 1973.

APPENDICES AND TABLES

Experimental Data, Tables 1 through 16.

Detailed Reaction Kinetic Mechanism, Table 17.

Thermochemical Data, Table 18

Equilibrium Constants, Table 19

Transport Parameters, Table 20

TABLE 1a FLAME 1 C-1
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F001C1NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.01

Upper Burner Flow Rates:

CH₄: 7.6 lpm)

N₂: 24.8 lpm

Lower Burner Flow Rates:

O₂: 15.4 lpm

N₂: 17.6 lpm

CO₂: 4.5 lpm

NO: 0.0 lpm to 0.07 lpm

NO premixed with Oxidant

Inlet % flowrates				Exhaust					analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
10.9	22.0	6.40	—	0.32	16.500	0.041	0.035	0.05	0.900	0.930	4.810	22
10.9	22.0	6.44	143	0.277	16.682	0.044	0.036	0.045	1.135	1.069	5.31	130
10.9	22.0	6.43	600	0.384	16.865	0.051	0.039	0.048	1.193	1.118	5.02	350
11.0	21.1	6.2	959	0.359	16.778	0.052	0.053	0.051	1.337	1.061	4.210	485

TABLE 1 b FLAME 1 C-1

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_4 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_x(measured) - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (deat'd) (ppmv)	% NO _x (deat'd)
1	0	22	93	85	0	0	-
2	143	130	91	83	94	49	34
3	600	350	89	84	284	316	53
4	959	485	88	82	394	565	59

TABLE 2a FLAME 1 C-2
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F001C2NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 0.95

Upper Burner Flow Rates:

CH₄: 8.0 lpm)

N₂: 24.5 lpm

Lower Burner Flow Rates:

O₂: 15.2 lpm

N₂: 20.0 lpm

CO₂: 4.3 lpm

NO: 0.0 lpm to 0.07 lpm

NO fed 1 cm from flame, horizontal probe

Inlet % flowrates			Exhaust						analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
11.1	21.1	5.97	-	0.654	15.23	0.05	0.03	0.039	1.12	1.01	2.32	30
11.1	21.1	5.97	139	0.299	15.94	0.041	0.031	0.043	1.15	0.949	2.51	45
11.1	21.1	5.97	278	0.312	15.59	0.049	0.037	0.043	1.08	0.942	2.44	52
11.1	21.1	5.97	389	0.32	15.3	0.042	0.043	0.034	1.30	0.91	2.89	340
11.1	21.1	5.97	971	0.34	15.41	0.049	0.038	0.042	1.13	0.93	2.73	522

TABLE 2 b FLAME 1 C-2

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_6 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{x,out}(corr'd) = \left(\frac{(NO_{x,measured}) - Thermal(NO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	30	97	97	0	0	-
2	139	45	93	91	14	125	90
3	278	52	96	93	21	257	93
4	389	340	96	94	294	95	24
5	971	522	96	93	464	506	52

TABLE 3a FLAME 1 C -3
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F001C3NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen,Carbon dioxide and Nitrogen

Stoichiometric ratio: 0.9

Upper Burner Flow Rates:

CH₄: 8.6 lpm)

N₂: 24.8 lpm

Lower Burner Flow Rates:

O₂: 14.9 lpm

N₂: 27.7 lpm

CO₂: 4.44 lpm

NO: 0.0 lpm to 0.07 lpm

NO fed through ϕ 0.05" diameter vertical probe 1 cm from flame

Inlet				% flowrates				Exhaust				analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)			
10.7	18.55	5.52	-	0.17	14.94	0.07	0.06	-	0.34	0.621	2.31	22			
10.7	18.54	5.53	75	0.21	14.35	0.08	0.05	-	0.92	0.532	2.29	28			
10.7	18.54	5.53	187	0.10	14.59	0.04	0.02	-	0.66	0.45	1.82	35			
10.7	18.54	5.52	448	0.13	14.01	0.01	0.03	-	0.84	0.694	1.21	37			
10.16	16.27	7.47	203	0.531	14.53	-	0.047	-	1.05	1.013	.906	29			
10.16	16.26	7.47	610	0.47	14.11	-	0.065	-	1.13	1.21	.879	32			
10.16	16.25	7.47	889	0.338	14.63	0.06	0.07	0.046	1.97	1.198	.98	47			

TABLE 3 b FLAME 1 C-3

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_6 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_x(measured) - Thermal/NO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	22	89	89	0	0	-
2	75	28	95	90	5.6	69.5	93
3	187	35	96	90	12	175	94
4	203	37	97	98	15	188	93
5	448	29	106	93	7	441	98
6	610	32	106	96	10	600	98
7	889	47	97	98	24	865	97

TABLE 4a FLAME 1 C-4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F001C4-0709-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 0.85

Upper Burner Flow Rates:

CH₄: 5.3 lpm)

N₂: 19.0 lpm

Lower Burner Flow Rates:

O₂: 9.0 lpm

N₂: 3.6 lpm

CO₂: 1.3 lpm

NO: 0.0 lpm to 0.04 lpm

NO fed through coaxial bottom burner

Measured bottom position of luminous zone 1.65 cm above bot. burner.

Inlet % flowrates				Exhaust								analysis		
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)		
13.9	23.56	3.40	-	0.014	13.538	-	-	-	4.47	0.13	5.53	68		
13.9	23.56	3.40	209	0.014	13.69	-	-	-	4.49	0.15	5.33	102		
13.9	23.56	3.40	471	0.013	14.25	-	-	-	4.73	0.18	4.69	127		
14.01	23.79	3.43	740	0.015	14.86	-	-	-	4.95	0.206	4.04	188		
14.01	23.78	3.44	1057	0.082	15.446	0.01	0.008	-	5.14	0.49	4.38	550		

* Indicates probable onset of leak on top burner.

TABLE 4 b FLAME 1 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	68	95	89	0	0	-
2	209	102	94	98	33	176	84
3	471	127	90	91	53	418	89
4	740	188	87	94	109	631	85
5	1057	550	83	89	414	642	61

TABLE 5a FLAME 2 C-4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F002C4-0710-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.1

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 20.0 lpm

Lower Burner Flow Rates:

O₂: 11.4 lpm

N₂: 3.6 lpm

CO₂: 2.24 lpm

NO: 0.0 lpm to 0.086 lpm

NO fed through coaxial bottom burner

Z_f = 1.80 cm

Inlet % flowrates				Exhaust								analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ [*] (%)	CO (%)	O ₂ (%)	NO _x (ppmv)			
12.25	26.86	5.28	—	0.049	13.27	0.008	0.005	—	5.342	0.664	13.64	90			
12.25	26.86	5.28	235	0.046	13.80	0.008	—	—	5.22	0.75	13.09	172			
12.24	26.84	5.27	659	0.039	14.125	0.004	—	—	4.94	0.80	12.43	455			
12.24	26.83	5.27	1271	0.032	14.09	0.005	—	—	4.89	0.81	12.3	595			
12.23	26.81	5.27	2022	0.036	14.00	0.003	—	—	4.94	0.81	12.82	648			

* Indicates a leak on top burner.

TABLE 5 b FLAME 2 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_2 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%C_2H_2 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{x,out}(corr'd) = \left(\frac{(NO_x(measured) - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	90	91	91	0	0	-
2	235	172	89	90	73	162	69
3	659	455	88	90	325	334	51
4	1271	595	88	91	452	819	64
5	2022	648	89	89	497	1525	75

TABLE 6a FLAME 3 C-4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F003C4-0810-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.2

Upper Burner Flow Rates:

CH₄: 6.8 lpm)

N₂: 24.7 lpm

Lower Burner Flow Rates:

O₂: 15.3 lpm

N₂: 19.8 lpm

CO₂: 4.2 lpm

NO: 0.0 lpm to 0.086 lpm

NO fed through coaxial bottom burner

Z_f = 1.89 cm

Inlet % flowrates				Exhaust									analysis		
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ [*] (%)	CO (%)	O ₂ (%)	NO _x (ppmv)			
9.60	21.61	5.93	-	0.022	10.95	0.004	0.007	-	5.017	0.247	13.25	45			
9.60	21.58	6.06	141	0.023	11.05	0.003	-	-	4.81	0.33	12.91	107			
9.59	21.57	6.06	395	0.022	11.22	-	-	-	4.63	0.40	12.68	249			
9.58	21.56	6.06	775	0.020	11.22	-	-	-	4.55	0.42	12.52	395			
9.58	21.55	6.06	1211	0.022	11.30	-	-	-	5.20	0.50	12.00	460			

* Indicates a leak on top burner.

TABLE 6 b FLAME 3 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_6 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_6 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	45	96	93	0	0	-
2	141	107	97	94	59	82	58
3	395	249	97	93	194	201	51
4	775	395	97	93	333	443	57
5	1211	460	92	98	394	817	67

TABLE 7a FLAME 4 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F004C4-0811-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.01

Upper Burner Flow Rates:

CH₄: 7.2 lpm)

N₂: 24.2 lpm

Lower Burner Flow Rates:

C₂: 14.6 lpm

N₂: 21.6 lpm

CO₂: 4.1 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.93 cm

Inlet			% flowrates			Exhaust						analysis			
CH ₄	O ₂		CO ₂	NO	H ₂	CO ₂	C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	CH ₄ *	CO	O ₂	NO _x		
(%)	(%)		(%)	(ppmv)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(ppmv)		
10.04	20.4		5.69	-	0.016	11.11	-	0.004	-	4.90	0.374	10.16	20		
9.54	20.5		5.72	140	0.021	11.47	0.004	-	-	4.93	-	10.70	70		
9.53	20.47		5.75	393	0.019	11.54	-	-	-	4.61	0.42	10.53	191		
10.06	20.4		5.73	755	0.018	12.40	-	-	-	4.58	0.41	9.84	268		
10.09	20.45		5.74	1205	0.022	12.53	-	-	-	4.49	0.44	9.45	430		
10.06	20.4		5.73	1229	0.031	12.4	-	-	-	4.76	0.452	9.17	449		
10.07	20.4		5.59	1677	0.03	12.96	-	-	-	4.74	0.46	9.08	550		

* Indicates a leak on top burner.

TABLE 7 b FLAME 4 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_x(measured) - Thermal(NO_x)) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	20	96	96	0	0	-
2	140	70	93	95	47	93	66
3	393	191	92	93	158	235	60
4	755	268	91	90	224	531	70
5	1205	430	91	91	373	832	69
6	1229	449	90	92	390	839	68
7	1677	550	86	89	463	1213	72

TABLE 8a FLAME 5 C4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F005C4-0826-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.07

Upper Burner Flow Rates:

CH₄: 6.8 lpm)

N₂: 24.0 lpm

Lower Burner Flow Rates:

O₂: 14.6 lpm

N₂: 21.0 lpm

CO₂: 3.92 lpm

NO: 0.0 lpm to 0.018 lpm

NO fed through coaxial bottom burner

Z_f = 2.1 cm

Inlet % flowrates				Exhaust					analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ * (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
9.67	20.8	5.57	-	0.015	8.53	-	0.005	-	5.98	0.123	13.69	25
9.64	20.8	5.57	57	0.021	9.44	-	-	-	6.47	0.19	15.1	45
9.67	20.8	5.57	250	**	**	**	**	**	**	**	**	145

* Indicates a leak on top burner. , **Flame blew off during this expt.

TABLE 8 b FLAME 5 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	25	104	103	0	0	-
2	57	45	100	98	20	37	65
3	350	145	-	-	-	-	-
4	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-
6	-	-	-	-	-	-	-

TABLE 9a FLAME 6 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F006C4-0827-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 0.94

Upper Burner Flow Rates:

CH₄: 8.0 lpm)

N₂: 23.8 lpm

Lower Burner Flow Rates:

O₂: 14 lpm

N₂: 20.0 lpm

CO₂: 3.92 lpm

NO: 0.0 lpm to 0.064 lpm

NO fed through coaxial bottom burner

Z_f = 2.2 cm

Inlet % flowrates				Exhaust						analysis		
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ * (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
11.3	21.2	5.54	-	-	7.84	-	-	-	8.057	0.017	16.03	23
11.3	21.2	5.38	85	-	7.95	-	-	-	8.08	0.032	16.14	69
11.3	21.2	5.38	283	-	7.86	-	-	-	8.11	0.046	16.13	125
11.4	21.3	5.38	539	-	7.57	-	-	-	8.12	0.101	15.71	286
11.4	21.3	5.39	908	-	8.19	-	-	-	8.07	0.118	15.51	385

* Indicates a leak on top burner.

TABLE 9 b FLAME 6 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_6 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_6 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{x,out}(corr'd) = \left(\frac{(NO_{x,measured}) - Thermal(NO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	23	106	98	0	0	-
2	85	69	104	95	46	39	49
3	283	125	104	96	101	182	64
4	539	286	106	100	270	268	50
5	908	385	103	93	355	553	61

TABLE 10a FLAME 8 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F008C4NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.4

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 21.0 lpm

Lower Burner Flow Rates:

O₂: 14.8 lpm

N₂: 16.6 lpm

CO₂: 3.84 lpm

NO: 0.0 lpm to 0.104 lpm

NO fed through coaxial bottom burner

Z_f = 1.58 cm

Inlet			% flowrates		Exhaust					analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
8.46	24.1	6.25	6.25	-	0.008	16.74	-	-	-	0.32	0.083	8.14	54
8.46	24.1	6.25	6.25	163	0.011	16.29	-	-	-	0.31	0.1	8.55	126
8.46	24.1	6.25	6.25	423	0.018	15.93	-	-	-	0.52	0.16	8.78	333
8.46	24.1	6.24	6.24	911	0.019	15.83	-	-	-	0.50	0.18	8.73	418
8.49	23.8	6.20	6.20	1077	0.02	15.29	-	-	-	0.48	0.18	8.77	431
8.48	23.8	6.20	6.20	1696	0.02	15.21	-	-	-	0.49	0.17	8.83	455

First of a wider and more stable flames.

TABLE 10b FLAME 8 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_4 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - Thermal(NO_x)) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	54	91	93	0	0	-
2	163	126	94	93	67	96	59
3	423	333	89	90	250	173	41
4	911	418	89	91	328	583	64
5	1077	431	92	91	345	732	68
6	1696	455	93	91	369	1327	78

TABLE 11a FLAME 9 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F09C4NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.0

Upper Burner Flow Rates:

CH₄: 6.8 lpm)

N₂: 20.9 lpm

Lower Burner Flow Rates:

O₂: 13.7 lpm

N₂: 16.6 lpm

CO₂: 5.56 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.55 cm

Inlet % flowrates				Exhaust							analysis	
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)
10.7	21.6	8.75	—	0.164	19.7	0.006	—	—	0.98	0.82	2.50	73
10.7	21.6	8.75	126	0.138	19.4	0.006	—	0.01	0.92	0.75	2.76	142
10.7	21.6	8.74	440	0.125	19.1	0.005	—	0.01	0.95	0.73	2.83	252
10.7	21.5	8.74	880	0.123	19.1	0.005	—	—	0.93	0.74	2.81	331
10.7	21.5	8.74	1320	0.154	19.1	0.006	—	0.015	1.02	0.85	2.41	352
10.7	21.5	8.73	1884	0.154	19.0	0.007	—	—	1.036	0.86	2.52	352

TABLE 11 b FLAME 9 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (deat'd) (ppmv)	% NO _x (deat'd)
1	0	73	90	91	0	0	-
2	126	142	92	91	63	63	50
3	440	252	93	92	166	274	62
4	880	331	94	92	240	640	72
5	1320	352	93	94	261	1059	80
6	1884	352	93	94	261	1623	86

TABLE 12a FLAME 10 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F010C4NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.0

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 23.0 lpm

Lower Burner Flow Rates:

O₂: 10.5 lpm

N₂: 19.8 lpm

CO₂: 3.04 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.575 cm

Inlet			% flowrates			Exhaust						analysis			
CH ₄ (%)	O ₂ (%)		CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)		
8.45	17.1		4.94	-	0.260	12.3	0.010	-	0.017	1.64	0.92	2.72	40		
8.45	17.1		4.94	162	0.320	12.5	0.013	-	0.030	1.45	0.97	4.43	122		
8.45	17.1		4.94	439	0.264	12.4	0.009	-	0.025	1.43	0.96	3.42	260		
8.44	17.1		4.94	893	0.265	12.5	0.011	-	0.020	1.48	0.98	3.03	320		
8.44	17.0		4.93	1363	0.261	12.3	0.012	-	0.018	1.45	0.96	3.45	327		
8.43	17.0		4.93	1946	0.254	12.2	0.011	-	0.018	1.45	0.95	3.44	335		

TABLE 12 b FLAME 10 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	40	90	99	0	0	-
2	162	122	89	86	72	90	56
3	439	260	90	92	200	239	54
4	893	320	89	95	258	635	71
5	1363	327	91	92	263	1100	81
6	1946	335	91	93	271	1675	86

TABLE 13 a-1 FLAME 11 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F011C4-08-04-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.2

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 21.8 lpm

Lower Burner Flow Rates:

O₂: 12.5 lpm

N₂: 18.8 lpm

CO₂: 3.84 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.64 cm

Inlet					% flowrates		Exhaust					analysis			
CH ₄ (%)	O ₂ (%)	CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)			
8.37	20.1	6.18	-	0.039	13.96	-	-	-	0.72	0.29	4.99	40			
8.36	20.1	6.17	1317	0.027	14.05	-	-	-	0.64	0.28	5.11	378			
8.35	20.1	6.17	1927	0.027	13.93	-	-	-	0.64	0.27	5.15	390			
8.37	20.1	6.18	257	0.035	13.81	-	-	-	0.66	0.29	5.10	182			
8.37	20.1	6.18	611	0.030	13.95	-	-	-	0.65	0.27	5.31	323			

TABLE 13 b-1 FLAME 11 C-4 RUN 0804

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_4_{inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	40	97	98	0	0	-
2	1317	378	97	96	326	991	75
3	1927	390	98	96	340	1586	82
4	257	182	99	97	139	118	46
5	611	323	98	96	275	336	55

TABLE 13 a-2 FLAME 11 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER: F011C4-08-11-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.2

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 21.8 lpm

Lower Burner Flow Rates:

O₂: 12.5 lpm

N₂: 18.8 lpm

CO₂: 3.84 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.64 cm

Inlet			% flowrates			Exhaust						analysis		
CH ₄	O ₂		CO ₂		NO	H ₂	CO ₂	C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	CH ₄	CO	O ₂	NO _x
(%)	(%)		(%)		(ppmv)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(ppmv)
8.37	20.1		6.18		-	0.041	13.72	-	-	-	0.72	0.29	5.17	45
8.37	20.1		6.18		80	0.045	16.50	-	-	-	0.70	0.32	4.67	106
8.37	20.1		6.18		241	0.043	16.19	-	-	-	0.66	0.32	4.69	174
8.37	20.1		6.18		354	0.042	16.03	-	-	-	0.70	0.32	4.89	223
8.37	20.1		6.18		643	0.044	16.15	-	-	-	0.72	0.32	4.71	330

TABLE 13 b-2 FLAME 11 C-4 RUN 0811

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2's + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	45	85	87	0	0	-
2	80	106	83	86	52	28	36
3	241	174	85	88	112	129	54
4	354	223	85	88	154	200	57
5	643	330	85	88	247	396	62

TABLE 13 a-3 FLAME 11 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F011C4-08-10-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.2

Upper Burner Flow Rates:

CH₄: 5.2 lpm)

N₂: 21.8 lpm

Lower Burner Flow Rates:

O₂: 12.5 lpm

N₂: 18.8 lpm

CO₂: 3.84 lpm

NO: 0.0 lpm to 0.12 lpm

NO fed through coaxial bottom burner

Z_f = 1.64 cm

Inlet			% flowrates			Exhaust					analysis			
CH ₄ (%)	O ₂ (%)		CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)	
8.37	20.1		6.18	-	0.041	13.72	-	-	-	0.72	0.29	5.17	41	
8.37	20.1		6.18	161	0.044	14.60	-	-	-	0.73	0.32	4.66	133	
8.37	20.1		6.18	418	0.048	14.0	-	-	-	0.71	0.34	4.68	283	
8.36	20.1		6.17	884	0.043	14.19	-	-	-	0.67	0.33	4.71	348	
8.36	20.1		6.17	1318	0.041	14.08	-	-	-	0.71	0.33	4.68	373	
8.35	20.1		6.17	1927	0.038	13.96	-	-	-	0.69	0.32	4.71	385	

TABLE 13 b-3 FLAME 11 C-4 RUN 0810

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_6 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_6 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_{x(measured)} - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	41	96	98	0	0	-
2	161	133	97	99	90	71	44
3	418	283	97	99	237	181	43
4	884	348	99	94	296	588	66
5	1318	373	96	98	322	956	76
6	1927	385	97	98	338	159	82

TABLE 14a FLAME 12 C 4
EXPERIMENTAL DATA FOR DIFFUSION FLAME

RUN NUMBER:F012C4-08-05-90NONOX

Fuel side: Methane and Nitrogen

Oxidant side: Oxygen, Carbon dioxide and Nitrogen

Stoichiometric ratio: 1.04

Upper Burner Flow Rates:

CH₄: 7.2 lpm)

N₂: 24.7 lpm

Lower Burner Flow Rates:

O₂: 15.0 lpm

N₂: 17.6 lpm

CO₂: 4.72 lpm

NO: 0.0 lpm to 0.14 lpm

NO fed through coaxial bottom burner

Z_f =1.56 cm

Inlet			% flowrates			Exhaust						analysis			
CH ₄ (%)	O ₂ (%)		CO ₂ (%)	NO (ppmv)	H ₂ (%)	CO ₂ (%)	C ₂ H ₄ (%)	C ₂ H ₆ (%)	C ₂ H ₂ (%)	CH ₄ (%)	CO (%)	O ₂ (%)	NO _x (ppmv)		
10.4	21.7		6.81	-	0.058	15.504	0.002	-	-	0.553	0.447	4.442	80		
10.4	21.7		6.81	217	0.092	16.15	-	-	-	0.629	0.548	3.640	189		
10.4	21.7		6.81	606	0.09	16.09	-	-	-	0.639	0.555	3.540	302		
10.4	21.7		6.81	866	0.089	16.65	0.003	-	-	0.635	0.556	3.00	358		
10.4	21.7		6.81	1385	0.085	16.270	0.002	-	-	0.614	0.538	3.62	370		
10.4	21.7		6.81	2018	0.085	16.350	-	-	-	0.600	0.560	3.48	379		

TABLE 14 b FLAME 12 C-4

REDUCED NO DATA AND ATOM BALANCE CLOSURES:

Exhaust NO ppm reduced to inlet flow rate conditions less Thermal NO_x

C balance:

$$(\%CH_4 + \%CO_2)_{inlet} = \left(\frac{n_d \times (\%CO_2 + 2 \times \%C_2H_4 + \%CH_4 + \%CO)_{exhaust}}{100} \right)$$

O balance:

$$2(\%O_2 + \%CO_2)_{inlet} = \left(\frac{n_d \times (2\%O_2 + 2\%CO_2 + \%CO)_{exhaust}}{100} \right) + n_{H_2O}$$

H balance:

$$4\%CH_{4inlet} = \left(\frac{n_d \times (4\%CH_4 + 2\%C_2H_2 + 2\%H_2 + 4\%C_2H_4 + 6\%C_2H_6)_{exhaust}}{100} \right) + 2n_{H_2O}$$

$$NO_{xout}(corr'd) = \left(\frac{(NO_x(measured) - ThermalNO_x) \times n_d}{100} \right)$$

Run No. #	NO in (ppmv)	NO _x out meas'd (ppmv)	n _d (C bal.)	n _d (O/H bal)	NO _x out(corr'd) (ppmv)	NO _x (dest'd) (ppmv)	% NO _x (dest'd)
1	0	80	104	92	0	0	-
2	217	189	99	93	105	112	52
3	606	302	100	94	215	391	64
4	866	358	96	94	264	602	70
5	1385	370	99	93	278	1107	80
6	2018	379	98	93	286	1732	86

TABLE 15
SPECIES AXIAL PROFILES FOR FLAME F011-Burner Spacing 29mm, no NO added
Z mm above bottom burner

TABLE 15
SPECIES AXIAL PROFILES FOR FLAME F011-

Burner Spacing 29mm, no NO added
Z mm above bottom burner

Z (mm)	CH ₄ (%)	N ₂ (%)	O ₂ (%)	CO ₂ (%)	CO (%)	H ₂ (%)	NO (ppmv)	NO _x (ppmv)	HCN (ppmv)	NH ₃ (ppmv)
5.45	-	55.85	33.74	10.42	-	-	2	3	*	*
10.35	0.07	58.13	30.57	11.24	-	-	2	12	*	*
15.05	0.34	67.17	19.13	11.66	1.32	0.36	2	28	*	*
18.35	4.13	74.62	9.15	9.33	1.74	0.87	3	35	*	*
20.30	7.10	77.89	4.09	7.81	1.83	1.08	7	35	*	*
24.00	11.29	79.90	0.90	5.04	1.58	1.10	21	30	*	*
26.65	12.99	80.11	0.55	3.86	1.42	0.98	22	24	*	*
28.85	13.68	80.12	0.52	3.41	1.31	0.89	19	21	*	*

* not measured
flame approximate bottom position at 16.2 mm

TABLE 16
SPECIES AXIAL PROFILES FOR FLAME F011-
Burner Spacing 29mm, NO added at 285 ppm of total oxidant flow
Z mm above bottom burner

Z (mm)	CH ₄ (%)	N ₂ (%)	O ₂ (%)	CO ₂ (%)	CO (%)	H ₂ (%)	NO (ppmv)	NO _x (ppmv)	HCN (ppmv)	NH ₃ (ppmv)
5.45	-	55.85	33.80	10.35	-	-	430	530	*	*
6.85	*	*	*	*	*	*	400	500	0.3	0.0
13.20	*	*	*	*	*	*	320	410	0.1	0.8
13.35	-	63.79	23.67	11.97	0.55	0.03	355	455	*	*
17.95	*	*	*	*	*	*	165	290	0.7	6.1
18.20	3.99	74.52	9.21	9.32	1.79	1.02	173	288	*	*
20.35	5.68	76.89	5.50	9.05	1.71	0.99	178	235	*	*
21.60	8.51	78.91	2.86	6.64	1.80	1.11	140	174	*	*
22.70	*	*	*	*	*	*	125	145	14.6	1.7
23.35	9.33	79.36	1.73	6.71	1.63	1.10	130	154	*	*
24.80	11.81	79.98	0.94	4.59	1.54	1.02	100	103	*	*
26.76	*	*	*	*	*	*	88	92	12.2	2.8
27.70	12.26	79.92	0.69	4.65	1.44	0.95	81	95	*	*

* not measured

Table 17 REACTION MECHANISM FOR 'CH₄/O₂/N₂' DIFFUSION FLAMEFORWARD RATE CONSTANT: $k_f = A * T^{*N} * \exp(-E/R/T)$ where $R [=]$ Kcal/Mole/K, $E [=]$ Kcal/Mole

STOICHOMETRIC REACTION		A	N	E
=====		=====	=====	=====
1	CO + O + M = CO ₂ + M,	0.268300E+23	-2.25000	6.16000
2	CH ₂ O + M = HCO + H + M,	0.360000E+18	0.00000	86.96000
3	H + CO + M = HCO + M,	0.700000E+15	0.00000	1.69000
4	O + O + M = O ₂ + M,	0.100000E+19	-1.00000	0.00000
5	H ₂ O ₂ + M = OH + OH + M,	0.130000E+18	0.00000	45.50000
6	H + OH + N ₂ = H ₂ O + N ₂ ,	0.219000E+23	-2.00000	0.00000
7	H + OH + O ₂ = H ₂ O + O ₂ ,	0.490000E+22	-1.76000	0.00000
8	H + OH + CO = H ₂ O + CO,	0.490000E+22	-1.76000	0.00000
9	H + OH + H ₂ = H ₂ O + H ₂ ,	0.980000E+22	-1.76000	0.00000
10	H + OH + H ₂ O = H ₂ O + H ₂ O,	0.192000E+24	-2.04000	0.00000
11	H + OH + CO ₂ = H ₂ O + CO ₂ ,	0.350000E+24	-2.44000	0.00000
12	H + H + N ₂ = H ₂ + N ₂ ,	0.543200E+19	-1.30000	0.00000
13	H + H + O ₂ = H ₂ + O ₂ ,	0.658000E+19	-1.32000	0.00000
14	H + H + CO = H ₂ + CO,	0.658000E+19	-1.32000	0.00000
15	H + H + H ₂ = H ₂ + H ₂ ,	0.537000E+17	-0.49300	0.00000
16	H + H + H ₂ O = H ₂ + H ₂ O,	0.187000E+20	-1.11000	0.00000
17	H + H + CO ₂ = H ₂ + CO ₂ ,	0.246000E+22	-2.29000	0.00000
18	H + O ₂ + N ₂ = HO ₂ + N ₂ ,	0.745000E+19	-1.00000	0.00000
19	H + O ₂ + O ₂ = HO ₂ + O ₂ ,	0.711000E+20	-1.44000	0.00000
20	H + O ₂ + CO = HO ₂ + CO,	0.711000E+20	-1.44000	0.00000
21	H + O ₂ + H ₂ = HO ₂ + H ₂ ,	0.177000E+19	-0.77000	0.00000
22	H + O ₂ + H ₂ O = HO ₂ + H ₂ O,	0.270000E+20	-0.85000	0.00000
23	H + O ₂ + CO ₂ = HO ₂ + CO ₂ ,	0.410000E+18	-0.50000	0.00000
24	CO + OH = CO ₂ + H,	0.151000E+08	1.30000	-0.76500
25	CO + O ₂ = CO ₂ + O,	0.690000E+08	1.00000	34.81000
26	CO + HO ₂ = CO ₂ + OH,	0.100000E+12	0.00000	10.00000
27	CH ₂ O + HO ₂ = HCO + H ₂ O ₂ ,	0.100000E+13	0.00000	8.00000
28	CH ₂ O + H = HCO + H ₂ ,	0.309000E+11	1.00000	3.31000
29	CH ₂ O + O = HCO + OH,	0.191300E+14	0.00000	3.10800
30	CH ₂ O + OH = HCO + H ₂ O,	0.420000E+11	0.87200	0.00000
31	HCO + HCO = CH ₂ O + CO,	0.140000E+13	0.50000	0.00000
32	HCO + O = OH + CO,	0.370000E+13	0.50000	0.00000
33	HCO + O = H + CO ₂ ,	0.370000E+13	0.50000	0.00000
34	HCO + H = H ₂ + CO,	0.330000E+15	0.00000	0.00000
35	HCO + OH = H ₂ O + CO,	0.639000E+13	0.50000	0.00000
36	HCO + O ₂ = CO + HO ₂ ,	0.580000E+14	-0.50000	0.00000
37	H ₂ + OH = H ₂ O + H,	0.573400E+07	2.00000	2.86830
38	H ₂ + O = OH + H,	0.799700E+06	2.25000	6.67740
39	H + O ₂ = OH + O,	0.146627E+18	-0.92986	17.30891
40	OH + OH = H ₂ O + O,	0.596000E+09	1.26000	0.00000
41	H ₂ O ₂ + H = H ₂ + HO ₂ ,	0.152000E+13	0.00000	3.71600
42	H ₂ O ₂ + H = H ₂ O + OH,	0.940000E+13	0.00000	3.49700
43	H ₂ O ₂ + O = OH + HO ₂ ,	0.850000E+06	2.00000	2.62000
44	H ₂ O ₂ + OH = H ₂ O + HO ₂ ,	0.184800E+07	2.00000	-1.08050
45	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂ ,	0.314000E+11	0.00000	-2.26540
46	H + HO ₂ = OH + OH,	0.150000E+14	0.00000	-0.55000
47	H + HO ₂ = H ₂ + O ₂ ,	0.420000E+13	0.00000	0.00000
48	H + HO ₂ = H ₂ O + O,	0.350000E+13	0.00000	0.50000
49	O + HO ₂ = OH + O ₂ ,	0.189000E+14	0.00000	-0.39280
50	OH + HO ₂ = H ₂ O + O ₂ ,	0.906000E+13	0.00000	-0.95360

Table 17 (cont'd)

STOICHIOMETRIC REACTION		A	N	E
=====		=====	=====	=====
51	H + OH + M = H2O + M,	0.750000E+24	-2.60000	0.00000
52	H + H + M = H2 + M,	0.100000E+19	-1.00000	0.00000
53	H2 + O2 = OH + OH,	0.170000E+14	0.00000	47.78000
54	H + O2 + M = H2O + M,	0.210000E+19	-1.00000	0.00000
55	CH4 + M = CH3 + H + M,	0.100000E+18	0.00000	88.00000
56	CH4 + OH = CH3 + H2O,	0.350000E+04	3.08000	2.00000
57	CH4 + H = CH3 + H2,	0.220000E+05	3.00000	8.75000
58	CH4 + O = CH3 + OH,	0.120000E+08	2.08000	7.63000
59	CH3 + O = CH2O + H,	0.680000E+14	0.00000	0.00000
60	CH3 + O = CH2 + OH,	0.500000E+14	0.00000	12.00000
61	CH3 + OH = CH2O + H2,	0.100000E+13	0.00000	0.00000
62	CH3 + OH = CH3O + H,	0.900000E+15	0.00000	15.40000
63	CH3 + OH = CH2 + H2O,	0.150000E+14	0.00000	5.00000
64	CH3 + O2 = CH2O + OH,	0.520000E+14	0.00000	34.57000
65	CH3 + O2 = CH3O + O,	0.700000E+13	0.00000	25.65000
66	CH3 + M = CH2 + H + M,	0.190000E+17	0.00000	91.60000
67	CH3 + H = CH2 + H2,	0.900000E+14	0.00000	15.10000
68	CH3O + M = CH2O + H + M,	0.100000E+15	0.00000	25.00000
69	CH3O + O = CH2O + OH,	0.100000E+14	0.00000	0.00000
70	CH3O + O2 = CH2O + H2O,	0.630000E+11	0.00000	2.60000
71	CH3O + H = CH2O + H2,	0.200000E+14	0.00000	0.00000
72	CH3O + OH = CH2O + H2O,	0.100000E+14	0.00000	0.00000
73	CH4 + CH2 = CH3 + CH3,	0.100000E+14	0.00000	9.50000
74	CH2 + O2 = CO2 + H2,	0.690000E+12	0.00000	0.50000
75	CH2 + O2 = CO + H2O,	0.190000E+11	0.00000	-1.00000
76	CH2 + O2 = HCO + OH,	0.430000E+11	0.00000	-0.50000
77	CH2 + O2 = CH2O + O,	0.200000E+14	0.00000	9.00000
78	CH2 + O = CO + H2,	0.500000E+14	0.00000	0.00000
79	CH2 + O = CH + OH,	0.500000E+14	0.00000	12.00000
80	CH2 + H = CH + H2,	0.730000E+18	-1.56000	0.00000
81	CH2 + OH = CH2O + H,	0.300000E+14	0.00000	0.00000
82	CH2 + OH = CH + H2O,	0.450000E+14	0.00000	3.00000
83	CH2 + CO2 = CO + CH2O,	0.110000E+12	0.00000	1.00000
84	CH + O = CO + H,	0.570000E+14	0.00000	0.00000
85	CH + OH = HCO + H,	0.300000E+14	0.00000	0.00000
86	CH + O2 = HCO + O,	0.330000E+14	0.00000	0.00000
87	CH + CO2 = HCO + CO,	0.340000E+13	0.00000	0.69000
88	CH + H = C + H2,	0.150000E+15	0.00000	0.00000
89	C + OH = CO + H,	0.500000E+14	0.00000	0.00000
90	C + O2 = CO + O,	0.200000E+14	0.00000	0.00000
91	C + CO2 = CO + CO,	0.600000E+09	0.00000	0.00000
92	C + CH4 = CH + CH3,	0.500000E+14	0.00000	24.00000
93	N + NO = N2 + O,	0.330000E+13	0.30000	0.00000
94	N + O2 = NO + O,	0.640000E+10	1.00000	6.28000
95	N + OH = NO + H,	0.380000E+14	0.00000	0.00000
96	NO2 + M = NO + O + M,	0.110000E+17	0.00000	66.00000
97	NO2 + O = NO + O2,	0.100000E+14	0.00000	0.60000
98	NO + H2O2 = NO2 + OH,	0.210000E+13	0.00000	-0.48000
99	CH + N2 = HCN + N,	0.190000E+12	0.00000	13.60000
100	CH2 + N2 = HCN + NH,	0.100000E+14	0.00000	74.00000

Table 17 (cont'd)

STOICHIOMETRIC REACTION		A	N	E
=====		=====	=====	=====
101	CH + N = CN + H,	0.100000E+14	0.00000	0.00000
102	C + NO = CN + O,	0.660000E+14	0.00000	0.00000
103	CH2 + N = HCN + H,	0.500000E+14	0.00000	0.00000
104	N + CH4 = NH + CH3,	0.100000E+14	0.00000	24.00000
105	CH + NO = HCN + O,	0.110000E+15	0.00000	0.00000
106	N + CO2 = NO + CO,	0.190000E+12	0.00000	3.40000
107	HCN + OH = CN + H2O,	0.150000E+14	0.00000	10.92900
108	HCN + O = CN + OH,	0.270000E+10	1.58000	26.60000
109	CN + H2 = HCN + H,	0.300000E+06	2.45000	2.23700
110	HCN + O = NCO + H,	0.140000E+05	2.64000	4.98000
111	HCN + O = NH + CO,	0.350000E+04	2.64000	4.98000
112	CN + O = CO + N,	0.180000E+14	0.00000	0.00000
113	CN + O2 = NCO + O,	0.560000E+13	0.00000	0.00000
114	CN + OH = NCO + H,	0.600000E+14	0.00000	0.00000
115	NCO + H = NH + CO,	0.500000E+14	0.00000	0.00000
116	NCO + O = NO + CO,	0.560000E+14	0.00000	0.00000
117	NCO + N = N2 + CO,	0.200000E+14	0.00000	0.00000
118	NCO + M = N + CO + M,	0.310000E+17	-0.50000	48.00000
119	NH + O2 = NO + OH,	0.140000E+12	0.00000	2.00000
120	NH2 + NO = N2 + H2O,	0.380000E+16	-1.25000	0.00000
121	NH + OH = N + H2O,	0.500000E+12	0.50000	2.00000
122	NH + N = N2 + H,	0.300000E+14	0.00000	0.00000
123	NH + H = N + H2,	0.300000E+14	0.00000	0.00000
124	NH2 + O = NH + OH,	0.680000E+13	0.00000	0.00000
125	NH2 + OH = NH + H2O,	0.450000E+13	0.00000	2.20000
126	NH2 + H = NH + H2,	0.690000E+14	0.00000	3.65000
127	N2O + M = N2 + O + M,	0.160000E+15	0.00000	51.60000
128	N2O + O = NO + NO,	0.100000E+15	0.00000	28.20000
129	N2O + O = N2 + O2,	0.100000E+15	0.00000	28.20000
130	N2O + H = N2 + OH,	0.760000E+14	0.00000	15.20000
131	NCO + NO = N2O + CO,	0.100000E+14	0.00000	-0.39000
132	NCO + H2 = HNCO + H,	0.860000E+13	0.00000	9.00000
133	HNCO + H = NH2 + CO,	0.200000E+14	0.00000	3.00000
134	NH + O2 = HNO + O,	0.100000E+14	0.00000	12.00000
135	NH + NO = N2O + H,	0.430000E+15	-0.50000	0.00000
136	NH + OH = HNO + H,	0.200000E+14	0.00000	0.00000
137	NH2 + O = HNO + H,	0.660000E+15	-0.50000	0.00000
138	NH2 + NO = N2H + OH,	0.880000E+16	-1.25000	0.00000
139	N2H + NO = N2 + HNO,	0.500000E+14	0.00000	0.00000
140	HNO + M = H + NO + M,	0.150000E+17	0.00000	48.68000
141	HNO + OH = NO + H2O,	0.360000E+14	0.00000	0.00000
142	HNO + H = H2 + NO,	0.500000E+13	0.00000	0.00000
143	NH3 + M = NH2 + H + M,	0.140000E+17	0.00000	90.60000
144	NH3 + O = NH2 + OH,	0.210000E+14	0.00000	9.00000
145	NH3 + H = NH2 + H2,	0.700000E+07	2.39000	10.17100
146	NH3 + OH = NH2 + H2O,	0.200000E+07	2.04000	0.56600
147	N2H + M = N2 + H + M,	0.200000E+15	0.00000	20.00000
148	N2H + H = N2 + H2,	0.370000E+14	0.00000	3.00000
149	NH + NH2 = N2H2 + H,	0.500000E+14	0.00000	0.00000
150	N2H2 + M = N2H + H + M,	0.500000E+17	0.00000	50.00000

Table 17 (cont'd)

STOICHOMETRIC REACTION		A	N	E
=====		=====	=====	=====
151	$\text{N}_2\text{H}_2 + \text{H} = \text{N}_2\text{H} + \text{H}_2,$	0.500000E+14	0.00000	1.00000
152	$\text{CH}_3 + \text{CH}_3 = \text{C}_2\text{H}_6,$	0.160000E+14	0.00000	-0.30600
153	$\text{CH}_3 + \text{CH}_3 = \text{C}_2\text{H}_4 + \text{H}_2,$	0.210000E+15	0.00000	19.20000
154	$\text{CH}_3 + \text{CH}_2 = \text{C}_2\text{H}_4 + \text{H},$	0.300000E+14	0.00000	0.00000
155	$\text{C}_2\text{H}_6 + \text{O} = \text{C}_2\text{H}_5 + \text{OH},$	0.250000E+14	0.00000	6.36000
156	$\text{C}_2\text{H}_6 + \text{H} = \text{C}_2\text{H}_5 + \text{H}_2,$	0.540000E+03	3.50000	5.20000
157	$\text{C}_2\text{H}_6 + \text{OH} = \text{C}_2\text{H}_5 + \text{H}_2\text{O},$	0.870000E+10	1.05000	1.81000
158	$\text{C}_2\text{H}_6 + \text{CH}_3 = \text{C}_2\text{H}_5 + \text{CH}_4,$	0.550000E+00	4.00000	8.28000
159	$\text{C}_2\text{H}_6 + \text{CH}_2 = \text{C}_2\text{H}_5 + \text{CH}_3,$	0.220000E+14	0.00000	8.66000
160	$\text{C}_2\text{H}_5 + \text{M} = \text{C}_2\text{H}_4 + \text{H} + \text{M},$	0.100000E+18	0.00000	31.00000
161	$\text{C}_2\text{H}_5 + \text{H} = \text{CH}_3 + \text{CH}_3,$	0.400000E+14	0.00000	0.00000
162	$\text{C}_2\text{H}_5 + \text{O}_2 = \text{C}_2\text{H}_4 + \text{H}_2\text{O}_2,$	0.320000E+13	0.00000	5.02000
163	$\text{C}_2\text{H}_4 + \text{M} = \text{C}_2\text{H}_3 + \text{H} + \text{M},$	0.260000E+18	0.00000	96.60000
164	$\text{C}_2\text{H}_4 + \text{M} = \text{C}_2\text{H}_2 + \text{H}_2 + \text{M},$	0.260000E+18	0.00000	79.35000
165	$\text{C}_2\text{H}_4 + \text{H} = \text{C}_2\text{H}_3 + \text{H}_2,$	0.110000E+15	0.00000	8.50000
166	$\text{C}_2\text{H}_4 + \text{OH} = \text{C}_2\text{H}_3 + \text{H}_2\text{O},$	0.480000E+13	0.00000	1.23000
167	$\text{C}_2\text{H}_4 + \text{O} = \text{HCO} + \text{CH}_3,$	0.160000E+10	1.20000	0.74600
168	$\text{C}_2\text{H}_4 + \text{OH} = \text{CH}_2\text{O} + \text{CH}_3,$	0.200000E+13	0.00000	0.96000
169	$\text{C}_2\text{H}_3 + \text{O}_2 = \text{HCO} + \text{CH}_2\text{O},$	0.400000E+13	0.00000	-0.25000
170	$\text{C}_2\text{H}_3 + \text{O} = \text{CH}_2\text{CO} + \text{H},$	0.330000E+14	0.00000	0.00000
171	$\text{C}_2\text{H}_3 + \text{H} = \text{C}_2\text{H}_2 + \text{H}_2,$	0.400000E+14	0.00000	0.00000
172	$\text{C}_2\text{H}_3 + \text{OH} = \text{C}_2\text{H}_2 + \text{H}_2\text{O},$	0.500000E+13	0.00000	0.00000
173	$\text{C}_2\text{H}_3 + \text{CH}_2 = \text{C}_2\text{H}_2 + \text{CH}_3,$	0.300000E+14	0.00000	0.00000
174	$\text{C}_2\text{H}_3 + \text{C}_2\text{H} = \text{C}_2\text{H}_2 + \text{C}_2\text{H}_2,$	0.300000E+14	0.00000	0.00000
175	$\text{C}_2\text{H}_3 + \text{M} = \text{C}_2\text{H}_2 + \text{H} + \text{M},$	0.800000E+15	0.00000	31.50000
176	$\text{C}_2\text{H}_2 + \text{M} = \text{C}_2\text{H} + \text{H} + \text{M},$	0.420000E+17	0.00000	107.00000
177	$\text{C}_2\text{H}_2 + \text{O} = \text{CH}_2 + \text{CO},$	0.220000E+11	1.00000	2.58000
178	$\text{C}_2\text{H}_2 + \text{O} = \text{C}_2\text{H} + \text{OH},$	0.320000E+16	-0.60000	15.00000
179	$\text{C}_2\text{H}_2 + \text{OH} = \text{CH}_2\text{CO} + \text{H},$	0.320000E+12	0.00000	0.20000
180	$\text{C}_2\text{H}_2 + \text{OH} = \text{C}_2\text{H} + \text{H}_2\text{O},$	0.600000E+13	0.00000	7.00000
181	$\text{C}_2\text{H} + \text{H}_2 = \text{C}_2\text{H}_2 + \text{H},$	0.410000E+06	2.39000	0.86000
182	$\text{C}_2\text{H} + \text{O}_2 = \text{CO} + \text{HCO},$	0.240000E+13	0.00000	0.00000
183	$\text{C}_2\text{H} + \text{O} = \text{CH} + \text{CO},$	0.500000E+14	0.00000	0.00000
184	$\text{CH}_2\text{CO} + \text{M} = \text{CH}_2 + \text{CO} + \text{M},$	0.360000E+16	0.00000	59.30000
185	$\text{CH}_2\text{CO} + \text{O} = \text{CH}_2\text{O} + \text{CO},$	0.200000E+14	0.00000	0.00000
186	$\text{CH}_2\text{CO} + \text{H} = \text{CH}_3 + \text{CO},$	0.110000E+14	0.00000	3.43000
187	$\text{CH}_2\text{CO} + \text{OH} = \text{CH}_2\text{O} + \text{HCO},$	0.280000E+14	0.00000	0.00000
188	$\text{CH}_2 + \text{CH} = \text{C}_2\text{H}_2 + \text{H},$	0.400000E+14	0.00000	0.00000
189	$\text{CH}_2 + \text{CH}_2 = \text{C}_2\text{H}_2 + \text{H}_2,$	0.320000E+14	0.00000	0.00000
190	$\text{CH} + \text{CH}_3 = \text{C}_2\text{H}_3 + \text{H},$	0.300000E+14	0.00000	0.00000
191	$\text{CH} + \text{CH}_4 = \text{C}_2\text{H}_4 + \text{H},$	0.600000E+14	0.00000	0.00000
192	$\text{C} + \text{CH}_3 = \text{C}_2\text{H}_2 + \text{H},$	0.500000E+14	0.00000	0.00000
193	$\text{C} + \text{CH}_2 = \text{C}_2\text{H} + \text{H},$	0.500000E+14	0.00000	0.00000

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$$\text{CO/R} = A1 + A2*T + A3*T**2 + A4*T**3 + A5*T**4$$

$$s/p = A1*\log(T) + A2*T + A3/2*T**2 + A4/3*T**3 + A5/4*T**4 + A7$$

$$u/Dt = A_1 + A_2/2 * T + A_3/3 * T^2 + A_4/4 * T^3 + A_5/5 * T^4 + A_6/T$$

$$u/P_T = A_1 + A_2/2*T + A_3/3*T**2 + A_4/4*T**3 + A_5/5*T**4 + A_6/T$$

The first set of data fits temperature range 1000 - 3000 K

The first set of data fits temperature range 1000 - 3000 K

The second set of data fits temperature range 300 - 1000 K

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Table 18 (cont'd)

SPECIES	A1	A2	A3	A4	A5	A6	A7
HNC0	0.513004E+01, 0.237222E+01, 0.659689E+01, 0.391418E+01, 0.360363E+01, 0.373863E+01, 0.499644E+01, 0.310920E+01, 0.619313E+01, 0.326704E+01, 0.482091E+01, 0.350778E+01, 0.556263E+01, 0.325240E+01, 0.231686E+01, 0.377297E+01, 0.509478E+01, 0.798038E+00, 0.275543E+01, 0.412629E+01, 0.274149E+01, 0.345206E+01, 0.318900E+01, 0.404595E+01, 0.462408E+01, 0.345892E+01, 0.473067E+01, 0.261892E+01, 0.243708E+01, 0.250000E+01, 0.232923E+01, 0.456441E+01, 0.424157E+01, 0.614217E+00, 0.141237E+01, 0.134110E+01, 0.241782E+00, 0.205006E+01, 0.429551E+01, 0.185869E+01, 0.209485E+01, 0.286170E+01, 0.247441E+01, 0.195008E+01, 0.100968E+01, 0.259692E+01, 0.247749E+01, 0.266594E+01, 0.546652E+01, 0.246606E+01, 0.72033-E+01, 0.768674E+00, 0.551449E+01, 0.250989E+01,	0.435514E-02, 0.136640E-01, 0.386941E-02, 0.140110E-01, 0.336444E-03, 0.192392E-02, 0.262509E-02, 0.662010E-02, 0.143275E-02, 0.982113E-02, 0.247900E-02, 0.720240E-02, 0.208606E-02, 0.700107E-02, 0.628415E-02, 0.829757E-03, 0.932961E-02, 0.217881E-01, 0.329058E-02, 0.164858E-02, 0.140320E-02, 0.549836E-03, 0.133823E-02, 0.341818E-02, 0.252603E-02, 0.206471E-02, 0.282583E-02, 0.864396E-02, 0.132339E-02, 0.34339E-02, 0.567671E-02, 0.591643E-02, 0.557648E-02, 0.244290E-01, 0.160120E-01, 0.118606E-01, 0.235885E-01, 0.11462E-01, 0.933088E-02, 0.198950E-01, 0.190216E-01, 0.102180E-01, 0.108287E-01, 0.106561E-01, 0.192829E-01, 0.800764E-02, 0.151151E-01, 0.941500E-02, 0.173260E-02, 0.917032E-02, 0.309088E-02, 0.211811E-01, 0.413944E-02, 0.121716E-01,	0.162690E-05, 0.133322E-04, 0.155162E-05, 0.174043E-04, 0.100289E-06, 0.470352E-05, 0.109284E-05, 0.260701E-05, 0.612552E-06, 0.832847E-05, 0.946441E-06, 0.755746E-05, 0.464411E-06, 0.881237E-06, 0.226536E-05, 0.212512E-05, 0.118019E-04, 0.336270E-05, 0.134568E-04, 0.11604E-05, 0.564617E-05, 0.460010E-06, 0.203585E-05, 0.528993E-06, 0.798192E-05, 0.106095E-05, 0.115581E-05, 0.681106E-05, 0.909078E-07, 0.832161E-11, 0.297669E-05, 0.190817E-04, 0.213337E-05, 0.382825E-04, 0.781972E-05, 0.679804E-05, 0.116027E-04, 0.170299E-04, 0.447349E-05, 0.220928E-04, 0.971538E-04, 0.135967E-04, 0.499798E-05, 0.131416E-06, 0.943689E-05, 0.169886E-04, 0.773219E-05, 0.946148E-05, 0.722049E-06, 0.496985E-05, 0.133290E-05, 0.169803E-04, 0.158787E-05, 0.786184E-05,	0.280356E-09, 0.644755E-08, 0.281415E-09, 0.120128E-07, 0.163182E-10, 0.311130E-08, 0.203091E-09, 0.149664E-08, 0.115787E-09, 0.176506E-08, 0.165488E-09, 0.429792E-08, 0.165038E-09, 0.289398E-08, 0.340187E-09, 0.121269E-07, 0.126988E-09, 0.563083E-09, 0.209038E-09, 0.405052E-08, 0.802177E-10, 0.303363E-08, 0.959193E-10, 0.611393E-08, 0.198792E-09, 0.955567E-08, 0.212637E-09, 0.222759E-08, 0.228641E-10, 0.942783E-14, 0.749752E-09, 0.176502E-07, 0.408612E-09, 0.308432E-07, 0.185851E-08, 0.150392E-07, 0.277031E-08, 0.247764E-07, 0.104816E-08, 0.143477E-07, 0.239369E-08, 0.212403E-07, 0.113214E-08, 0.617073E-08, 0.224435E-08, 0.234847E-07, 0.190823E-08, 0.164360E-07, 0.137217E-09, 0.206342E-08, 0.254616E-09, 0.229638E-08, 0.279776E-09, 0.353516E-09,	-0.182760E-13, 0.104029E-11, 0.190594E-13, 0.335658E-11, 0.362867E-15, 0.616753E-12, 0.139152E-13, 0.109220E-11, 0.804013E-14, 0.596328E-12, 0.108991E-13, 0.942579E-12, 0.113667E-13, 0.182701E-11, 0.214700E-13, 0.416738E-11, 0.358597E-13, 0.258652E-11, 0.156763E-13, 0.104999E-11, 0.527709E-14, 0.124011E-11, 0.648479E-14, 0.159191E-11, 0.137994E-13, 0.361959E-11, 0.145641E-13, 0.806503E-13, 0.137623E-14, 0.381080E-17, 0.735385E-13, 0.562603E-11, 0.305289E-13, 0.954114E-11, 0.174296E-12, 0.630286E-11, 0.260557E-12, 0.928765E-11, 0.972239E-13, 0.390482E-11, 0.231037E-12, 0.812764E-11, 0.101980E-12, 0.303131E-11, 0.210449E-12, 0.878111E-11, 0.184471E-12, 0.647777E-11, 0.962338E-14, 0.200156E-11, 0.160596E+05, 0.582440E+04, 0.752929E+04, 0.193210E-11, 0.185842E-13, 0.115409E-11,	-0.906958E+05, -0.840485E+05, 0.348837E+05, 0.355146E+05, 0.491470E+05, 0.492580E+05, 0.222606E+05, 0.228588E+05, 0.648184E+05, 0.655891E+05, 0.686859E+05, 0.689943E+05, 0.548979E+05, 0.556091E+05, -0.642655E+04, -0.669085E+04, 0.929966E+04, 0.103799E+05, 0.220011E+05, 0.216975E+05, 0.415305E+05, 0.412803E+05, 0.982833E+04, 0.974539E+04, 0.228999E+04, 0.281523E+04, 0.816177E+04, 0.110737E+05, 0.561070E+05, 0.561286E+05, 0.452111E+01, 0.418064E+01, 0.117795E+02, 0.161173E+01, -0.173544E+01, 0.257382E+05, 0.262825E+05, 0.516308E+02, 0.535373E+04, -0.111436E+05, 0.112978E+05, 0.119905E+02, 0.178992E+02, 0.133871E+02, 0.143286E+02, 0.119673E+02, 0.108393E+02, 0.138516E+02, 0.185270E+02, 0.119537E+02, 0.137562E+02, 0.140068E+02, -0.347126E+01, 0.121721E+02, -0.126081E+02, 0.204063E+02, -0.314225E+01, 0.123996E+02,	
C2H2							
C2H4							
C2H6							
CH3CHO							
C2H3							
C2H5							
CH3CO							
O3							
N03							
HN02							

Table 18 (continued)

SPECIES	A1	A2	A3	A4	A5	A6	A7
HNO3	O 705911E+01, O 143771E+01, C 442076E+00, O 267394E+01, O 377080E+01, O 210620E+01, O 472350E+01, O 333684E+01, O 136049E-01, -O 447781E+00, O 361221E+01, O 378371E+01, O 441534E+01, O 350134E+01, O 337119E+01, O 161800E+01, O 258107E+01, O 253287E+01,	O 567694E-02, O 209036E-01, O 221193E-02, O 849195E-02, O 787150E-02, O 721660E-02, O 610204E-02, O 658812E-02, O 191822E-02, O 536910E-02, O 748532E-03, -O 302336E-02, O 161439E-02, O 205359E-02, O 603997E-02, O 130631E-01, -O 146962E-03, -O 158876E-03,	-O 223489E-05, -O 145746E-04, -O 592949E-06, -O 981654E-05, -O 265638E-05, O 533847E-05, -O 191321E-05, O 299793E-05, -O 840404E-06, -O 397756E-06, -O 198206E-06, O 994928E-05, -O 163289E-06, O 717041E-06, -O 230385E-05, -O 1571E-04, O 743881E-07, O 306821E-06,	O 401555E-09, O 119720E-08, O 941958E-10, O 653736E-08, O 394443E-09, -O 737764E-08, O 276074E-09, -O 587197E-08, O 164487E-09, -O 404593E-08, O 337490E-10, -O 981891E-08, -O 855985E-10, O 492135E-09, O 406279E-09, O 160561E-07, -O 794811E-11, -O 267701E-09,	-O 270805E-13, O 191173E-11, -O 685276E-14, -O 173563E-11, -O 211262E-13, O 207561E-11, -O 145484E-13, O 212296E-11, -O 116727E-13, O 211349E-11, -O 239074E-14, O 330318E-11, O 161479E-13, -O 967117E-12, -O 271314E-13, -O 609364E-11, O 582010E-16, O 874888E-13,	-O 189200E+05, -O 173854E+05, O 633838E+05, O 638241E+05, O 127833E+03, O 978601E+03, -O 393292E+04, -O 331683E+04, -O 657139E+03, -O 942807E+02, -O 119782E+04, -O 106381E+04, O 278803E+05, O 283335E+05, O 241817E+05, O 246753E+03, O 852163E+05, O 852404E+05,	-O 107783E+02, O 182463E+02, -O 115881E+01, O 768986E+01, O 292957E+01, O 131522E+02, -O 852438E-01, O 804682E+01, -O 800702E+01, O 168408E+01, O 367033E+01, O 364163E+01, O 904289E+00, O 639184E+01, O 498059E+01, O 137947E+02, O 431289E+01, O 460624E+01,

Table 19 Equilibrium Constants of Species

The data shown below fit modified Arrhenius expression:

$$K_{p,i} = A * T^N * \exp(-E/R/T)$$

where $R = 1.987 * 10^{-3}$, [=] Kcal/Mole/K,

E [=] Kcal/Mole,

T [=] K

SPECIES	A	N	E
AR	0.10000000E+01	0.00000	0.00000
HE	0.10000000E+01	0.00000	0.00000
NE	0.10000000E+01	0.00000	0.00000
M	0.10000000E+01	0.00000	0.00000
C(S)	0.10000000E+01	0.00000	0.00000
H2	0.10000000E+01	0.00000	0.00000
N2	0.10000000E+01	0.00000	0.00000
O2	0.10000000E+01	0.00000	0.00000
CH4	0.91501490E-01	-1.30880	-18.12005
CH3	0.12659590E+03	-0.92997	35.02684
CH2	0.10942560E+06	-0.69568	92.75912
CH	0.98995510E+07	-0.34124	142.42220
C2H	0.15185170E+10	-0.72901	146.56569
CO	0.44973550E+07	-0.60557	-25.70979
CO2	0.70695720E+01	-0.22837	-93.85992
CH2O	0.22087240E+02	-0.92851	-27.63321
HCO	0.60114120E+05	-0.71864	10.85438
H2O	0.44514290E+00	-0.72481	-57.58922
H	0.57402340E+01	0.63772	51.78321
OH	0.23855150E+02	-0.17626	9.65523
O	0.76485410E+02	0.43322	59.43514
C3	0.39985250E-04	0.24392	33.80483
NH3	0.22708190E-03	-0.68432	-11.29351
NH2	0.37929920E+00	-0.48854	45.46653
NH	0.11481070E+02	-0.00468	84.15144
N	0.33892710E+02	0.52741	112.73841
N2H4	0.27943690E-12	0.17238	21.32647
HCN	0.46461080E+03	-0.28741	32.46957
CN	0.54930820E+07	-0.43393	98.35054
NCO	0.24066000E+02	0.05174	47.86087
HNCO	0.20848250E+00	-0.35489	-14.22454
C2N2	0.65778360E+02	0.14675	74.12702
C2N	0.51783650E+07	0.03590	133.53236
CNN	0.66433400E+02	0.03170	139.85102
CN2	0.11186410E+02	0.21923	113.16164
NO	0.41119610E+01	0.01346	21.57882
NO2	0.42889430E-03	0.01717	7.68731
N2O	0.36310090E-05	0.47950	19.06228
NO3	0.46248130E-10	0.74380	16.11318

Table 19 (cont'd)

SPECIES	A	N	E
HN02	0.33504530E-06	0.60229	-18.66886
HN03	0.15614360E-12	0.59833	-33.22463
CH30	0.13286590E-01	-0.91604	3.50447
CH20H	0.23163320E+00	-1.02170	-3.98950
H02	0.12430530E-01	-0.14977	2.26538
H202	0.51218650E-05	-0.15591	-32.74775
HNO	0.17053500E-01	-0.23728	23.56979
C2H2	0.10482000E+06	-0.65848	54.65442
C2H4	0.15422000E+01	-1.24340	12.23952
C2H6	0.13695890E-05	-1.49970	-21.00259
CH2CO	0.11476650E+03	-0.79547	-11.08547
CH3CHO	0.50588560E-03	-1.11440	-40.29437
C2H3	0.73203610E+05	-1.29840	71.79826
C2H5	0.56073050E-01	-1.48610	27.52591
CH3CO	0.90340430E+01	-1.23120	-4.13276
C	0.17233620E+09	-0.00015	171.29887
N2H	0.20986270E-01	-0.07174	58.31050
N2H2	0.66937420E-05	-0.24923	50.28600

Table 20 Transport Parameters

SPECIES	M(g/mol)	ϵ/k , (K)	σ , (A)	μ_d (debye)	Zrot	n	$\alpha(10^{25} \text{ cm}^3)$
CH4	16.043,	142.100,	3.790,	0.000,	8.000,	3.,	26.000,
O2	32.000,	102.600,	3.480,	0.000,	2.600,	2.,	16.000,
N2	28.016,	82.000,	3.738,	0.000,	2.800,	2.,	17.600,
CO	28.011,	104.500,	3.698,	0.010,	2.000,	2.,	19.500,
H2	2.016,	59.700,	2.827,	0.000,	2.600,	2.,	7.900,
NH3	17.032,	309.900,	3.215,	0.760,	37.100,	3.,	22.600,
HCN	27.027,	569.100,	3.630,	1.180,	3.100,	2.,	25.900,
NO	30.008,	117.200,	3.489,	0.015,	2.000,	2.,	17.000,
CO2	44.011,	200.900,	3.943,	0.000,	12.000,	2.,	26.500,
CH	13.019,	68.600,	3.370,	0.000,	0.000,	0.,	14.000,
CH2	14.027,	90.000,	3.570,	0.000,	0.000,	0.,	18.000,
CH3	15.035,	122.000,	3.630,	0.000,	0.000,	0.,	22.000,
HCO	29.019,	200.000,	3.700,	0.000,	0.000,	0.,	22.000,
CH2O	30.027,	340.400,	4.304,	0.710,	0.000,	0.,	24.600,
CH3O	31.035,	340.000,	4.300,	0.000,	0.000,	0.,	0.000,
CN	26.019,	75.000,	3.856,	0.000,	0.000,	0.,	20.000,
H2O	18.016,	506.000,	2.710,	1.230,	12.600,	3.,	14.700,
H	1.008,	37.000,	2.250,	0.000,	0.000,	0.,	4.000,
OH	17.008,	79.800,	3.147,	4.000,	8.000,	2.,	0.000,
O	16.000,	106.700,	3.050,	0.000,	0.000,	0.,	8.000,
H02	33.008,	168.000,	3.068,	0.000,	0.000,	0.,	20.000,
N	14.008,	71.400,	3.298,	0.000,	0.000,	0.,	9.000,
HNO	31.016,	117.000,	3.655,	0.880,	0.000,	0.,	21.000,
NH	15.016,	65.300,	3.312,	0.000,	0.000,	0.,	13.000,
NH2	16.024,	312.000,	3.106,	0.000,	0.000,	0.,	17.000,
N2O	44.016,	248.800,	3.776,	0.010,	3.000,	2.,	30.000,
NO2	46.008,	404.300,	3.712,	0.028,	3.000,	3.,	25.000,
NCO	42.019,	106.700,	4.110,	0.200,	0.000,	0.,	28.000,
H2O2	34.016,	289.300,	4.196,	0.750,	0.000,	0.,	21.000,
HE	4.000,	10.220,	2.576,	0.000,	0.000,	0.,	2.040,
NEON	20.183,	54.960,	2.567,	0.000,	0.000,	0.,	0.000,
ARGON	39.944,	113.500,	3.465,	0.000,	0.000,	0.,	16.300,
HNCO	43.027,	106.700,	4.110,	0.200,	0.000,	0.,	28.000,
C	12.011,	68.600,	3.370,	0.000,	0.000,	0.,	14.000,
C2H	25.030,	209.000,	4.100,	0.000,	2.500,	0.,	25.000,
C2H2	26.038,	209.000,	4.100,	0.000,	2.500,	0.,	0.000,
C2H3	27.046,	209.000,	4.100,	0.000,	0.000,	0.,	0.000,
C2H4	28.054,	280.800,	3.971,	0.000,	1.500,	0.,	0.000,
C2H5	29.062,	252.300,	4.302,	0.000,	1.500,	0.,	0.000,
C2H6	30.070,	252.300,	4.302,	0.000,	1.500,	0.,	0.000,
N2H	29.024,	71.400,	3.798,	0.000,	1.000,	0.,	0.000,
N2H2	30.032,	71.400,	3.798,	0.000,	1.000,	0.,	0.000,
CH2CO	42.038,	436.000,	3.970,	0.000,	2.000,	0.,	0.000,

END

**DATE
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12/23/91