NASA/TM—2004-213046

New Reduced Two-Time Step Method for Calculating Combustion and Emission Rates of Jet-A and Methane Fuel With and Without Water Injection

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April 2004

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ABSTRACT

A simplified kinetic scheme for Jet-A, and methane fuels with water injection was developed to be used in numerical combustion codes, such as the National Combustor Code (NCC) or even simple FORTRAN codes that are being developed at Glenn. The two time step method is either an initial time averaged value (step one) or an instantaneous value (step two). The switch is based on the water concentration in moles/cc of 1×10^{-20}. The results presented here results in a correlation that gives the chemical kinetic time as two separate functions. This two step method is used as opposed to a one step time averaged method previously developed to determine the chemical kinetic time with increased accuracy. The first time averaged step is used at the initial times for smaller water concentrations. This gives the average chemical kinetic time as a function of initial overall fuel air ratio, initial water to fuel mass ratio, temperature, and pressure. The second instantaneous step, to be used with higher water concentrations, gives the chemical kinetic time as a function of instantaneous fuel and water mole concentration, pressure and temperature (T4). The simple correlations would then be compared to the turbulent mixing times to determine the limiting properties of the reaction.

The NASA Glenn GLSENS kinetics code calculates the reaction rates and rate constants for each species in a kinetic scheme for finite kinetic rates. These reaction rates were then used to calculate the necessary chemical kinetic times. Chemical kinetic time equations for fuel, carbon monoxide and NO_x were obtained for Jet-A fuel and methane with and without water injection to water mass loadings of 2/1 water to fuel.

A similar correlation was also developed using data from NASA's Chemical Equilibrium Applications (CEA) code to determine the equilibrium concentrations of carbon monoxide and nitrogen oxide as functions of overall equivalence ratio, water to fuel mass ratio, pressure and temperature (T3). The temperature of the gas entering the turbine (T4) was also correlated as a function of the initial combustor temperature (T3), equivalence ratio, water to fuel mass ratio, and pressure.

INTRODUCTION

A simplified kinetic scheme for Jet-A, and methane fuels with water injection was developed to be used in numerical combustion codes, such as the National Combustor Code (NCC) or even simple FORTRAN codes that are being developed at Glenn. The two step kinetic scheme presented here results in a correlation that gives the chemical kinetic time as two separate functions. This two step method is used as opposed to a one step time averaged method (Reference 1) to determine the chemical kinetic time with increased accuracy. The first time averaged step is used at initial with smaller water concentrations of less than 1×10^{-20} moles/cc. This gives the average chemical kinetic time as a function of initial overall fuel air ratio, initial water to fuel mass ratio, temperature, and pressure. The second instantaneous step, to be used with higher water concentrations, gives the chemical kinetic time as a function of instantaneous fuel and water mole fractions, pressure and temperature (T4). The simple correlations would then be used with the turbulent mixing times to determine the limiting properties of the reaction.

Water injection into gas turbine engines can be useful in many ways. This includes reduced NO_x formation, a lower temperature entering into the turbine (T4) and improving the efficiency and performance of the engine. Water injection has been used in industrial applications, including turbo machinery and diesel engines. Aeronautical applications are still being developed and studied. (Reference 2). The chemical kinetic times for Jet-A fuel and methane with water injection is the focus of the research presented here.

Reaction rates are kinetically limited at low temperatures and mixing limited at very high temperatures. According to the Magnussen model (Reference 3), the fuel oxidation rate will be determined by the maximum of either the chemical kinetic time or the turbulent mixing times of the fuel and air. However, for large numerical solutions it is very tedious to use detailed classical calculations to compare both the kinetic and turbulent mixing times to determine the limits of the reaction. Detailed chemical kinetic schemes are extremely time consuming for two and three dimensional computer calculations for combustors.

Large mechanisms with many intermediate species and very fast radical reactions which cause the equations to be stiff (extremely fast compared to the overall rate, requiring a large number of small time steps), making them very difficult to integrate. Calculations for these extensive mechanisms are repetitive and complex. Using the simplified kinetic scheme developed here to calculate the three chemical kinetic times greatly reduces the amount of time required to compare kinetic reaction times with turbulent mixing times and will reduce the time required to obtain a converged solution. The advantage of extracting the chemical kinetic time for only the species of interest from a detailed computation is that we have only the differential equations of interest to solve, resulting in a much smaller set of equations.

This method is for use in Computational Fluid Dynamics (CFD) calculations where chemical kinetics is important. The current version of NCC requires the user to decide to use either chemical kinetics or the turbulent mixing rates for computing the overall conversion rate. Following detailed conventional methods would not allow for the calculation of both in a reasonable amount of time. The derived method allows for a quick and easy comparison over the complete spectrum of conditions. This scheme is intended for use in numerical combustion codes, but it can also be used as a quick and accurate method to calculate chemical reaction rates.

We have also curve fitted T4 and the equilibrium concentrations of CO_e, and NO_{x_e} using data generated by the NASA Chemical Equilibrium Application code (CEA). Jet-A fuel was represented as $C_{12}H_{23}$, using Krishna Kundu's twenty three step mechanism (References 4 and

5). The methane combustion was represented using the GRI-mech version 2.1 mechanism (Reference 10).

GLSENS (Reference 6) was used to integrate the system of equations at constant temperature and pressure, at over 2000 conditions to derive the rate expressions. We have massively correlated the output from GLSENS, the NASA detailed kinetics code, into simple exponential expressions for the chemical kinetic times. It may be reasoned that the presented equations are only as good as the overall mechanism that calculates the data. However, performing the calculations in the conventional manner is also only as good as the mechanism equations and constants that go into them. The first sections of the report, including Mixing and Kinetics, Model Equations, H_2O Mass Balance, Determination of the Chemical Kinetic Time, and the kinetic schemes pertain to both Jet-A and methane fuels. The Jet-A equilibrium and chemical kinetic time correlations will then be presented, followed by the methane correlations. Suggestions for using the correlations and a comparison of NO_x production data (Reference 2) and the NO_x produced by the chemical kinetic time correlations will then be given.

MIXING AND KINETICS

The Magnussen model (Reference 3) proposes that the maximum of either the turbulent mixing or the chemical kinetic times will be the limiting factor of a chemical reaction. This model could be explored by numerically calculating both times to compare them. However, using detailed mechanisms, this is a long and tedious process. The calculations would be extremely complicated for the detailed chemical kinetic time. By using the equations presented here to determine the chemical kinetic times and using conventional numerical methods to determine mixing times, the Magnussen model can be applied in a much more convenient way.

$$\text{Net rate} \quad \varpi_r = \min\left(\frac{A\varepsilon}{k} y_{fuel}, \frac{A\varepsilon}{k}\frac{y_{oxygen}}{r_f}, \varpi_{kinetic}\right) \tag{1}$$

Where $\frac{k}{A\varepsilon}$ equals the turbulent mixing time, τ_m, with k being the turbulent kinetic energy, ε is the dissipation rate, y is the mass fraction, and r_f, is the stoichiometric coefficient written on a mass fraction basis. The mixing constant, A, is usually given as 4.0. The factor $\frac{y_{fuel}}{\varpi_{kinetic}}$ is the chemical kinetic time τ_c computed in this report from the correlations presented.

In order to obtain the chemical source term ϖ_r, a comparison is made of the mixing rate, $\frac{1}{\tau_m}$ and the chemical kinetic rate $\frac{1}{\tau_c}$, and the lowest rate or the longest time is used in the expression; see Figure 1. This may also be represented by the following relationship:

$$\tau = \max(\tau_m, \tau_c) \tag{2}$$

MODEL EQUATIONS

The following equations can be used to model the chemical system.

$$C_x H_y + (x/2 + y/4)\, O_2 \xrightarrow{\tau_{\text{Fuel}}} x\, CO + y/2\, H_2O \tag{S1}$$

$$CO + \frac{1}{2} O_2 \xrightarrow{\tau_{\text{CO}}} CO_2 \tag{S2}$$

$$N_2 + O_2 \xrightarrow{2\tau_{\text{NO}}} 2NO \tag{S3}$$

The following first order reaction was used to represent the rate of fuel burning. (In this report, t and τ are given in milliseconds, except τ_{NO_x} which is in $\frac{ms \cdot cc}{gmol}$, while concentrations are given in gmoles/cc):

$$\frac{dFuel}{dt} = -\frac{Fuel}{\tau_{Fuel}} \tag{3}$$

For a constant τ_{Fuel}, the fuel concentration is then represented by a simple exponential decay expression, where F_0 is the initial fuel concentration.

$$Fuel = F_o e^{\left(\frac{-t}{\tau_F}\right)} \tag{4}$$

The carbon monoxide reaction rate was represented by Equations (5) and (5a). The fuel concentration is multiplied by a factor of 12 because the Jet-A fuel takes the formula $C_{12}H_{23}$. Equation (6) is the solution to the differential equation showing the CO concentration as a function of initial fuel concentration, CO equilibrium concentration and the chemical kinetic times for fuel and CO.

$$\frac{dCO}{dt} = -\frac{(CO - COeq)}{\tau_{CO}} + \frac{12Fuel}{\tau_{Fuel}} \tag{5}$$

and

$$\frac{dCO_2}{dt} = \frac{CO}{\tau_{CO}} \tag{5a}$$

$$CO - CO_{eq} = e^{\frac{-t}{\tau_{CO}}}\left[CO(t=0) - CO_{eq} - \frac{12F_o\tau_{CO}}{\tau_f - \tau_{CO}}\right] + \frac{12F_o\tau_{CO}}{\tau_f - \tau_{CO}}\, e^{-\frac{t}{\tau_f}} \qquad (6)$$

Finally, the nitrogen oxide formation rate, a species important for combustor emissions, was modeled as a simple zero order expression.

$$\frac{dNOx}{dt} = \frac{1}{\tau_{NOx}}^{*} \quad (7) \qquad \text{or} \qquad NOx = \frac{t}{\tau_{NOx}} \qquad (8)$$

$^{*}\tau_{NOx}$ has units of $\frac{ms \cdot cc}{gmol}$

H$_2$O MASS BALANCE

The inlet mixture contains only fuel, H_2O, and air, so the initial mole fractions can be easily calculated using the method of LSENS (Reference 7). This procedure is described in detail below. The mixture is completely specified by fixing the equivalence ratio, Eratio, and the water to fuel ratio, H2OF (weight H_2O/weight fuel). We have chosen to keep the weight of the H_2O separate from the weight of the fuel so that the stoichiometric fuel/air ratio is always 0.068 for all Jet-A water to fuel ratios and 0.059 for all methane water to fuel ratios. This H_2O mass balance was used for both Jet-A and methane fuels. The term MWF can be used to represent the molecular weights of either fuel.

$$\text{Let } y_i = \frac{moles \quad i}{mole \quad mixture} \quad (9); \qquad \text{let } x_i = \frac{moles\ i}{molesO_2\ in\ air} \qquad (10)$$

For the general chemical equation:

$$C_{n_c}H_{n_h}O_{n_o} + \frac{4n_c + n_n - 2n_o}{4}O_2 = n_cCO_2 + \frac{n_h}{2}H_2 0 \qquad (11)$$

$$\text{let} \quad \phi = \frac{f/o_2}{\left(f/o_2\right)_{stoich}} \quad (12)\ ; \qquad \frac{y_f}{y_{o_2}} = \frac{4\phi}{4n_c + n_h - 2n_0} \qquad (13)$$

The above equations are the same as with water injection and n_o is equal to zero for Jet-A and methane. The sum of the mole fractions of all species in the system is equal to one.

$$y_f + y_{H_2O} + y_{0_2} + y_{N_2} + y_{Ar} + y_{CO} = 1.0 \tag{14}$$

$$\text{let H2OF=} \frac{lbs\ H_2O}{lb\ \ fuel}\ ; \quad H2OM = \frac{moles\ H_2O}{mole\ \ fuel} = \frac{H2OF * MWF}{18} \tag{15}$$

where MWF for Jet-A is 167 and MWF for methane is 16.

$$y_{H_2O} = y_f\,(\frac{H2OF * MWF}{18}) \tag{16}$$

$$y_f = \frac{4\phi}{4n_c + n_h + 2n_o}\, y_{o_2} \tag{17}$$

Or,

$$y_{O_2} = \frac{4n_C + n_H - 2n_O}{4\phi\left(1 + \dfrac{H2OF * MW}{18}\right) + \left(4n_C + n_H - 2n_O\right)\left(1 + x_{N_2} + x_{Ar} + x_{CO_2}\right)} \tag{18}$$

(See the computer code modifications in Appendix C)

DETERMINATION OF CHEMICAL KINETIC TIME

With the approach derived here, a simple direct comparison can be made between the mixing and chemical kinetic times and the minimum rate used for the computation as shown in Figure 1. The integration was performed for 2160 cases shown below for Jet-A and methane fuels with water injection.

Table Input

Input Parameter	**Range**
Pressure	1 to 40 atmospheres (increments of 10 atm)
Temperature	1000 to 2500K (increments of 500K)
Lean Equivalence ratios	0.3 to 1.0 (increments of 0.1)
Rich Equivalence ratios	1.0 to 2.0 (increments of 0.1)
Water to fuel mass ratio	0.0 to 2.0 (increments of 0.5)
Step One Time	1×10^{-6} to 2 ms
Step Two Time	0.05 to 6 ms

Calculations were performed isothermally using GLSENS for each condition over a time of 0 to 6 milliseconds. By computing the progress isothermally, the chemical rate constants were fixed and the chemical kinetic time was determined as a unique value of temperature, pressure and instantaneous mole fractions of fuel and water. GLSENS computes the cumulative rate of reaction for each species from all equations in the mechanism, so it is a simple matter to then compute the chemical kinetic time for each species. For the fuel equation (3) the chemical kinetic time is given as

$$\tau_f = -\frac{Fuel}{\left(\frac{dFuel}{dt}\right)} \tag{19}$$

This simple calculation was done using additional steps in Subroutine Out2 in the GLSENS code (see Appendix D). Values for the chemical kinetic time were calculated for each concentration at each output time and each set of conditions. For time step 1, the trapezoidal rule (using $1/\tau$) was then used to average the chemical kinetic time to calculate the best value for each set of conditions and the final numbers regressed over the complete set of cases to obtain the final correlation.

A correlation could then be developed that determines the chemical kinetic time as a function of the initial overall cell fuel/air ratio, water to fuel mass ratio, pressure and temperature. The data was correlated using the same method as previously mentioned for the equilibrium equations. Two correlations for each step for each of the three species, one for the lean side and one for the rich side, were obtained. This results in a total of 12 Jet-A correlations and 12 Methane correlations. As OH is formed, the reaction rates get faster and the chemical kinetic time gets smaller. Chemical kinetic time was correlated using two different steps to increase the accuracy of the calculation. Step one is an average chemical kinetic time taken over 2.0 milliseconds. Step two is an instantaneous value that depends on the instantaneous amounts of fuel, water and oxygen. Since we were not tracking the radical concentrations, we were using H_2O to indicate the state of the radical species. In other words for the reactions

$H2 + OH = H2O + H$
$CO + OH = CO2 + H$
$CH4 + OH = CH3 + H2O$
$N + OH = NO + H$ etc.

The radicals could be correlated with H2O because of the first reaction.

The user should want to switch from step one to step two when the molar concentration of water is greater than 1×10^{-20} moles/cc. Step two can not be used with small concentrations of water because if the value of the water concentration was zero, the entire correlation time would go to zero.

JET-A KINETIC SCHEME FOR STEP 1(AVERAGE) AND STEP 2 (INSTANTANEOUS) METHODS

The following is GLSENS input for the 23 step, 16 species mechanism from Krishna Kundu that was used for the Jet-A calculations. The water and fuel were added as a liquid to the equilibrium program, but they were added as gases to the kinetic program to make up the reacting mixture. We did not alter the mechanism equations to compute the chemical kinetic times for water injection. The additional water took part in the reaction set as the rate equations dictated.

```
Jet-A Mechanism used in GLSENS
 &RTYPE  GLOBAL=.TRUE., GRONLY=.FALSE.,  &END
  H2     +   OH      =   H2O   +   H      1.17E+11    1.1     3626.
  H2     +   O       =   H     +   OH     2.50E+15    0.      6000.
  H      +   O2      =   O     +   OH     4.00E+14    0.     18000.
  N2     +   O2      >2.0O     +   N2     1.00E+18    0.    122239.
  H2     +2.0O       >   O2    +   H2     5.00E+17     .5        0.
  H2     +2.0H       =2.0H2               4.00E+20   -1.        0.
  H      +   O2      =   HO2              1.00E+15   -1.1       0.
  O      +   HO2     =   OH    +   O2     1.50E+13    0.        0.
  H      +   HO2     =   H2    +   O2     1.50E+13    0.        0.
  CO     +   OH      =   CO2   +   H      4.17E+11    0.0     1000.
  CO     +   HO2     >   CO2   +   OH     5.80E+13    0.     22934.
  CH     +   O       =   CO    +   H      1.00E+10     .5        0.
  CH     +   NO      =   CO    +   NH     1.00E+11    0.        0.
  CH     +   O2      =   CO    +   OH     3.00E+10    0.        0.
  C2H2   +   O2      =2.0CO    +   H      3.00E+12    0.     49000.
  N2     +2.0N       =   N2    +   N2     1.00E+15    0.        0.
  N      +   O2      =   NO    +   O      6.30E+09    1.      6300.
  N      +   OH      =   NO    +   H      3.00E+13    0.        0.
  NH     +   O       =   NO    +   H      1.50E+13    0.        0.
  NH     +   NO      =   N2    +   OH     2.00E+15    -.8       0.

  O      +   N2      +   HO2     >2.0NO      +   H    +  O
  .1       .5   1.        1.50E+07  1.      45900.
          2.0NO      +   H       >   N2      +   HO2
          1.1   1.        2.50E+10   .16     8000.
             N2      +   O       >   NO      +   N
           .5   1.        4.75E+10   .29    75010.
             N       +   NO      >   N2      +   O
          1.    1.        3.00E+12   .2         0.
  H2     +   N2      +2.0CH      >2.0CH      +2.0NH
  .1      1.    1.        1.00E+16  0.      78000.
          2.0NH      +2.0CH      >2.0CH      +   N2   +  H2
          2.    1.        1.95E+15  0.          0.
             N2      +   C12H23  >6.0C2H2    +11.0H   +  N2
           .8    .8       2.50E+09   .0     30000.
             N2      +   C12H23  >12.0CH     +11.0H   +  N2
           .8    .8       2.50E+10   .0     30000.
```

For example the last three body mechanism step the rate is given by $2.5\times10^{10}\,T^{0}e^{-30000/RT}\,N_2^{0.8}C_{12}H_{2}3^{0.8}$ in an irreversible step.

Note the fuel is $C_{12}H_{23}$. The last two steps are irreversible fuel breakup reactions to CH and C_2H_2.

Note, some reactions are bimolecular and some are trimolecular expressions. The code follows the method of LSENS developed by Radhakrishnan (Reference 7).

PARTIAL METHANE KINETICS SCHEME

Whereas Jet-A is broken down in an irreversible molecule breaking step which has a given rate, methane, CH4 is broken down by radicals OH, H, O, etc so the fast reaction is delayed until the radical pool builds up. This forces the modeling scheme to use a two step method to predict the chemical time constants. We have just listed the CH4 reactions to illustrate this process. The complete GRI-mech mechanism is listed in Appendix B. The complicated nature of the methane mechanism makes it very difficult to obtain a correlation with so few variables over a wide range of conditions (so the resulting R^2 is low).

CH4 partial mechanism showing free radical attack

OH	CH4	=	CH3	H2O	1.000E+08	1.600	3120.00
OH	CO	=	H	CO2	4.760E+07	1.228	70.00
N	OH	=	NO	H	7.333E+13	.000	1120.00
2.0O		=	O2	M	1.200E+17	-1.000	.00
H	H	=	H2	M	1.000E+18	-1.000	.00
O	H2	=	H	OH	5.000E+04	2.670	6290.00
H	O2	=	O	OH	8.300E+13	.000	14413.00
H	HO2	=	O2	H2	2.800E+13	.000	1068.0
OH	H2	=	H	H2O	2.160E+08	1.510	3430.00
O	CH4	=	OH	CH3	1.020E+09	1.500	8600.00
OH	CH2	=	CH	H2O	1.130E+07	2.000	3000.00
OH	CH3	=	CH3OH	M	6.300E+13	.000	.00
CH	CH4	=	H	C2H4	6.000E+13	.000	.00
CH2	CH4	=	2.0CH3		2.460E+06	2.000	8270.00
CH3	CH2O	=	HCO	CH4	3.320E+03	2.810	5860.00
CH3	CH3OH	=	CH2OH	CH4	3.000E+07	1.500	9940.00
CH3	CH3OH	=	CH3O	CH4	1.000E+07	1.500	9940.00
CH3	C2H4	=	C2H3	CH4	2.270E+05	2.000	9200.00
CH3	C2H6	=	C2H5	CH4	6.140E+06	1.740	10450.00
N	O2	=	NO	O	2.650E+12	.000	6400.00
NO	O	=	NO2	M	1.060E+20	-1.410	.00

JET-A EQUILIBRIUM CORRELATIONS WITH AND WITHOUT WATER INJECTION

Equilibrium correlations were generated by using Microsoft Excel to perform a multivariate linear regression on the large data set generated by the CEA program of Reference 8. (A detailed procedure describing the regression used for both equilibrium and finite rate chemical times can be found in Appendix A). CEA has a plot f option for direct tabulation of the output data, for ‘f/a, P, T H2O, CO, NO’. Although the equilibrium correlations were not usually used in the calculation of the chemical kinetic times, we feel that these equations could still be very useful for other calculations. Table 1 shows the Jet-A equilibrium correlations for

T4, CO and NO_x for both the lean and rich cases. Figures 2 is a parity plot showing the strength of the lean Jet-A CO equilibrium correlation. This plot shows a minimal amount of scatter, mostly at an equivalence ratio of 1.0, indicating a strong correlation (R^2 values greater than 0.9). Note that the units of CO_{eq} and $NO_{x_{eq}}$ are moles/cc. This parity plot is typical of all the variables because of the high R^2 values obtained. This was a correlation for all of the range of independent variables in the Table Input.

Table 1. EQUILIBRIUM Lean Jet-A with Water Injection Correlations

Species	**Lean** **(f/a ≤ 0.068)**	**R-squared**	
T4	$T4 = 1725\ (T3)^{0.241}\left(f/a\right)^{0.442}(1+h2o/f)^{(-0.151)}\ P^{0.00301}$	**0.949**	(20)
CO	$CO_{eq} = 22.6(f/a)^{2.22}(1+h2o/f)^{0.0658}P^{0.524}\exp\left[\frac{-31647}{T}\right]$	**0.995**	(21)
NO_x	$NOx_{eq} = 2.65e^{-8}(f/a)^{(-1.52)}(1+h2o/f)^{(-0.133)}\ P^{0.980}\ \exp\left[\frac{-9953}{T}\right]$	**0.958**	(22)

Table 2. EQUILIBRIUM Rich Jet-A with Water Injection Correlations

Species	**Rich** **(f/a > 0.068)**	**R-squared**	
T4	$T4 = 163(T3)^{0.186}\left(f/a\right)^{(-0.613)}(1+h2o/f)^{(-0.296)}\ P^{0.00231}$	**0.959**	(23)
CO	$CO_{eq} = 3.85e^{-4}(f/a)^{2.86}(1+h2o/f)^{(-0.369)}\ P^{0..995}\ \exp\left[\frac{185}{T}\right]$	**0.990**	(24)
NO_x	$NOx_{eq} = 1.80e^{-8}(f/a)^{(-6.08)}(1+h2o/f)^{0.418}P^{0.530}\exp\left[\frac{-38952}{T}\right]$	**0.993**	(25)

CHEMICAL KINETIC TIMES FOR JET-A WITH AND WITHOUT WATER INJECTION

Step OneEquations for Jet-A

The following form of equation was used for the Jet-A step one correlations:

$$\tau = A(P)^a(f/a)^b(1+\frac{h2o}{fuel})^c \exp\frac{D}{T} \qquad (26)$$

where τ is the chemical kinetic time in milliseconds, *P* is pressure in atm, f/a is the initial or overall mass fuel air ratio as in reference 1, $\frac{h2o}{fuel}$ is the initial mass water to fuel ratio and *T* is the temperature in Kelvin. The correlation is switched to Step Two when the water molar concentration is greater than 1×10^{-20}.

The initial or overall fuel air ratio can be determined as follows:

$$f\,/\,a = (\,fuel + \frac{(CO + CO_2)}{12})*167\,/\,\frac{0.79}{28N_2} \tag{27}$$

The coefficients for each of the parameters in the correlations may be found in Table 3. R-square values have been included to demonstrate the strength of the correlation. R-squared is a measure of the error that the model accounts for; an R-squared value of one is ideal.

Table 3. Step One Jet-A With Water Injection Chemical Kinetic Time Correlations

Component	Rich or lean	A	a	D	b	c	R-squared	
Fuel	Lean	7.47×10^{-5}	-0.60	14202	0.238	0.0712	1.00	(28)
CO	Lean	7.13×10^{-2}	-0.758	9295	-0.314	0.159	0.933	(29)
NO_x	Lean	1.00×10^{6}	-1.30	26139	0.110	1.30	0.994	(30)
Fuel	Rich	8.19×10^{-5}	-0.60	14206	0.296	0.153	1.00	(31)
CO	Rich	1.39×10^{-3}	-0.882	6803	-0.222	-0.328	0.988	(32)
NO_x	Rich	93.2	-1.67	27755	-0.0582	0.529	0.983	(33)

All of the results presented here are correlated over the complete conditions listed in Table Input. Parity plots for the lean step one correlations have been created and may be found in Figures 3-5. The x-axis contains values for the chemical kinetic time generated by the full mechanism GLSENS at each condition. The y-axis contains values calculated using the chemical kinetic time correlations above at the same set of conditions. This demonstrates how close the calculated value is to the expected value and is a good measurement of the strength of the correlations. Figure 6 shows an increase in the step one chemical kinetic time with a higher water to fuel ratio. Data from the previous Jet-A chemical kinetic time correlation without water injection has also been included on this plot for comparison. In order to compare the correlations, we took various values of f/a, *p*, and *T* and obtained predictions for the previous correlation (Ref. 1 as “No Water Injection”). Then these prediction are plotted using the overall factor found here (x axis). Note that the previous work gave a much faster time (averaged over a total time as high as 10 milliseconds and accounted for the lower τ. This difference in results caused us to switch to an instantaneous correlation (Step Two) for longer times.

Step Two Equations for Jet-A

The following form of equation was used for the Jet-A step two fuel and NO_x correlations. This form of the equation produced the best fit:

$$\tau = A(P)^{a}(cfuel)^{b}(co2)^{c}(cH2O)^{d}\exp\frac{E}{T} \tag{34}$$

and for the Jet-A step two CO correlation:

$$\tau = A(P)^{a}(cfuel)^{b}(cco)^{c}(co2)^{d}(cH2O)^{e}\exp\frac{F}{T} \tag{35}$$

where P is pressure in atm, cfuel is the instantaneous molar concentration of fuel, cco is the instantaneous molar concentration of CO. We added CO as a parameter in order to attempt to raise the R^2 value for the CO correlation. We have preceded the symbol with a c to indicate molar concentration was used and a y for mole fraction. The CO2 is the instantaneous molar concentration of O2, cH2o is the instantaneous molar concentration of water, and T is the temperature in Kelvin. We have correlated to only the major species hoping that H_2O will track the minor species (OH, H, O, etc.) to allow good overall correlation and easy use of the equations.

The coefficients for each parameter are given in Table 4. Parity plots for the step two lean Jet-A correlations can be found in Figures 7-9. These figures show a minimal amount of scattering for the fuel and NO$_x$, which is consistent with the high R-squared values as seen in Table 4. However, the CO plot shows considerably more scattering with an R-squared value of 0.578 for the lean case and 0.389 for the rich case.

Table 4. Step Two Jet-A With Water Injection Chemical Kinetic Time Correlations

Component	Rich or Lean	A	Pressure	1/T	cfuel	cCO	cO2	cH2O	R-squared	
Fuel	Lean	7.31E-06	-0.173	12412	0.0792	-	-0.164	-0.115	0.927	(36)
CO	Lean	9.28E-07	-0.164	8893	-0.15	0.268	-0.549	-0.0588	0.578	(37)
NO$_x$	Lean	2.67E-03	-0.628	28071	-0.186	-	-0.558	0.0458	0.93	(38)
Fuel	Rich	1.35E-04	-0.352	12962	0.0147	-	-0.0743	-0.0373	0.953	(39)
CO	Rich	0.373	-0.422	4387	-0.287	0.206	0.227	0.115	0.389	(40)
NO$_x$	Rich	28.9	-0.00805	19595	-0.117	-	-0.158	-0.16	0.438	(41)

METHANE EQUILIBRIUM CORRELATIONS WITH AND WITHOUT WATER INJECTION

The rich and lean Methane equilibrium correlations can be found in Tables 5 and 6, respectively. A parity plot for the rich Methane CO equilibrium correlation can be found in Figure 10.

Table 5. EQUILIBRIUM Lean Methane With Water Injection Correlations

Species	Lean (f/a ≤ 0.058)	R-Squared	
T4	$T4 = 1565(f/a)^{0.435}(1+\frac{h2o}{f})^{-0.069}(T3)^{0.258}(P)^{0.00284}$	**0.944**	(42)
CO	$COeq = 3.37x10^{6}(f/a)^{1.90}(1+\frac{h2o}{f})^{0.00705}(P)^{-0.477}\exp\frac{-33388}{T}$	**0.998**	(43)
NO_x	$NOxeq = 2.44x10^{-2}(f/a)^{-1.13}(1+\frac{h2o}{f})^{-1.07}(P)^{-0.017}\exp\frac{-11415}{T}$	**0.953**	(44)

Table 6. EQUILIBRIUM Rich Methane With Water Injection Correlations

Species	Rich (f/a > 0.058)	R-Squared	
T4	$T4 = 177(f/a)^{-0.559}(1+\frac{h2o}{f})^{-0.146}(T3)^{0.176}(P)^{0.00167}$	**0.976**	(45)
CO	$COeq = 72.2(f/a)^{2.55}(1+\frac{h2o}{f})^{-0..358}(P)^{-0.00393}\exp\frac{-31365}{T}$	**0.911**	(46)
NO_x	$NOxeq = 0.218(f/a)^{-4.43}(1+\frac{h2o}{f})^{0.427}(P)^{-0.493}\exp\frac{-41408}{T}$	**0.998**	(47)

CHEMICAL KINETIC TIMES FOR METHANE WITH AND WITHOUT WATER INJECTION

Step One Equations for Methane

The step one Methane chemical kinetic time correlations are of the following form:

$$\tau = A(P)^{a}(f/a)^{b}(1+\frac{h2o}{fuel})^{c}\exp\left[\frac{D}{T}\right] \tag{48}$$

where P is pressure in atm, f/a is the initial or overall fuel air ratio, $\frac{h2o}{fuel}$ is the initial water to fuel ratio and T is the temperature in Kelvin.

The initial or overall fuel air ratio can be determined as follows:

$$f/a = (fuel + (CO + CO_2)) * 16 / \frac{0.79}{28N_2} \tag{49}$$

A summary of these correlations can be found in Table 7. Parity plots for the lean step one methane with water injection correlations can be found in Figures 11-13. These parity plots show minimal scatter, which is consistent with the high R-squared values of the lean correlations. Figure 14 shows an increase in step one chemical kinetic time with a higher water to fuel ratio.

Table 7. Step One Methane With Water Injection Chemical Kinetic Time Correlations

Component	Rich or Lean	A	a	D	b	c	R-squared	
Fuel	Lean	$2.09\text{x}10^{-4}$	-1.07	22625	0.222	0.0675	0.996	(50)
Co	Lean	$9.99\text{x}10^{-4}$	-1.00	2434	0.101	0.0959	0.999	(51)
NO_x	Lean	29395	-2.11	34859	0.0315	0.329	0.996	(52)
Fuel	Rich	0.0274	-0.328	14216	0.111	-0.829	0.75	(53)
Co	Rich	$1.30\text{x}10^{-3}$	-1.00	2433	0.215	0.195	0.999	(54)
NO_x	Rich	43928	-2.00	32649	0.284	0.641	0.999	(55)

Step Two Equations for Methane

The following form of equation was used for all lean Methane step two correlations:

$$\tau = A(P)^a (cfuel)^b (ch20)^c (1 + \frac{ch2o}{cfuel})^d \exp\left[\frac{E}{T}\right] \tag{56}$$

The following form of equation was used for the rich Methane step two correlations for fuel and NO_x:

$$\tau = A(P)^a (cfuel)^b (co2)^c (cH2O)^d \exp\frac{E}{T} \tag{57}$$

and for the rich Methane step two CO correlation:

$$\tau = A(P)^a (cfuel)^b (cco)^c (co2)^d (cH2O)^e \exp\frac{F}{T} \tag{58}$$

Table 8 provides a summary of these correlations, and lean parity plots can be found in Figures 15-17.

Table 8. Step Two Methane With Water Injection Chemical Kinetic Time Correlations

Compo-nent	A	Pressure	1/T	cfuel	cCO	cO2	cH2O	$1+\frac{ch2o}{cfuel}$	R-squared	
Fuel (lean)	3.50x10^{-9}	-0.0713	14149	-0.307	-	-	-0.465	-0.221	0.416	(59)
CO (lean)	3.07x10^{-3}	-1.09	2291	0.0957	-	-	-9.82x10^{-4}	0.131	0.999	(60)
NO_x (lean)	1.48x10^{5}	-2.28	37437	0.239	-	-	- 0.0206	0.778	0.986	(61)
Fuel (rich)	9.99x10^{-11}	-0.761	19950	0.050	-	-0.549	-0.350	-	0.483	(62)
CO (rich)	1.64E-10	0.0722	7880	-0.261	0.0568	-0.636	-0.00341	-	0.816	(63)
NO_x (rich)	1.67E+06	-2.45	24117	0.05	-	0.119	-0.281	-	0.792	(64)

TWO STEP METHANE CHEMICAL KINETIC TIMES WITHOUT WATER INJECTION

The step two methane chemical kinetic times were also correlated without water injection. The previous correlations are a massive regression over all water injection values. If one were not using water injection, the relations would be useful, but the following relations resulted in a higher R^2 factor. The equations are of the same form as the methane step two correlations with water injection. The results can be found in Table 9:

Table 9. Step Two Methane Without Water Injection Chemical Kinetic Time Correlations

Compo-nent	A	Pressure	1/T	cfuel	cCO	cO2	cH2O	$1+\frac{ch2o}{cfuel}$	R-squared	
Fuel (lean)	1.86x10^{-9}	0.479	13446	0.182	-	0.0528	-0.704	0.349	0.767	(65)
CO (lean)	1.43x10^{-3}	-1.04	2371	0.0461	-	-	-5.7x10^{-4}	-	0.999	(66)
NO_x (lean)	10.0	-1.92	38229	0.0389	-	-	-0.200	-	0.992	(67)
Fuel (rich)	2.02x10^{-14}	0.498	14860	0.252	-	-0.776	-0.756	0.254	0.995	(68)
CO (rich)	6.73x10^{-13}	0.244	8229	-0.274	-0.237	-0.802	0.217	-	0.806	(69)
NO_x (rich)	0.0574	-1.22	26010	-0.103	-	-0.0583	-0.617	-	0.959	(70)

COMBINED LEAN AND RICH STEP TWO METHANE TIMES

In this case the program would not have to choose between the rich and lean fuel/air zones, but could use the correlation directly. The lean and rich step two methane chemical kinetic times were also combined into one large data set and correlated. The results of this correlation can be found in Table 10. The fuel correlation is in the following form:

$$\tau = A(P)^a (cfuel)^b (co2)^c (cH2O)^d \exp\frac{E}{T} \qquad (71)$$

while the CO and NO_x correlations are modeled by the following form:

$$\tau = A(P)^a (cfuel)^b (ch20)^c (1+\frac{ch2o}{cfuel})^d \exp\left[\frac{E}{T}\right] \qquad (72)$$

Table 10. Combined Step Two Methane With Water Injection Chemical Kinetic Time Correlations

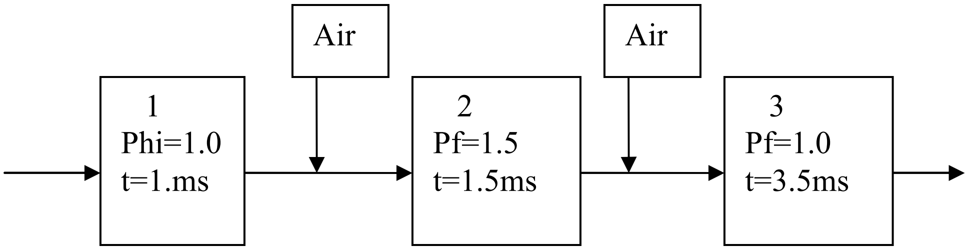
Compo-nent	A	Pressure	1/T	cfuel	cO2	cH2O	$1+\frac{ch2o}{cfuel}$	R-squared	
Fuel	$6.20\text{x}10^{-9}$	-0.290	14259	-0.0532	-0.332	-0.429	-	0.433	(73)
CO	$1.18\text{x}10^{26}$	-5.37	-1877	4.68	-	-0.106	4.90	0.627	(74)
NO_x	$2.42\text{x}10^{-14}$	0.585	37951	-2.92	-	0.0539	-2.98	0.879	(75)

COMPARISON TO NO_X DATA WITH WATER INJECTION

An important result of water injection into Jet-A and methane fuels is the reduction of NO_x formation. The NO_x concentrations calculated using the chemical kinetic time correlations were compared to water injection data presented in reference 2. This reduction is with constant T4. So the equations from Table 1 Lean T4 is solved for the increased f/a with an increase in $h2o/f$, then the NO_x value Table 3 Step One Lean is solved for the new NO_x value. Figures 18 and 19 show the ratio of NO_x with water injection to NO_x without water injection versus weight fraction ratio of water to air for Jet-A and methane respectively from the correlations, at a fuel air ratio of 0.05 as shown in reference 2. The Jet-A predicted data behaves very similarly to the given experimental data while there is more of a difference in the methane prediction. Although the temperature is constant and the kinetic mechanism remains the same there is a change in kinetics rate due to water dilution. The residence time of the combustor is decreased because of the increased throughput with water addition (t corrected results) and the molecular weight of the mixture is decreased with water addition (T constant).

TANKS IN SERIES MODEL FOR PREDICTING EMISSIONS

A tanks-in-series Fortran program was developed to simulate CO and NO_x production, so that it may be compared to the water injection data in reference 9. This model accounts for the increase in fuel/air ratio in the initial fuel injection and mixing process. Figure 20-23 show the results of this comparison.



Pf is the ratio of the tank f/a to the exit f/a. The f/a for tank 2 was limited to stoichiometric, to prevent it from going overstoichimetric as the exit f/a was increased. Reference 9 uses 15 reactors with the complete GRI Mech 2.11 mechanism compared to only the three reactors used here. Obviously one can adjust the times and equivalence ratios of the tanks, or add tanks until the output of the emissions matched the experimental data. We chose to not manipulate the parameters and determine the outcome. The results were very good.

The Fortran computer code is given in Appendix F. In this calculation we only use Step One, because it is a well stirred reactor. We had to compute the dilution factors due to Air addition between stages. We had chosen the equivalence ratio for the first stage to be one. Pf is the ratio of the equivalence ratio of the stage to the exit value. The following equation is the balanced reaction used to model the combustion of the methane fuel:

$$\phi CH_4 + (1+\frac{x}{4})O_2 + (1+\frac{x}{4})(\frac{79}{21})N_2 + (\frac{16}{18})(\frac{H2O}{F})\phi \rightarrow$$

$$\phi CO_2 + (\frac{x}{2}+\frac{16}{18}\frac{H2O}{F}\phi)H2O + [(1-\phi)(1+\frac{x}{4}))]O_2 + (1+\frac{x}{4})(\frac{79}{21})N_2$$

where x is the ratio of hydrogen to carbon, and is equal to 4 for methane. The $\frac{H2O}{F}$ term is the initial water to fuel ratio and ϕ is the overall equivalence ratio.

This equation was used to obtain a wet to dry correction so that the generated NO_x and CO data could be compared to existing data. The concentrations were corrected to 15% O2.

SUGGESTIONS FOR USING THE REDUCED EQUATIONS

In this section we show how our correlations might be used in a typical kinetics program the calculate the amount of reaction

The fuel equations that we use are:

$$\frac{dFuel}{dt} = -\frac{Fuel}{\tau_{Fuel}} \qquad (76)$$

where for step one:

$$\tau_{Fuel(lean)} = 7.47x10^{-5}(f/a)_o^{0.238}(P)^{-0.60}(1+\frac{h2o}{fuel})^{0.0712}\exp\frac{14202}{T} \tag{77}$$

Equation (76) is the "net" rate, so one does not have to compute the reverse rate. Then

$$\frac{dF}{dt} = -\frac{F\exp^{\frac{-14202}{T4}}}{7.47x10^{-5}(f/a)_o^{0.238}(P)^{-0.60}(1+\frac{h2o}{fuel})^{0.0712}} \Rightarrow -\frac{F}{C}e^{-\frac{E}{RT}} \tag{78}$$

The denominator C is a constant since we take the initial conditions as being held constant throughout the reaction and one can treat the T4 constant as an activation energy (14202×1.987) = 28219.

One can relate $(f/a)_o$ to F of a mixture by:

$$F_o = C_{12}H_{23} + \frac{1}{12}(CO+CO_2)\,\frac{moles}{cc} \tag{79}$$

$$\rho = \frac{P}{82.056T}x\frac{moles}{cc}mix \tag{80}$$

$$x_{Fo} = \frac{F_o}{\rho} = \frac{f\,{}^{gm}/_{167}}{\frac{fgm}{167}+\frac{Agm}{29}+\frac{H2O}{18F}F} = \frac{(f/a)_o}{(f/a)_o + 5.76 + 9.28\frac{H2O}{F}(f/a)_o} \tag{81}$$

Note, *gm* is the grams of component. If some fuel had reacted one can use Equation (81) to find f/a_o;

$$\left(f/a\right)_o = \frac{5.76\,F/\rho}{1-F/\rho(1+9.28\frac{H2O}{F})} \tag{82}$$

Given Equation (78) above

$$\frac{dF}{dt} \Rightarrow -\frac{F}{C}e^{-\frac{E}{RT}} \text{ which is directly usable by an Arrhenius .kinetics code} \tag{83}$$

Then the mass balance equation is

$$C_{12}H_{23} + (6 + \frac{23}{4})O_2 = 12CO + \frac{23}{2}H2O \tag{84}$$

To avoid fractional coefficients, one could use any number of methods, such as:

$$C_{12}H_{23} + (6)O_2 = 12CO + 23H2O \tag{85}$$

For CO

$$\frac{dCO}{dt} = \frac{-CO}{\tau_{CO}} \tag{86}$$

And for NO_x

$$\frac{dNOx}{dt} = \frac{1}{\tau_{NOx}} = \frac{1}{C'}e^{\frac{-26139}{T}} \tag{87}$$

$$N_2 + O_2 = 2NO \tag{88}$$

So

$$\frac{dN2}{dt} = \frac{1}{2}\frac{dNO}{dt} = \frac{1}{2C'}e^{\frac{-26139}{T}} \tag{89}$$

This completes the equations that one would need to simulation of the chemical kinetics. In our model we have only three rates and seven species, therefore the step size can be large and the rates are no longer coupled. This should be very fast.

SIMULATION OF GLSENS WITH THE TWO STEP MODEL WITHOUT WATER INJECTION

In this example we compare directly the new two time step method with the complete kinetic mechanism for an arbitrary constant temperature of 2000K and at a constant pressure of two atmospheres. The initial fuel/air ratio was taken as 0.0526 with zero water injection. We used a simple Fortran code with a Newton integration method given in Appendix G. The results are shown in Figures 24 and 25. The results from methane was one reason for creating the two step method with step two trying to follow the instantaneous reaction times though correlation with H_2O as the tracking species. Step 2 is very important for prediction of combustion stability and blowout for methane.

Figure 24 shows the rapid decreases in the chemical reaction time. This model is not as fast as the full kinetics version so the concentration decrease (Figure 25) lags the full kinetics version as well. The kinetics calculations in comparison the mixing times from (1.e-5 to 1.e-3 seconds) maybe much more relevant and accurate.

CONCLUSIONS

Much work still needs to be done to explore possible benefits and detriments of water injection in combustion. A simplified kinetic scheme for Jet-A and methane fuels with water injection resulted in a two time step correlation that calculates chemical kinetic times for fuel, CO, and NO_x. These chemical kinetic time equations can then be used in a numerical combustor code to compare the chemical kinetic time with the turbulent mixing time. Strong step one Jet-A correlations were developed ($R^2 > 0.9$). The Jet-A step two correlations for CO and NO_x are slightly weaker, but still thought to be effective. The Methane step one correlations were all very strong, while the rich step two correlations had considerably smaller R-squared values. However, because we are trying to correlate so many values over a wide range of conditions, we will accept a small amount of scatter. These twenty four equations are believed to be extremely useful in the comparison of kinetic reaction and turbulent mixing times and in the computation of kinetic rate results.

APPENDIX A

MULTIPLE LINEAR REGRESSION WITH EXCEL

Performing Multiple Linear Regression on a Logarithmic Equation

This regression technique may be used to develop a correlation between a dependent variable and one or more independent variables. First the equation to be used must be linearized. An example of an exponential equation used here is shown below.

$$A = BC^{c}D^{d}\exp\left(\frac{e}{T}\right) \qquad \text{(Non-linear form)} \qquad \text{(A1)}$$

$$\ln(A) = \ln(B) + c\ln(C) + d\ln(D) + \frac{e}{T} \qquad \text{(Linear form)} \qquad \text{(A2)}$$

Columns of data containing the independent variables (natural log of C, natural log of D, 1/T,) and the independent variable (natural log of A) were contained in an Excel spreadsheet. (It is easiest to have the independent variables adjacent to each other, followed by the dependent variable.)

The multiple variable regression analysis is located in the Data Analysis Toolpak. The Data Analysis Toolpak must be added into the spreadsheet if it is not already running in Excel. In order to add it, select the ‘Add ins’ button from the Tools menu. Click on the Analysis Toolpak option and click OK to accept this choice. Then choose ‘Data Analysis’ from the Tools menu and double click on ‘regression’. Click on the ‘Input Y Range’ box and highlight the column that contains the logarithm of the dependent variable and press return. Click on the ‘Input X Range’ box and highlight the columns containing all of the independent variables. (In this case ln(C), ln(D) and 1/T). Press OK to begin the regression. The regression data will be contained in a new worksheet. The variable labeled ‘intercept’ will be equal to the natural log of coefficient B. The remaining coefficients (c,d, and e) will be given as X Variable 1,X Variable 2 and X Variable 3 respectively. This process is quick and accurate for Excel 2002 and was used for all equations given in this report. Excel has to capability to handle one dependent variable and multiple independent variables. As many as 12,000 points were used in the regressions.

APPENDIX B

COMPLETE GRI-MECH VERSION 2.1 (REF. 10) CH4 MECHANISM USED

```
 &RTYPE   GLOBAL=.TRUE., GRONLY=.FALSE.,   &END
2.0O                   =  O2           M          1.200E+17 -1.000     .00
   THIRDBODY
H2      2.40        H2O       15.40     CH4         2.00     CO         1.75
CO2     3.60        C2H6      3.00      N2          0.83     END
   O           H       =  OH           M          5.000E+17 -1.000     .00
   THIRDBODY
H2      2.00        H2O       6.00      CH4        2.00      CO         1.50
CO2     2.00        C2H6      3.00      N2          0.5      END
   O           H2      =  H            OH         5.000E+04  2.670   6290.00
   O           HO2     =  OH           O2         2.000E+13   .000       .00
   O           H2O2    =  OH           HO2        9.630E+06  2.000   4000.00
   O           CH      =  H            CO         5.700E+13   .000       .00
   O           CH2     =  H            HCO        8.000E+13   .000       .00
   O           CH3     =  H            CH2O       8.430E+13   .000       .00
   O           CH4     =  OH           CH3        1.020E+09  1.500   8600.00
   O           CO      =  CO2          M          6.020E+14   .000   3000.00
   THIRDBODY
H2        2.00      O2        6.00      H2O        6.00      CH4        2.00
CO        1.50      CO2       3.50      C2H6       3.00      END
   O           HCO     =  OH           CO         3.000E+13   .000       .00
   O           HCO     =  H            CO2        3.000E+13   .000       .00
   O           CH2O    =  OH           HCO        3.900E+13   .000   3540.00
   O           CH2OH   =  OH           CH2O       1.000E+13   .000       .00
   O           CH3O    =  OH           CH2O       1.000E+13   .000       .00
   O           CH3OH   =  OH           CH2OH      3.880E+05  2.500   3100.00
   O           CH3OH   =  OH           CH3O       1.300E+05  2.500   5000.00
   O           C2H     =  CH           CO         5.000E+13   .000       .00
   O           C2H2    =  H            HCCO       1.020E+07  2.000   1900.00
   O           C2H2    =  OH           C2H        4.600E+19 -1.410  28950.00
   O           C2H2    =  CO           CH2        1.020E+07  2.000   1900.00
   O           C2H3    =  H            CH2CO      3.000E+13   .000       .00
   O           C2H4    =  CH3          HCO        1.920E+07  1.830    220.00
   O           C2H5    =  CH3          CH2O       1.320E+14   .000       .00
   O           C2H6    =  OH           C2H5       8.980E+07  1.920   5690.00
   O           HCCO    =  H         2.0CO         1.000E+14   .000       .00
   O           CH2CO   =  OH           HCCO       1.000E+13   .000   8000.00
   O           CH2CO   =  CH2          CO2        1.750E+12   .000   1350.00
   O2          CO      =  O            CO2        2.500E+12   .000  47800.00
   O2          CH2O    =  HO2          HCO        1.000E+14   .000  40000.00
   H           O2      =  HO2          M          2.800E+18  -.860        .00
   THIRDBODY
O2        .00       H2O        .00      CO          .75      CO2        1.50
C2H6      1.50      N2         0.0      END
   H         2.0O2     =  HO2          O2         3.000E+20 -1.720        .00
   H           O2      =  O            OH         8.300E+13   .000  14413.00
   H           H       =  H2           M          1.000E+18 -1.000        .00
   THIRDBODY
H2        .00       H2O        .00      CH4         2.00     CO2         .00
C2H6       3.00     N2         0.63     END
2.0H           H2      =2.0H2                      9.000E+16  -.600        .00
2.0H           H2O     =   H2           H2O        6.000E+19 -1.250        .00
```

```
2.0H           CO2     =   H2          CO2         5.500E+20 -2.000        .00
   H           OH      =   H2O         M           2.200E+22 -2.000        .00
   THIRDBODY
H2          .73     H2O        3.65       CH4         2.00     C2H6       3.00
N2          0.38    END
   H           HO2     =   O           H2O         3.970E+12   .000     671.00
   H           HO2     =   O2          H2          2.800E+13   .000    1068.00
   H           HO2     =2.0OH                      1.340E+14   .000     635.00
   H           H2O2    =   HO2         H2          1.210E+07  2.000    5200.00
   H           H2O2    =   OH          H2O         1.000E+13   .000    3600.00
   H           CH      =   C           H2          1.100E+14   .000        .00
   H           CH2     =   CH3         M           2.500E+16  -.800        .00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       N2         0.7        END
   H           CH3     =  CH4         M           1.270E+16  -.630     383.00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       N2         0.7        END
   H           CH4     =  CH3         H2          6.600E+08  1.620  10840.00
   H           HCO     =  CH2O        M           1.090E+12   .480    -260.00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       END
   H           HCO     =  H2          CO          7.340E+13   .000        .00
   H           CH2O    =  CH2OH       M           5.400E+11   .454    3600.00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       END
   H           CH2O    =  CH3O        M           5.400E+11   .454    2600.00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       END
   H           CH2O    =  HCO         H2          2.300E+10  1.050    3275.00
   H           CH2OH   =  CH3OH       M           1.800E+13   .000        .00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       END
   H           CH2OH   =  H2          CH2O        2.000E+13   .000        .00
   H           CH2OH   =  OH          CH3         1.200E+13   .000        .00
   H           CH3O    =  CH3OH       M           5.000E+13   .000        .00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       END
   H           CH3O    =  H           CH2OH       3.400E+06  1.600        .00
   H           CH3O    =  H2          CH2O        2.000E+13   .000        .00
   H           CH3O    =  OH          CH3         3.200E+13   .000        .00
   H           CH3OH   =  CH2OH       H2          1.700E+07  2.100    4870.00
   H           CH3OH   =  CH3O        H2          4.200E+06  2.100    4870.00
   H           C2H     =  C2H2        M           1.000E+17 -1.000        .00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       N2         0.7        END
   H           C2H2    =  C2H3        M           5.600E+12   .000    2400.00
   THIRDBODY
H2         2.00     H2O        6.00       CH4        2.00       CO         1.50
CO2        2.00     C2H6       3.00       N2         0.7        END
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   H           C2H3    =  C2H4        M          6.080E+12   .270      280.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      END
   H           C2H3    =  H2          C2H2       3.000E+13   .000         .00
   H           C2H4    =  C2H5        M          1.080E+12   .454     1820.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2        0.7       END
   H           C2H4    =  C2H3        H2         1.325E+06  2.530    12240.00
   H           C2H5    =  C2H6        M          5.210E+17  -.990     1580.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2        0.7       END
   H           C2H5    =  H2          C2H4       2.000E+12   .000         .00
   H           C2H6    =  C2H5        H2         1.150E+08  1.900     7530.00
   H           CH2CO   =  HCCO        H2         5.000E+13   .000     8000.00
   H           CH2CO   =  CH3         CO         1.130E+13   .000     3428.00
   H           HCCOH   =  H           CH2CO      1.000E+13   .000         .00
   H2          CO      =  CH2O        M          4.300E+07  1.500    79600.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      END
   OH          H2      =  H           H2O        2.160E+08  1.510     3430.00
   OH          OH      =  H2O2        M          7.400E+13  -.370         .00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2        0.7       END
2.0OH                  =  O           H2O        3.570E+04  2.400    -2110.00
   OH          HO2     =  O2          H2O        2.900E+13   .000     -500.00
   OH          H2O2    =  HO2         H2O        1.750E+12   .000      320.00
   OH          H2O2    =  HO2         H2O        5.800E+14   .000     9560.00
   OH          C       =  H           CO         5.000E+13   .000         .00
   OH          CH      =  H           HCO        3.000E+13   .000         .00
   OH          CH2     =  H           CH2O       2.000E+13   .000         .00
   OH          CH2     =  CH          H2O        1.130E+07  2.000     3000.00
   OH          CH3     =  CH3OH       M          6.300E+13   .000         .00
   THIRDBODY
H2         2.00     H2O       6.00      CH4       2.00      CO        1.50
CO2        2.00     C2H6      3.00      END
   OH          CH3     =  CH2         H2O        5.600E+07  1.600     5420.00
   OH          CH4     =  CH3         H2O        1.000E+08  1.600     3120.00
   OH          CO      =  H           CO2        4.760E+07  1.228       70.00
   OH          HCO     =  H2O         CO         5.000E+13   .000         .00
   OH          CH2O    =  HCO         H2O        3.430E+09  1.180     -447.00
   OH          CH3O    =  H2O         CH2O       5.000E+12   .000         .00
   OH          C2H     =  H           HCCO       2.000E+13   .000         .00
   OH          C2H2    =  H           CH2CO      2.180E-04  4.500    -1000.00
   OH          C2H2    =  C2H         H2O        3.370E+07  2.000    14000.00
   OH          C2H2    =  CH3         CO         4.830E-04  4.000    -2000.00
   OH          C2H3    =  H2O         C2H2       5.000E+12   .000         .00
   OH          C2H4    =  C2H3        H2O        3.600E+06  2.000     2500.00
   OH          C2H6    =  C2H5        H2O        3.540E+06  2.120      870.00
   OH          CH2CO   =  HCCO        H2O        7.500E+12   .000     2000.00
2.0HO2                 =  O2          H2O2       1.300E+11   .000    -1630.00
2.0HO2                 =  O2          H2O2       4.200E+14   .000    12000.00
   HO2         CH2     =  OH          CH2O       2.000E+13   .000         .00
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   HO2         CH3     =  O2          CH4         1.000E+12   .000        .00
   HO2         CH3     =  OH          CH3O        2.000E+13   .000        .00
   HO2         CO      =  OH          CO2         1.500E+14   .000   23600.00
   HO2         CH2O    =  HCO         H2O2        1.000E+12   .000    8000.00
   C           O2      =  O           CO          5.800E+13   .000     576.00
   C           CH2     =  H           C2H         5.000E+13   .000        .00
   C           CH3     =  H           C2H2        5.000E+13   .000        .00
   CH          O2      =  O           HCO         3.300E+13   .000        .00
   CH          H2      =  H           CH2         1.107E+08  1.790    1670.00
   CH          H2O     =  H           CH2O        1.713E+13   .000    -755.00
   CH          CH2     =  H           C2H2        4.000E+13   .000        .00
   CH          CH3     =  H           C2H3        3.000E+13   .000        .00
   CH          CH4     =  H           C2H4        6.000E+13   .000        .00
   CH          CO      =  HCCO        M           5.000E+13   .000        .00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2         0.7       END
   CH          CO2     =  HCO         CO          3.400E+12   .000     690.00
   CH          CH2O    =  H           CH2CO       9.460E+13   .000    -515.00
   CH          HCCO    =  CO          C2H2        5.000E+13   .000        .00
   CH2         O2      =  OH          HCO         1.320E+13   .000    1500.00
   CH2         H2      =  H           CH3         5.000E+05  2.000    7230.00
2.0CH2                 =  H2          C2H2        3.200E+13   .000        .00
   CH2         CH3     =  H           C2H4        4.000E+13   .000        .00
   CH2         CH4     =2.0CH3                     2.460E+06  2.000    8270.00
   CH2         CO      =   CH2CO       M           8.100E+11   .500    4510.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2         0.7       END
   CH2         HCCO    =   C2H3        CO          3.000E+13   .000        .00
   CH3         O2      =   O           CH3O        2.675E+13   .000   28800.00
   CH3         O2      =   OH          CH2O        3.600E+10   .000    8940.00
   CH3         H2O2    =   HO2         CH4         2.450E+04  2.470    5180.00
2.0CH3                 =   C2H6        M           2.120E+16  -.970     620.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2         0.7       END
2.0CH3                 =   H           C2H5        4.990E+12   .100   10600.00
   CH3         HCO     =   CH4         CO          2.648E+13   .000        .00
   CH3         CH2O    =   HCO         CH4         3.320E+03  2.810    5860.00
   CH3         CH3OH   =   CH2OH       CH4         3.000E+07  1.500    9940.00
   CH3         CH3OH   =   CH3O        CH4         1.000E+07  1.500    9940.00
   CH3         C2H4    =   C2H3        CH4         2.270E+05  2.000    9200.00
   CH3         C2H6    =   C2H5        CH4         6.140E+06  1.740   10450.00
   HCO         O2      =   HO2         CO          7.600E+12   .000     400.00
   CH2OH       O2      =   HO2         CH2O        1.800E+13   .000     900.00
   CH3O        O2      =   HO2         CH2O        4.280E-13  7.600   -3530.00
   C2H         O2      =   HCO         CO          5.000E+13   .000    1500.00
   C2H         H2      =   H           C2H2        4.070E+05  2.400     200.00
   C2H3        O2      =   HCO         CH2O        3.980E+12   .000    -240.00
   M           C2H4    =   H2          C2H2        8.000E+12   .440   88770.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00      CO        1.50
CO2        2.00     C2H6      3.00      N2         0.7       END
   C2H5        O2      =  HO2         C2H4        8.400E+11   .000    3875.00
   HCCO        O2      =  OH       2.0CO          1.600E+12   .000     854.00
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2.0HCCO                 =2.0CO           C2H2        1.000E+13   .000
.00
   N           NO        =   N2          O           3.500E+13   .000
330.00
   N           O2        =   NO          O           2.650E+12   .000
6400.00
   N           OH       =   NO          H           7.333E+13   .000    1120.00
   N2O         O        =   N2          O2          1.400E+12   .000   10810.00
   N2O         O        =2.0NO                      2.900E+13   .000   23150.00
   N2O         H        =   N2          OH          4.400E+14   .000   18880.00
   N2O         OH       =   N2          HO2         2.000E+12   .000   21060.00
   M           N2O      =   N2          O           1.300E+11   .000   59620.00
   THIRDBODY
H2         2.00     H2O       6.00       CH4        2.00      CO         1.50
CO2        2.00     C2H6      3.00       N2         0.625     END
   HO2         NO        =   NO2         OH          2.110E+12   .000    -
480.00
   NO          O        =   NO2         M           1.060E+20 -1.410         .00
   THIRDBODY
H2         2.00     H2O       6.00       CH4        2.00      CO         1.50
CO2        2.00     C2H6      3.00       END
   NO2         O        =   NO          O2          3.900E+12   .000    -240.00
   NO2         H        =   NO          OH          1.320E+14   .000     360.00
   NH          O        =   NO          H           5.000E+13   .000         .00
   NH          H        =   N           H2          3.200E+13   .000     330.00
   NH          OH       =   HNO         H           2.000E+13   .000         .00
   NH          OH       =   N           H2O         2.000E+09  1.200         .00
   NH          O2       =   HNO         O           4.610E+05  2.000    6500.00
   NH          O2       =   NO          OH          1.280E+06  1.500     100.00
   NH          N        =   N2          H           1.500E+13   .000         .00
   NH          H2O      =   HNO         H2          2.000E+13   .000   13850.00
   NH          NO       =   N2          OH          2.160E+13  -.230         .00
   NH          NO       =   N2O         H           4.160E+14  -.450         .00
   NH2         O        =   OH          NH          7.000E+12   .000         .00
   NH2         O        =   H           HNO         4.600E+13   .000         .00
   NH2         H        =   NH          H2          4.000E+13   .000    3650.00
   NH2         OH       =   NH          H2O         9.000E+07  1.500    -460.00
   M           NNH      =   N2          H           3.300E+08   .000         .00
   M           NNH      =   N2          H           1.300E+14  -.110    4980.00
   THIRDBODY
H2         2.00     H2O       6.00       CH4        2.00      CO         1.50
CO2        2.00     C2H6      3.00       N2         0.7       END
   NNH         O2       =   HO2         N2          5.000E+12   .000         .00
   NNH         O        =   OH          N2          2.500E+13   .000         .00
   NNH         O        =   NH          NO          7.000E+13   .000         .00
   NNH         H        =   H2          N2          5.000E+13   .000         .00
   NNH         OH       =   H2O         N2          2.000E+13   .000         .00
   NNH         CH3      =   CH4         N2          2.500E+13   .000         .00
   H           NO       =   HNO         M           8.950E+19 -1.320     740.00
   THIRDBODY
H2         2.00     H2O       6.00       CH4        2.00      CO         1.50
CO2        2.00     C2H6      3.00       N2         0.7       END
   HNO         O        =   NO          OH          2.500E+13   .000         .00
   HNO         H        =   H2          NO          4.500E+11   .720     660.00
   HNO         OH       =   NO          H2O         1.300E+07  1.900    -950.00
   HNO         O2       =   HO2         NO          1.000E+13   .000   13000.00
   CN          O        =   CO          N           7.700E+13   .000         .00
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   CN          OH       =   NCO         H          4.000E+13   .000        .00
   CN          H2O      =   HCN         OH         8.000E+12   .000    7460.00
   CN          O2       =   NCO         O          6.140E+12   .000    -440.00
   CN          H2       =   HCN         H          2.100E+13   .000    4710.00
   NCO         O        =   NO          CO         2.350E+13   .000        .00
   NCO         H        =   NH          CO         5.400E+13   .000        .00
   NCO         N        =   N2          CO         2.000E+13   .000        .00
   NCO         O2       =   NO          CO2        2.000E+12   .000   20000.00
   M           NCO      =   N           CO         8.800E+16  -.500   48000.00
   THIRDBODY

H2         2.00     H2O       6.00      CH4        2.00       CO         1.50
CO2        2.00     C2H6      3.00      N2         0.7        END
   NCO         NO       =   N2O         CO         2.850E+17 -1.520     740.00
   NCO         NO       =   N2          CO2        5.700E+18 -2.000     800.00
   M           HCN      =   H           CN         1.040E+29 -3.300
126600.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00       CO         1.50
CO2        2.00     C2H6      3.00      N2         0.7        END
   HCN         O        =   NCO         H          1.107E+04  2.640    4980.00
   HCN         O        =   NH          CO         2.767E+03  2.640    4980.00
   HCN         O        =   CN          OH         2.134E+09  1.580   26600.00
   HCN         OH       =   HOCN        H          1.100E+06  2.030   13370.00
   HCN         OH       =   HNCO        H          4.400E+03  2.260    6400.00
   HCN         OH       =   NH2         CO         1.600E+02  2.560    9000.00
   H           HCN      =   H2CN        M          1.400E+26 -3.400    1900.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00       CO         1.50
CO2        2.00     C2H6      3.00      N2         0.7        END
   H2CN        N        =   N2          CH2        6.000E+13   .000     400.00
   C           N2       =   CN          N          6.300E+13   .000   46020.00
   CH          N2       =   HCN         N          2.857E+08  1.100   20400.00
   CH2         N2       =   HCN         NH         1.000E+13   .000   74000.00
   C           NO       =   CN          O          1.900E+13   .000        .00
   C           NO       =   CO          N          2.900E+13   .000        .00
   CH          NO       =   HCN         O          5.000E+13   .000        .00
   CH          NO       =   H           NCO        2.000E+13   .000        .00
   CH          NO       =   N           HCO        3.000E+13   .000        .00
   CH2         NO       =   H           HNCO       3.100E+17 -1.380    1270.00
   CH2         NO       =   OH          HCN        2.900E+14  -.690     760.00
   CH2         NO       =   H           HCNO       3.800E+13  -.360     580.00
   CH3         NO       =   HCN         H2O        9.600E+13   .000   28800.00
   CH3         NO       =   H2CN        OH         1.000E+12   .000   21750.00
   HNCO        O        =   NH          CO2        9.800E+07  1.410    8500.00
   HNCO        O        =   HNO         CO         1.500E+08  1.570   44000.00
   HNCO        O        =   NCO         OH         2.200E+06  2.110   11400.00
   HNCO        H        =   NH2         CO         2.250E+07  1.700    3800.00
   HNCO        H        =   H2          NCO        1.050E+05  2.500   13300.00
   HNCO        OH       =   NCO         H2O        4.650E+12   .000    6850.00
   HNCO        OH       =   NH2         CO2        1.550E+12   .000    6850.00
   M           HNCO     =   NH          CO         1.180E+16   .000   84720.00
   THIRDBODY
H2         2.00     H2O       6.00      CH4        2.00       CO         1.50
CO2        2.00     C2H6      3.00      N2         0.7        END
   HCNO        H        =   H           HNCO       2.100E+15  -.690    2850.00
   HCNO        H        =   OH          HCN        2.700E+11   .180    2120.00
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   HCNO        H       =   NH2         CO         1.700E+14  -.750    2890.00
   HOCN        H       =   H           HNCO       2.000E+07  2.000    2000.00
   HCCO        NO      =   HCNO        CO         2.350E+13   .000        .00
   CH3         N       =   H2CN        H          6.100E+14  -.310     290.00
   CH3         N       =   HCN         H2         3.700E+12   .150     -90.00
   NH3         H       =   NH2         H2         5.400E+05  2.400    9915.00
   NH3         OH      =   NH2         H2O        5.000E+07  1.600     955.00
   NH3         O       =   NH2         OH         9.400E+06  1.940    6460.00
   NH       +  NO      =   N2      +   OH          2.00E+15   -.8       0.

    H            O2            H2O      =    HO2           H2O
1.         1.          1.       9.380E+18 -.760         .00
    H            O2            N2       =    HO2           N2
1.         1.          1.       3.750E+20 -1.720       .00
    OH           CH2           OH       =    H2O           CH2O
1.         1.          1.       5.000E+12  .000         .00
    OH           CH3           OH       =    CH2           OH           H2O
1.         1.          1.       1.440E+06  2.000    -840.00
    OH           CH3           OH       =    CH3O          H2O
1.         1.          1.       6.300E+06  2.000    1500.00
                 HCO           H2O      =    H             CO           H2O
            1.          1.      2.244E+18 -1.000    17000.00
                 NCO           OH       =    NO            H            CO
            1.          1.      2.500E+12   .000         .00
                 NCO           OH       =    NO            H            CO
            1.          1.      2.500E+12   .000         .00
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APPENDIX C

MODIFICATIONS TO GLSENS FOR WATER INJECTION

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C  WATER INJECTION MODIFICATION FOR CH4 TO SUBROUTINE INIT
15     IF (FUEL.EQ.BLANK) GO TO 80
C   SPECIAL COMPOSITION INPUT
       DO 20 J=1,NRS
       IF (FUEL.NE.DSPNM(J)) GO TO 20
       JFUEL=J
       GO TO 30
20     CONTINUE
       WRITE (LWRITE,25) FUEL
25     FORMAT(//,7H0(INIT),5X,'***** WARNING: INPUT FUEL NAME "',A8,
      1 '" IS NOT IN REACTANT LIST *****',//)
       NEXT=.TRUE.
       RETURN
   30 IF (ERATIO.NE.0.) GO TO 35
       IF (FLAIR.EQ.0.) GO TO 80
C  FUEL-OXIDANT MASS RATIO SPECIFIED
       TERM1 = AIRMW*FLAIR/MW(JFUEL)
       FRO2 = 1.0/(1.0 + NOXRAT + ARAT + CRAT)
       TERM2 = 1.0/(1.0 + TERM1)
       CONCO2 = DBLE(FRO2*TERM2)
       GO TO 40
C  FUEL-OXIDANT EQUIVALENCE RATIO SPECIFIED
   35 H2OMF=H2OF*16./18.
       TERM1 = 4.0*ERATIO*(1.+H2OMF)
       TINP = 4.0*SCC + SCH - 2.0*SCOX
       ERAT=ERATIO
       TERM2 = 1.0 + NOXRAT + ARAT + CRAT
       FRO2 = 1.0/TERM2
       TERM2 = 1.0/(TERM1 + TINP*TERM2)
       CONCO2 = DBLE(TINP*TERM2)
C
   40 IF (MOLEF) GO TO 42
C  WARNING: MOLEF = .FALSE. FOR SIMPLIFIED COMPOSITON INPUT.
C            SET MOLEF = .TRUE.
       MOLEF = .TRUE.
       WRITE (LWRITE,41)
   41 FORMAT(//,7H0(INIT),5X,'**** WARNING: SIMPLIFIED COMPOSITION ',
      1 'INPUT USED BUT MOLEF SET EQUAL TO .FALSE. IN NAMELIST START',/,
      2 30X,'MOLEF HAS BEEN SET EQUAL TO .TRUE. ****',//)
C    SIGMA = MOLES/GRAM MIXTURE
   42 SIGMA(JFUEL) = DBLE((TERM1*TERM2)/(dble(1.+H2OMF)))
       DO 45 I = 1,LS
       IF (O2.NE.DSPNM(I)) GO TO 45
       SIGMA(I) = CONCO2
       GO TO 50
45     CONTINUE
50     SIGMA(27) =SIGMA(JFUEL)*DBLE(H2OMF)
       DO 55 I = 1,LS
       IF (N2.NE.DSPNM(I)) GO TO 55
       SIGMA(I) = DBLE(NOXRAT)*CONCO2
       GO TO 60
55     CONTINUE
```

```
60     DO 65 I = 1,LS
       IF (AR.NE.DSPNM(I)) GO TO 65
       SIGMA(I) = DBLE(ARAT)*CONCO2
       GO TO 70
65     CONTINUE
70     DO 75 I = 1,LS
       IF (CO2.NE.DSPNM(I)) GO TO 75
       SIGMA(I) = DBLE(CRAT)*CONCO2
       GO TO 80
75     CONTINUE
C
   80    READ (LDAT,85) DSP,TINP
```

Additional equations specific to the program.

$$Term2 = \frac{1}{Term1 + TINP + Term2} \tag{C1}$$

$$conc\ O_2 = y_{O_2} = \frac{TINP * 1}{Term2} \tag{C2}$$

$$y_f = \frac{4Eratio}{4n_C + n_H - 2n_O} * y_{O_2} = \frac{Term1}{TINP} * TINP * Term2 \tag{C3}$$

$$yH2O = y_{fuel} * H2OF * \frac{167}{18} \tag{C4}$$

$$y_{N_2} = \eta_{N_2} * y_{O_2} \tag{C5}$$

let y_{Ar}=0.0, and y_{CO2}=0.0

APPENDIX D

MODIFICATIONS TO OUT2 OF GLSENS FOR OBTAINING OUTPUT FOR THE CH4 COMPUTATIONS

```
C      ALREADY DONE IN DIFFUN
C  ch4.f dec 14,2003
420   foa=eratio*0.059
      tn=timil
      trr=sngl(T)
418 if(time.gt.0.)goto 427
      write(10,1)
    1 format(' TITLE= P atm  T K  f/a   conc fuel   co       nox
     3coequil  time ')
C     calculate the initial conditions for the averaging
      write(11,417)ch4e
  417 format('  ch4e ',e13.4)
      nc=1
      nco=1
      t0=0.
      stco=0.
      areaf=0.
      tauf=0.
      tauco=0.
      tauno=0.
      areaco=0.
      areano=0.
      atauf=0.
      atauco=0.
      atauno=0.
  427 continue
      cco=sngl(dabs(prc(9)))
      cnox=sngl(dabs(prc(31)+2.d0*prc(33)+prc(34)))
      xnox=sngl(prc(31)/(prc(31)+2.d0*prc(33)+prc(34)))
      cfuel=sngl(dabs(prc(14)))
C     write(10,423)nc,P,T,foa,cfuel,cco,cnox,ccoe,
C    1timil
  423 format(i4,f5.1,f8.1,1p,8e10.3)
C  Begin Step One calculations
C     calculate the initial conditions for the averaging
      if(nc.lt.2)goto 1500
      if(nc.eq.2)tstart=timil
      if(nc.eq.2)t0=timil
      O2=sngl(prc(2))
      if(nc.eq.2)taufo=-sngl(prc(14)/W(14))*1.e3
C     if(nc.eq.2)edd=15.*taufo
      if(tn.eq.t0)goto 424
      if(W(14).ne.0.)tauf=-sngl(prc(14)/W(14))*1.e3
      if(tauf.le.0.)goto 424
C     if(cfuel.lt.1.e-25)goto 424
      areaf=areaf+(1./taufo+1./tauf)/2.*(tn-t0)
      timet=timil-tstart
      atauf=timet/areaf
      if(nc/10*10.eq.nc)write(11,423)nc,P,T,foa,cfuel,O2,tauf,atauf,
     1timil
      taufo=tauf
```

```
  424 if(nc.eq.2)tauni=sngl(1.D0/(W(31)+2.d0*W(33)+W(34)))*1.e3
      tauno=sngl(1.D0/(W(31)+2.d0*W(33)+W(34)))*1.e3
      if(t0.eq.tn)goto 339
      if(tauno.lt.0.)go to 339
      areano=areano+(1./tauno+1./tauni)/2.*(tn-t0)
      atauno=timet/areano
      tauni=tauno
      xrate=sngl(W(31)+2.d0*W(33)+W(34))
      if((nc/10*10).eq.nc)write(13,501)nc,P,T,xrate,cnox,tauno,xnox,
     1atauno,eratio,timil
  339 denm=sngl(w(15))
      cco2=sngl(prc(15))
C     if(w(15).lt.0.)next=.true.
      if(nc.eq.2)tauci=(sngl(dabs(prc(9))))/denm*1.e3
      tauco=(sngl(dabs(prc(9))))/denm*1.e3
      if(t0.eq.tn) goto 504
      if(tauco.le.0.)goto 503
C     if(stco.eq.0.)stco=timil
      timco=timil
      rfuel=cfuel/tauf*1.e3
      areaco=areaco+(1./tauco+1./tauci)/2.*(tn-t0)
      atauco=timco/areaco
      tauci=tauco
      nco=nco+1
  338 format(i7,1p8e11.3)
      rfuel2=sngl(w(14))
      dcodt=-((sngl(prc(9)))-ccoe)/tauco*1.e3
  503 if((nc/10*10).eq.nc)write(12,423) nc,P,T,foa,cco,ccoe,tauco,
     1atauco,timil
      if(nco.lt.100)write(15,338)nc,timco,tauci,tauco,atauco,areaco
  504 t0=tn
  431 format (f12.2,3e13.5,f8.3,f8.3,e13.5)
  501 format(i4,f7.4,f7.1,4e12.5,f6.3,f9.3)
C  Begin step Two calculations
      pl=log(P)
      tol=1./T
      h2ol=prc(27)
      h2osl=sngl(prc(27))
      h2ol=dlog(prc(27))
C     if(cfuel.lt.1.e-20)cfuel=1.e-20
      fo=log(cfuel)
      fo2=sngl(prc(2))
      fo2l=log(fo2)
      tal=log(tauf)
      talc=log(tauci)
      taln=log(tauni)
      if(nc.eq.2)tolo=log(tfop)
      if( nc.gt.2)tolo=timil
      if(cfuel.le.1.e-24)goto 902
  425 format(i6,1p9e11.3)
C output fuel times
      write(26,900)foa,h2of,pl,tol,fo,fo2l,h2ol,tal,tolo
  900 format(2f7.3,1p,9e11.3)
  902 tal=log(tauci)
      if(cco.lt.1.e-20)goto 903
      col=log(cco)
      tolo=log(tcop)
```

```
      if(nc.gt.2) tolo=timil
C Output co times and concentrations
      write(27,900)foa,h2of,pl,tol,fo,col,fo2l,h2ol,tal,tolo
  903 continue
      tal=log(tauni)
      tolo=log(tnop)
      if(nc.gt.2) tolo=timil
C  output nox times and concentrations
     write(28,900)foa,h2of,pl,tol,fo,fo2l,h2ol,tal,tolo
 1500 nc=nc+1
C     if(nc.gt.4000)next=.true.
C     if(nc.gt.50)next=.true.
      if (timil.gt.1.)go to 502
      DO 435 IJ=1,MAX
      IF (IJ.GT.LS.OR.IJ.GT.LR) GO TO 435
      TCON(IJ)=SNGL(PRC(IJ)/W(IJ))
      FMOL=SNGL(SIGMA(IJ)*MIXMW)
      WRITE (LWRITE,175) DSPNM(IJ),PRC(IJ),FMOL,W(IJ)
      GO TO 435
430   WRITE (LWRITE,185) IJ,RATE(IJ),PRX(IJ),EQUIL(IJ)
C430    continue
435   CONTINUE
```

APPENDIX E

RUN INPUT FOR GLSENS

```
Run input for Jet-A for GLSENS TYPICAL FOR STEP ONE
TIME      PRESSURE                      C12H23
 &prob TCON=.TRUE.,CT0=1.0,
 IPRINT=1,end=1.e-2,,&end
 &start time=0.,ERATIO=0.3,SCC=12.0,SCOX=0.,SCH=23.,
 NOXRAT=3.76,ARAT=0.,CRAT=0.,T=1000.,H2OF=0.&end
END
 &solver mxstep=2000.,emax=1.e-13,atolsp=1.e-13,maxstp=190000,&end
INIT
ALLSP     END
SENSVAR
ALLSP     END
REAC
FINIS
   RUN INPUT FOR JET-A FOR GLSENS TYPICAL FOR STEP TWO
REPEAT  MECHANISM
TIME      PRESSURE                      C12H23
 &prob TCON=.TRUE.,CT0=1.0,
 PRINT=5.e-5,1.e-4,1.5e-4,2.e-4,2.5e-4,
 3.e-4,4.e-4,5.e-4,1.e-3,1.5e-3,2.e-3,2.5e-3,3.e-3,3.5e-3,4.e-3,
 4.5e-3,5.e-3,5.5e-3,6.0e-3,&end
 &start time=0.,ERATIO=0.3,SCC=12.0,SCOX=0.,SCH=23.,
 NOXRAT=3.76,ARAT=0.,CRAT=0.,T=1000.,H2OF=0.0&end
END
 &solver mxstep=2000,emax=1.e-13,atolsp=1.e-13,maxstp=190000,&end
INIT
ALLSP     END
SENSVAR
ALLSP     END
REAC
FINIS
```

```
RUN INPUT FOR CH4 FOR GLSENS TYPICAL FOR STEP ONE
TIME      PRESSURE                      CH4
 &prob TCON=.TRUE.,CT0=1.0,
 IPRINT=1,end=5.e-4,,&end
 &start time=0.,ERATIO=0.4,SCC=1.0,SCOX=0.,SCH=4.,
 NOXRAT=3.76,ARAT=0.,CRAT=0.,T=1000.,H2OF=0.&end
END
 &solver mxstep=2000.,emax=1.e-15,atolsp=1.e-15,maxstp=190000,,&end
INIT
ALLSP     END
SENSVAR
ALLSP     END
REAC
FINIS
    RUN INPUT FOR CH4 FOR GLSENS TYPICAL FOR STEP TWO
TIME      PRESSURE                      CH4
 &prob TCON=.TRUE.,CT0=1.0,
 PRINT=5.e-6,1.e-5,2.5e-5,5.e-5,1.e-4,1.5e-4,2.e-4,2.5e-4,
```

```
 3.e-4,4.e-4,5.e-4,1.e-3,1.5e-3,2.e-3,2.5e-3,3.e-3,3.5e-3,4.e-3,
 4.5e-3,5.e-3,5.5e-3,6.0e-3,&end

 &start time=0.,ERATIO=0.3,SCC=1.0,SCOX=0.,SCH=4.0,
 NOXRAT=3.76,ARAT=0.,CRAT=0.,T=1000.,H2OF=0.0,&end
END
 &solver mxstep=20000,emax=1.e-14,atolsp=1.e-14,maxstp=300000,  &end
ALLSP     END
SENSVAR
ALLSP     END
REAC
FINIS
```

APPENDIX F

FORTRAN CODE FOR TANKS IN SERIES CALCULATION

```
C  IN FIGURE 8 OUTPUT THE PPM AS A FUNCTION OF TEMPERATURE AND COMPUTE
c EACH PHIN TO KEEP TEMPERATURE CONSTANT AS H INCREASES
C methane
C  H=h/a t=time
C  set up maximum reactors to be eight in series
C pf=f/a fraction in reactor, t=time milliseconds
   DIMENSION pf(8),t(8),TT(8),EFT(8),TAUF(8),TCO(8),TNOX(8),tim(8)
   DIMENSION fa(8),COE(8),rnox(10),hn(5),melissa(5)
   data pf/1.5,1.2,1.0,5*0./
   data t/1.,1.5,2.5,5*0.5/
   REAL NOX,melissa
      open(5,file='fort.5',form='formatted')
      open(10,file='fort.10',form='formatted')
      open(11,file='fort.11',form='formatted')
      open(12,file='fort.12',form='formatted')
      open(13,file='fort.13',form='formatted')
      open(14,file='fort.14',form='formatted')
   open(15,file='fort.15',form='formatted')
      write(12,111)
C 111 format(' h2o  phi  h2o/f  eftt  tt(4)  ppmco  ',
 111 format(' phi ',8X, 'h2o', 2X 'T4 ',9x,'O2    O2COR ',
   1'  ppmno,  cwcd')
   T3=700.
   P=200./14.696
C   read(5,5)p3,T3,pf,t
  5 format(2e10.3,/,8f5.2,/8f5.3)
c     p=p3/14.696
      WRITE(10,7)P,T3,((PF(I),T(I)),I=1,4)
      WRITE(13,7)P,T3,((PF(I),T(I)),I=1,4)
  7 FORMAT(' P=',F5.2,' T3= ',F5.0,/,' PF,T=',2(2F5.2' : ')/2(2F5.2' :
   1'),/,3x,'TEMP F  H=0.0   H=0.05  H=0.1   H=0.15 ')
   WRITE(15,7)P,T3,((PF(I),T(I)),I=1,4)
   WRITE(10,8)
  8 FORMAT(6x,'IR   h   FA(IR)  T4(IR)   EFF     nox
   1 Ttnox  TAUNOX')
   PHI=0.2
   DO 11 IP=1,8
   PHI=PHI+0.1
      H=-0.05
      DO 1 IH=1,4
   H=H+0.05
   PHIN=PHI
   DO 36 IX=1,10
  36  PHIN=PHI*(1.+H/(PHIN*0.059))**0.1586
C     WRITE(10,37)IX,PHIN,PHI,H
  37 FORMAT(I5,3F11.4)
      pf(1)=1./phin
   if(phin.ge.1.)write(13,17) Phi, Phin,H
  17 format(' phi=',e12.4,'phin=',e12.4,' h ',e12.4)
      if(PHIN.GT.1.) go to 500
      CO=0.
   NOX=0.
```

```
C  ITERATE TO SOLVE FOR T4 FOR EACH REACTOR, IR= CONDITIONS FOR EACH REACTOR.
(NO)
   tim(1)=0.
      DO 30 IR=1,3
      tim(ir)=tim(ir)+t(ir)
   FA(ir)=PHIN*0.059*PF(IR)
   If(fa(ir).gt.0.059)fa(ir)=0.059
   HF=H/FA(ir)
      IF(HF.GT.2.5)HF=2.5
   EFF=100.00
   EFTT=100.
      itI=0
C   DO 40 IT4=1,10
      itI=itI+1
C  EFTT= TOTAL INEFFICIENCY
   EFFO=EFF
C DO NOT USE RICH CORRELATIONS HERE AS RESULTS FLUCTUATE - NOT PHYSICAL
   IF(fa(ir).GT.0.0592) GO TO 66
C   DO LEAN CORRELATIONS
      T4E=457.*(T3)**0.258*FA(ir)**0.435*(1.+HF)**(-.069)*(P)
   1**0.00284*0.059**(-.435)
       eff=100.
   T4=T3+(T4E-T3)*EFF/100.
   TAUF(IR)=2.09e-4*FA(ir)**0.222*(1.+HF)**0.0675*P**(-1.07)*
   1EXP(22625./T4)
   TCO(IR)=9.99E-4*FA(ir)**(0.101)*(1.+HF)**.0959*p**(-1.00)*
   1EXP(2434./T4)
   TNOX(IR)=2.94E4*fa(ir)**.032*(1.+HF)**.329*p**(-2.1)*
   1EXP(34859./T4)
   COE(IR)=15569.*fa(ir)**1.90*(1.+HF)**.00705*P**(-.477)*
   1EXP(-33388./T4)*0.059**1.90
   goto 40
C   DO RICH CORRELATIONS
  66 T4E=859.*T3**0.176*fa(ir)**(-0.559)*(1.+HF)**(-0.146)*P**
   1(.00167)*0.059**.559
   T4=T3+(T4E-T3)*EFF/100.
   TAUF(IR)=2.74e-2*fa(ir)**.111*(1.+HF)**(-.829)*P**(-0.328)*
   1EXP(14216./T4)
   TCO(IR)=1.3E-3*fa(ir)**(.215)*(1.+HF)**(.195)*p**(-1.0)
   1*EXP(2433./T4)
   TNOX(IR)=43928.*fa(ir)**(.284)*(1.+HF)**.641*P**(-2.0)
   1*EXP(32649./T4)
   COE(IR)=5.3E-2*fa(ir)**2.55*(1.+HF)**(-.358)*P**(-.00393)*
   1EXP(-31365./T4)*0.059**(-2.55)
C   EFF EQUALS THE EFFICIENCY OF EACH REACTOR
C   IF CHANGE IN EFFICIENCY IS LESS THAN 0.1 ITS CONVERGED
C  67 EFF=(1.-EXP(-tim(IR)/TAUF(IR)))*100.
C   IF(ABS(EFF-EFFO).LT.0.01)GO TO 41
C     WRITE(10,96)IR,iTI,fa(ir),T4,EFF
  40 CONTINUE
  96 FORMAT(' IR= ',I10,' itI ',i4,' fa ',e10.3,' T4 ',F7.2,F7.2)
  41 TT(IR)=T4
      EFT(IR)=EFF
   FAE=fa(ir)*EFF/100.
      XFO=FAE/(FAE*(1.+HF*16./29.)+16./29.)
   FO=XFO*P/82.056/T4
   eftt=eftt*(100.-eff)
```

```
C     write(10,97) ir,phi,hf
  97 format(' ir ',i5,' phi ',f10.3,' hf ',f8.3)
 100 FORMAT(2X,4e12.4)
c CALCULATE CO FOR EACH REACTOR
   TTF=T(IR)/TAUF(IR)
   TTCO=T(IR)/TCO(IR)
   EXCO=EXP(-TTCO)
   TTAUF=T(IR)/TAUF(IR)
      FOT=FO*TTAUF/(TTCO-TTAUF)
      if(ir.eq.1)CO=COE(IR)-EXCO*COE(IR)+FOT*(EXP(-TTAUF)-EXCO)
      irb=ir
      IF(IR.GT.1)irb=ir-1
   CO=CO*FA(IR)/FA(IRB)*(1.+fa(irb)*29./16.)/(1.+fa(ir)*29./16.)
   IF(IR.GT.1)CO=COE(IR)+(CO-COE(IR))*EXCO+FOT*(EXP(-TTAUF)-EXCO)
C CACULATE NOX FOR EACH REACTOR
   TTNOX=T(IR)/TNOX(IR)
      IF(IR.EQ.1)nox=nox+TTnox
      NOX=NOX*FA(IR)/FA(IRB)*(1.+fa(irb)*29./16.)/(1.+fa(ir)*29./16.)
      IF(IR.GT.1)nox=nox+TTnox
      phio=fa(ir)/0.059
      WRITE(10,99)IR,IP,H,phio,T4e,EFF,NOX,TTNOX,TNOX(IR)
  99 FORMAT(' *',2I4,2F8.4,2F9.2,1P6E10.2)
 110 rnox(ih)=nox*1.e6*82.056*t4/p
      write(11,98)ir,PHIO,t(ir),ttf,ttco,CO,COE(IR),T4
  98 format(i3,1p7e10.2)
C END OF INDIVIDUAL REACTOR SEGMENT
  30 continue
 113 format(2x,f9.3,1p5e11.3)
   CWCD=(PHIN+(2.+(16./18.)*(HF)*PHIN)+(1.-PHIN)*2+(2.*79./21.))/
      1(PHIN+(1.-PHIN)*2.+(2.*79./21.))
   RHO=P/82.056/TT(3)
   O2=(1.-PHIN)*2.*phin/(9.524-phin)
   if(O2.lt.0.)O2=0.
   O2COR=5.9/(20.9-100.*O2)
   PPMCO=CO*1.E6/RHO*O2COR
   PPMCO=PPMCO*CWCD
   PPMNO=NOX*1.E6/RHO*O2COR
   PPMNO=PPMNO*CWCD
   hn(ih)=ppmno
      melissa(ih)=ppmco
   write(12,102)phi,hf,tt(3),o2,o2cor,ppmno,cwcd
 102 format(2f8.3,f7.1,f8.3,1p3e10.2)
c     write(13,113)phi,(rnox(ir),ir=1,4)
  1 continue
   Tf=tt(3)*1.8-460.
   write(13,113)tf,(hn(in),in=1,4)
      write(14,113)tf,(rnox(in),in=1,4)
      write(15,113)tf,(melissa(in),in=1,4)
  11 continue
 500  stop
      End
```

APPENDIX G

FORTRAN CODE FOR MODEL SIMULATION OF GLSENS CONSTANT TEMPERATURE AND PRESSURE PLUG FLOW REACTOR

```
C Moder Ch4 reaction
   OPEN(6,FILE='MELISSA.OUT',FORM='FORMATTED')
   foa=0.05263
      TK=2000.
   P=2.
      rho=P/82.056/TK
      yfo=foa/(foa+16./29.)
      fo=yfo*rho
C Step one equation - lean
      tauf1=2.09e-4*P**(-1.07)*foa**(0.222)*exp(22625./TK)
      TMIN=-TAUF1*LOG(1.-1.E-20/2./FO)
      WRITE(6,1)TMIN,TAUF1,fo
  1 FORMAT(' TMIN MS ',E12.4,' TAUF1 MS ',E12.4,' fo ',e12.4)
   write(6,2)
  2 format(8X,' TIME SEC  FUEL    H2O     TAUF MS  ')
C  CH4+2.O2=CO2+2.H2O
   NT=0
   F=FO
      H2O=0.
      TIME=0.
      TAUF=TAUF1
      DTIME=1.E-5
      DO 6 IT=1,50000
      TIME=TIME+DTIME
      DF=F*DTIME/TAUF
      F=F-DF
      H2O=H2O+2*DF
C step two equation
      IF(H2O.GT.1.E-20)TAUF=3.5E-9*P**(-0.0713)*F**(-0.307)*
   2H2O**(-0.465)*(1.+H2O/F)**(-0.221)*EXP(14149/TK)
       TSEC=TIME*1.E-3
      NT=NT+1
       IF (IT/100*100.EQ.IT)WRITE(6,10)NT,TSEC,F,H2O,TAUF
  10 FORMAT(I8,1P4E12.4)
  6 CONTINUE
   STOP
      END
```

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10. GRI-Mech Version 2.1 released 9/6/95 http:/www.gri.org/tech/res/

Figure 1
Magnussen Mixing Model

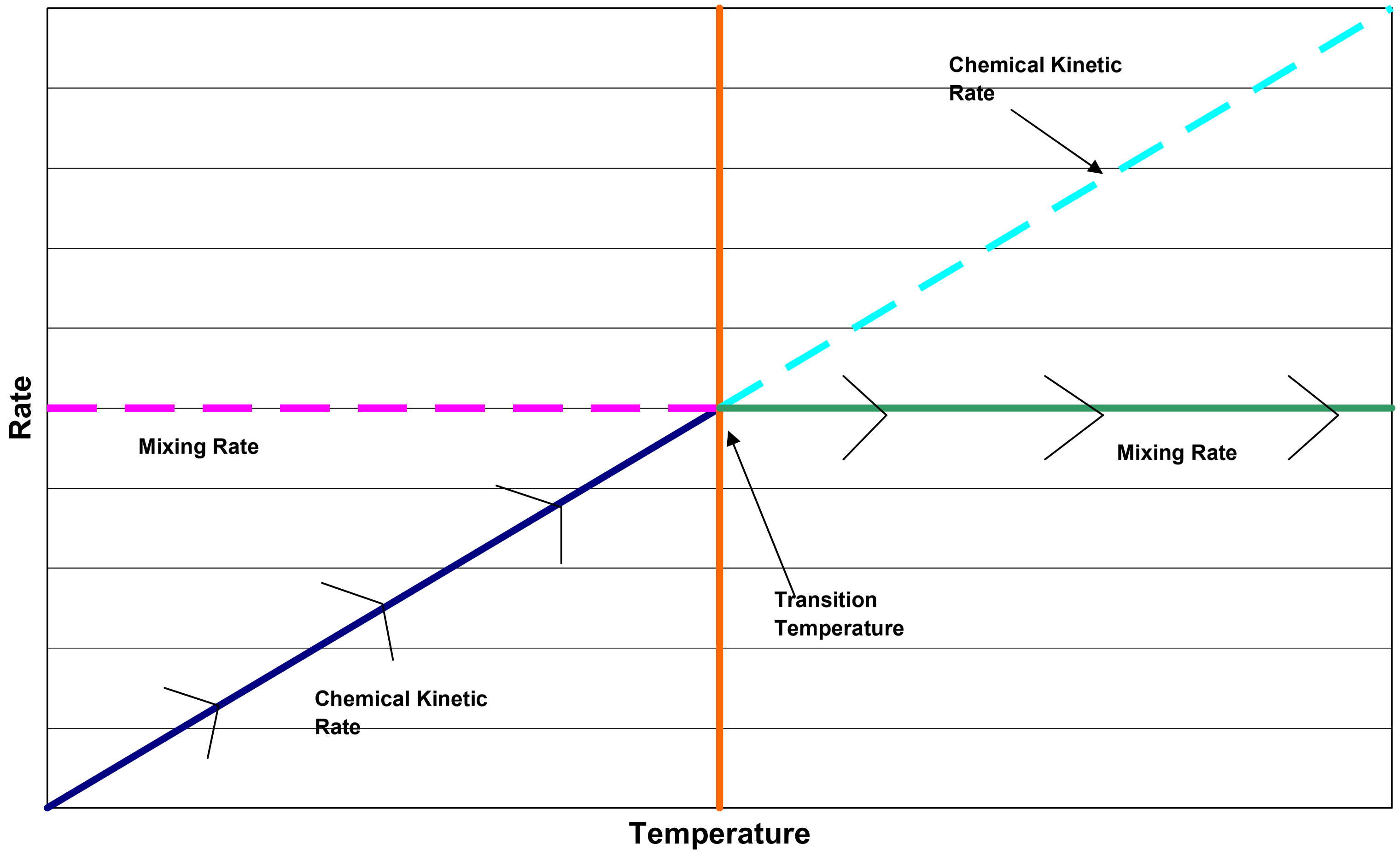


Figure 2

Equilibrium Jet A Water Injection COeq Parity

0.2< Eratio≤1.0

(lean)

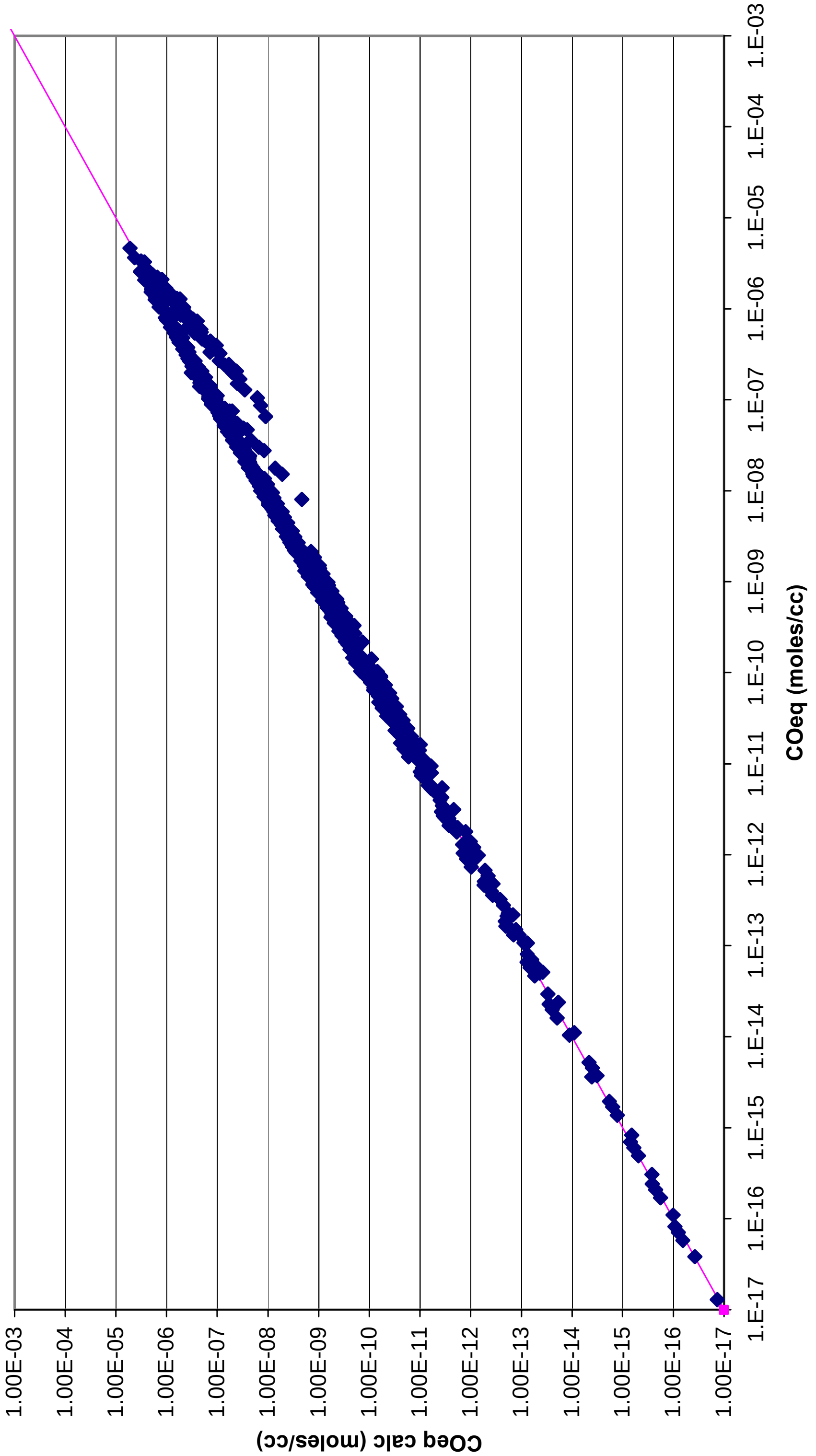


Figure 3
Kinetic Jet-A Water Injection Fuel Tau Parity
Step One
(lean)

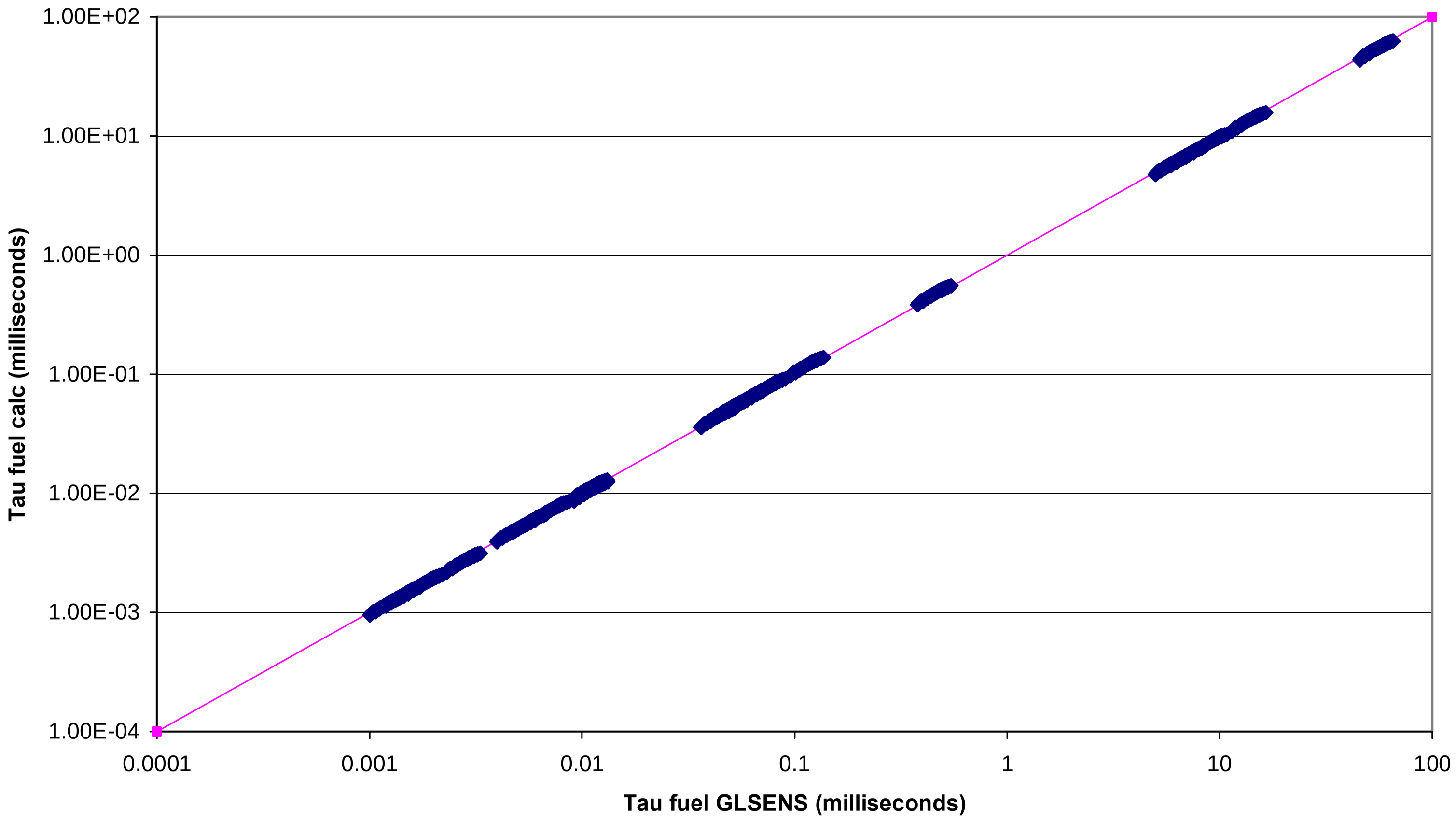


Figure 4
Kinetic Jet-A Water Injection CO Tau Parity
Step One
(lean)

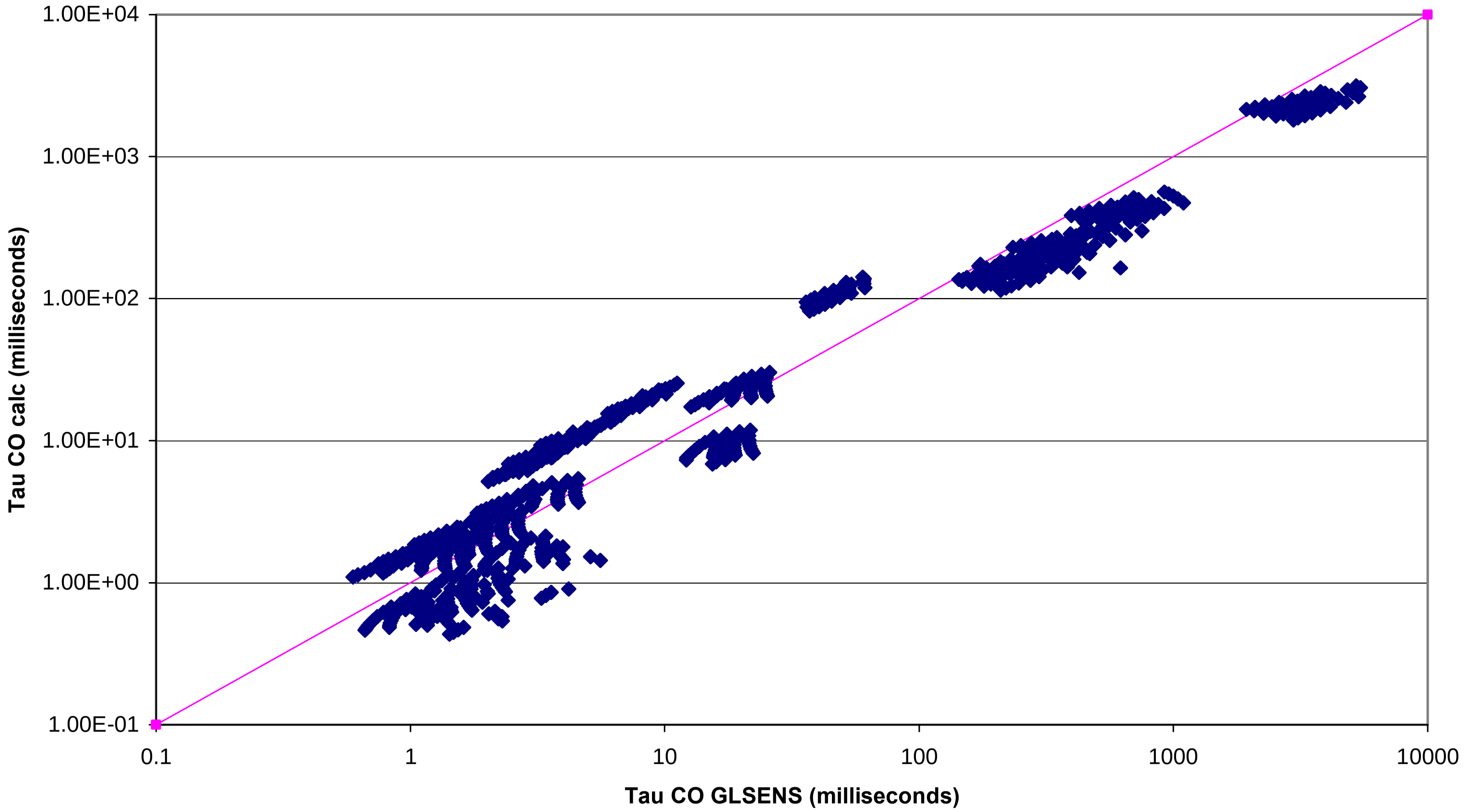


Figure 5
Kinetic Jet-A Water Injection Nox Tau Parity
Step One
(lean)

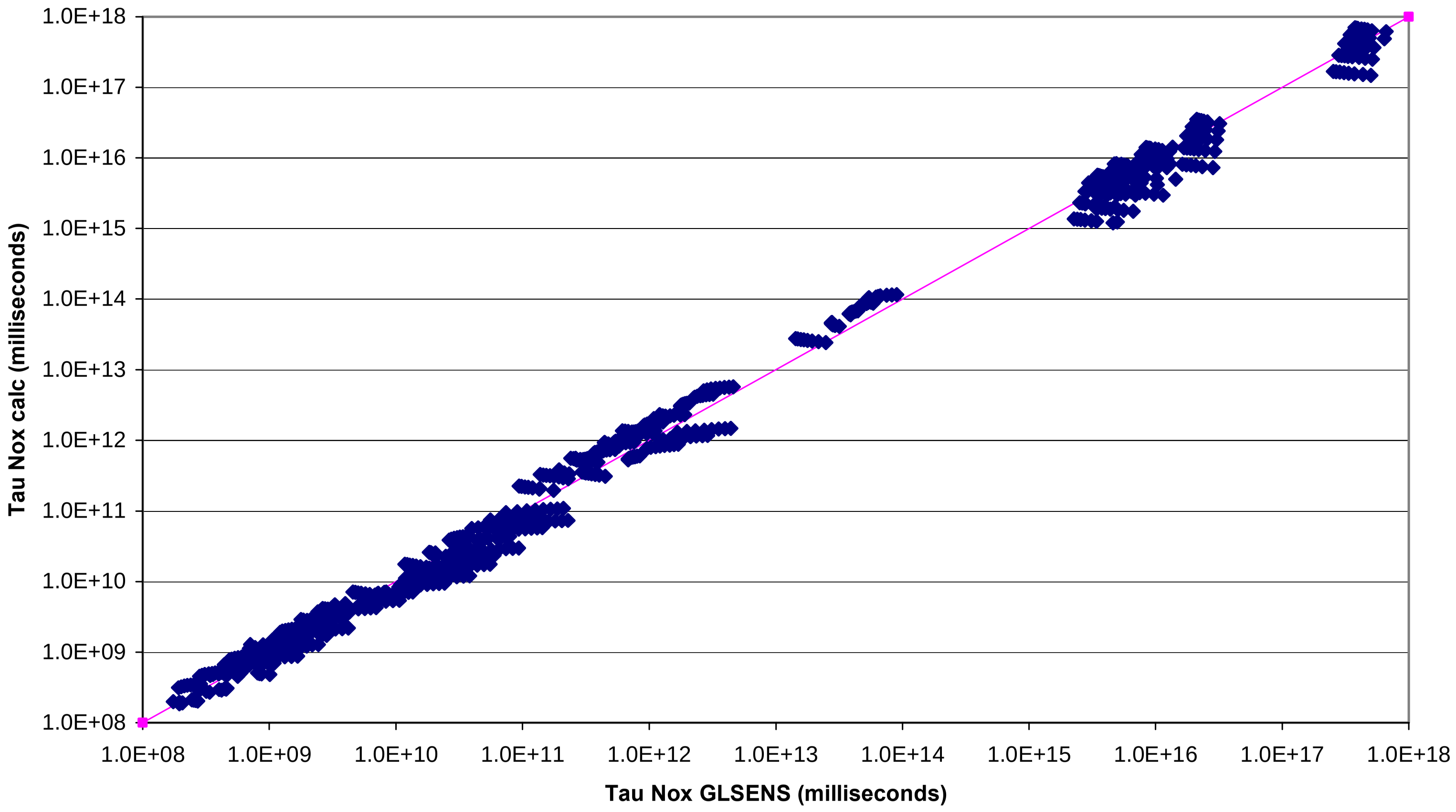


Figure 6
Jet-A Fuel Step One Lean Model

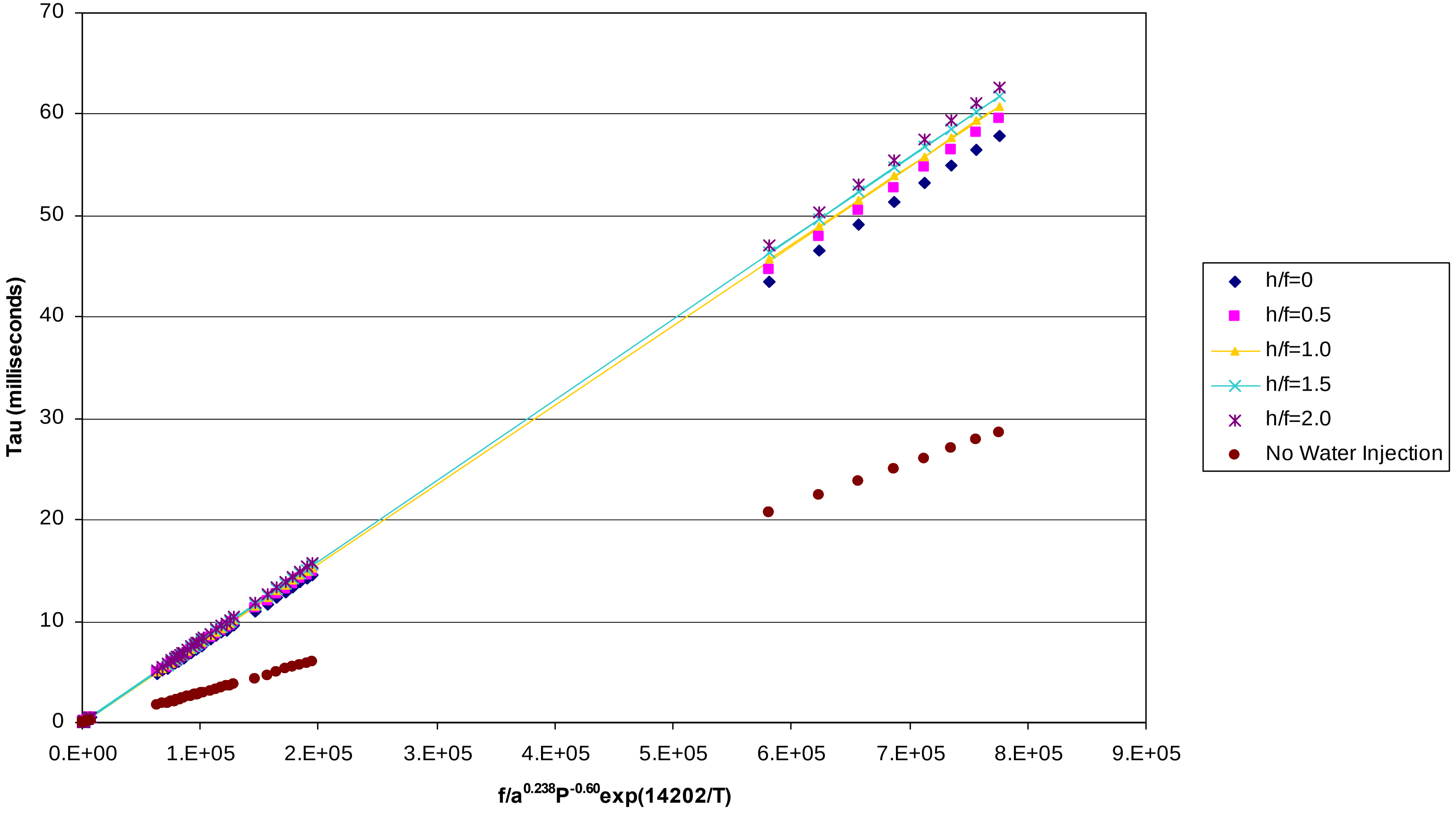


Figure 7
Kinetic Jet-A Fuel Tau Parity
Step Two
(lean)

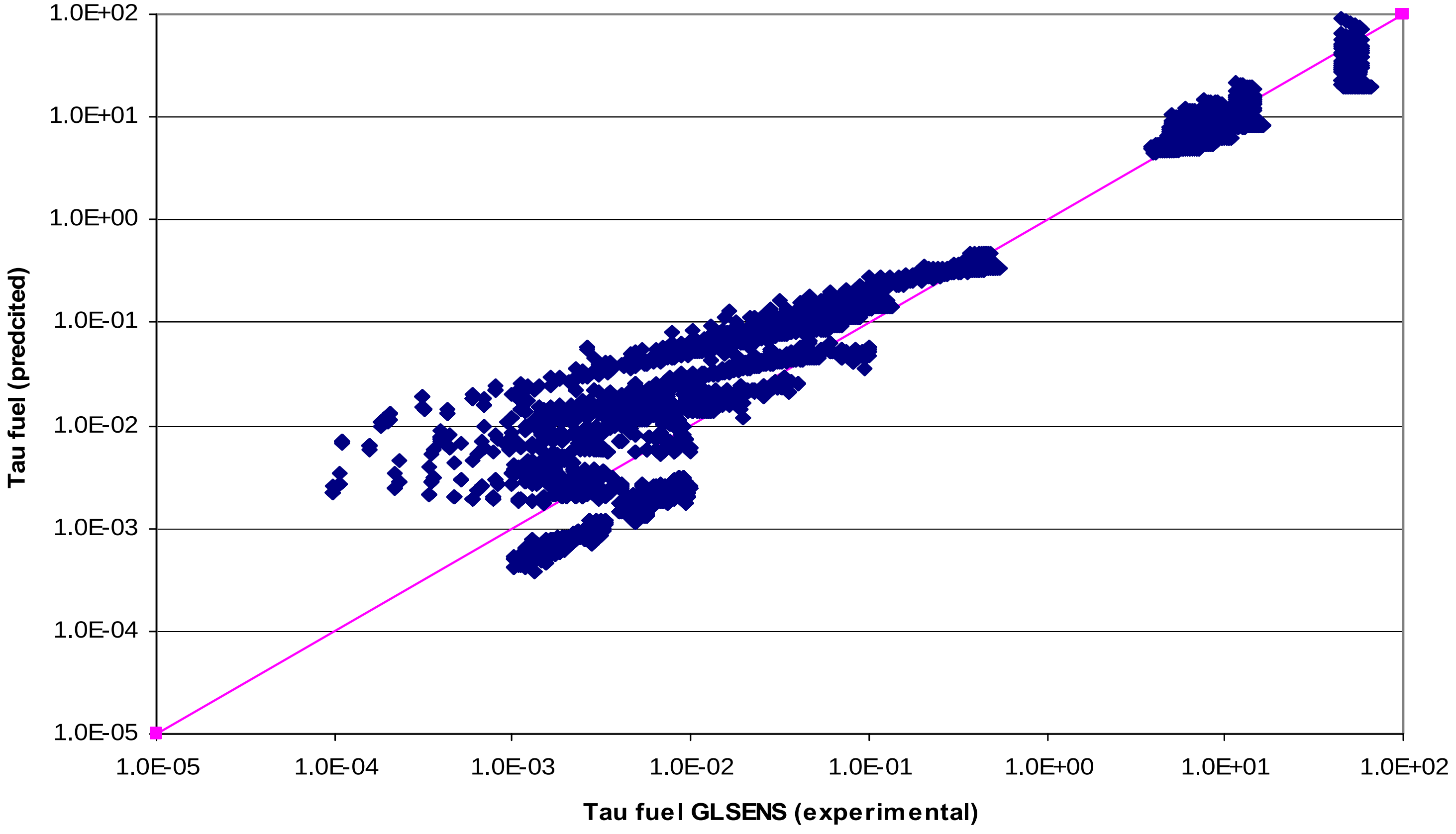


Figure 8
Kinetic Jet-A CO Tau Parity
Step Two
(lean)

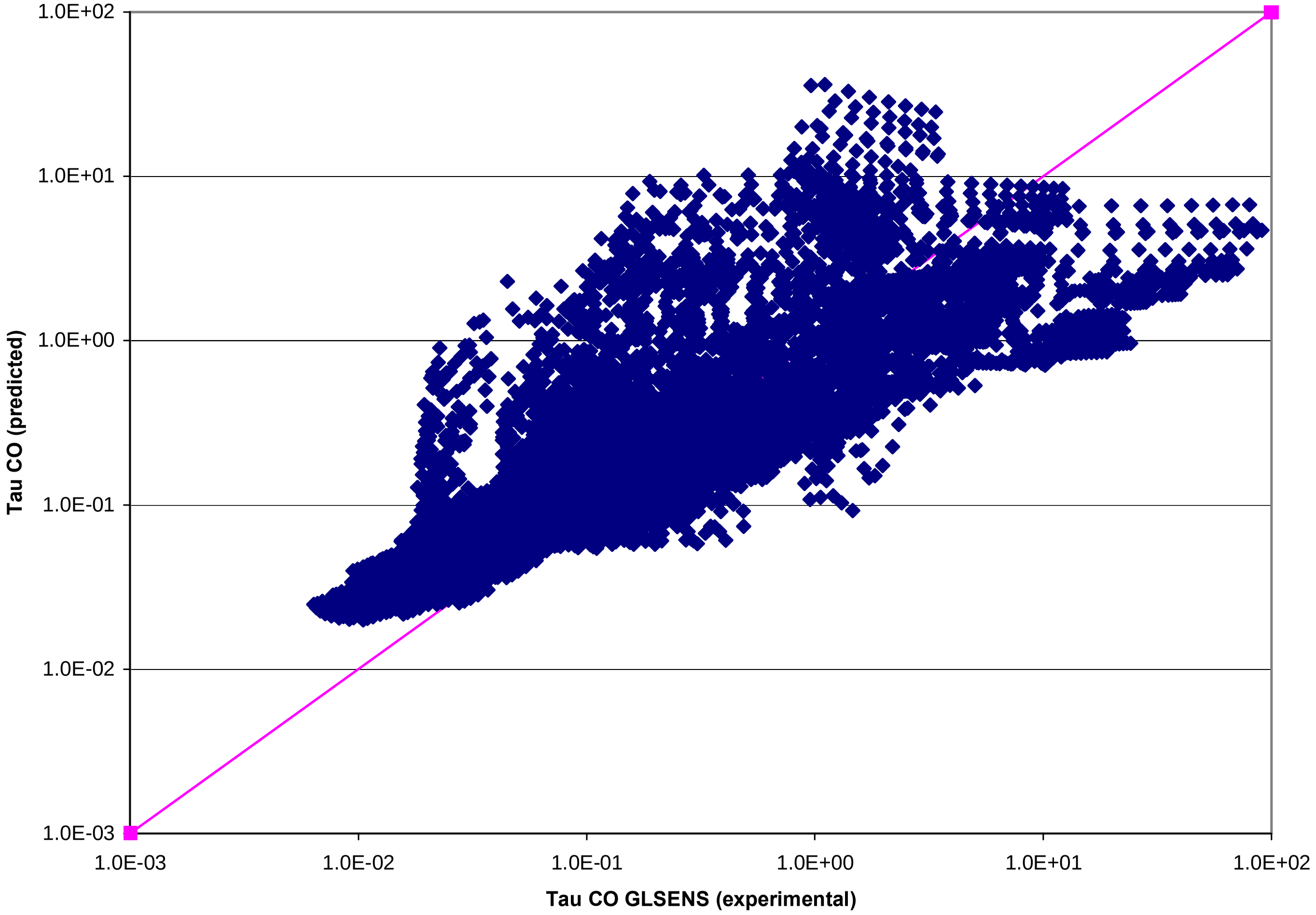


Figure 9
Kinetic Jet-A NOx Tau Parity
Step Two
(lean)

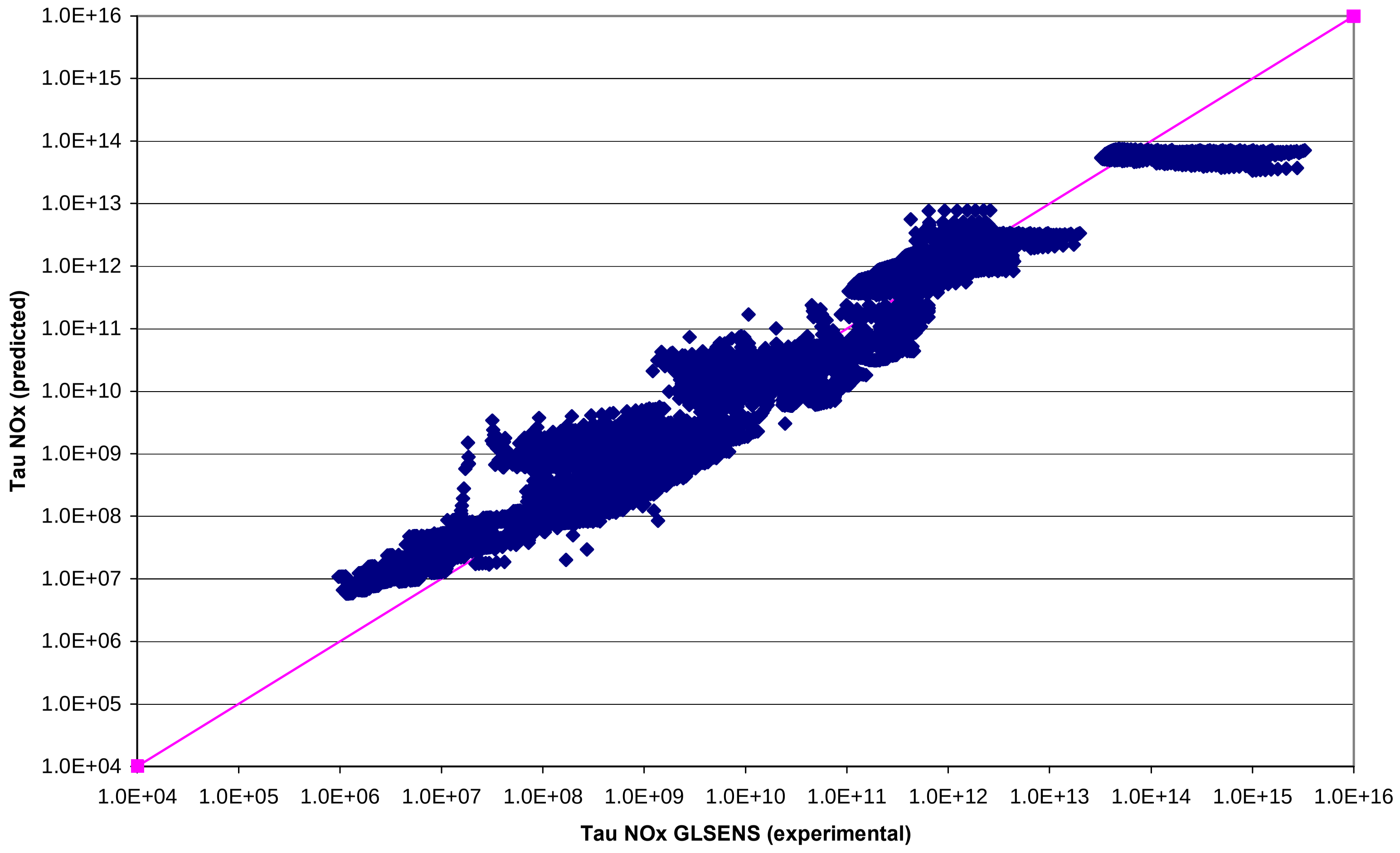


Figure 10
Equilibrium Methane CO Parity
(rich)

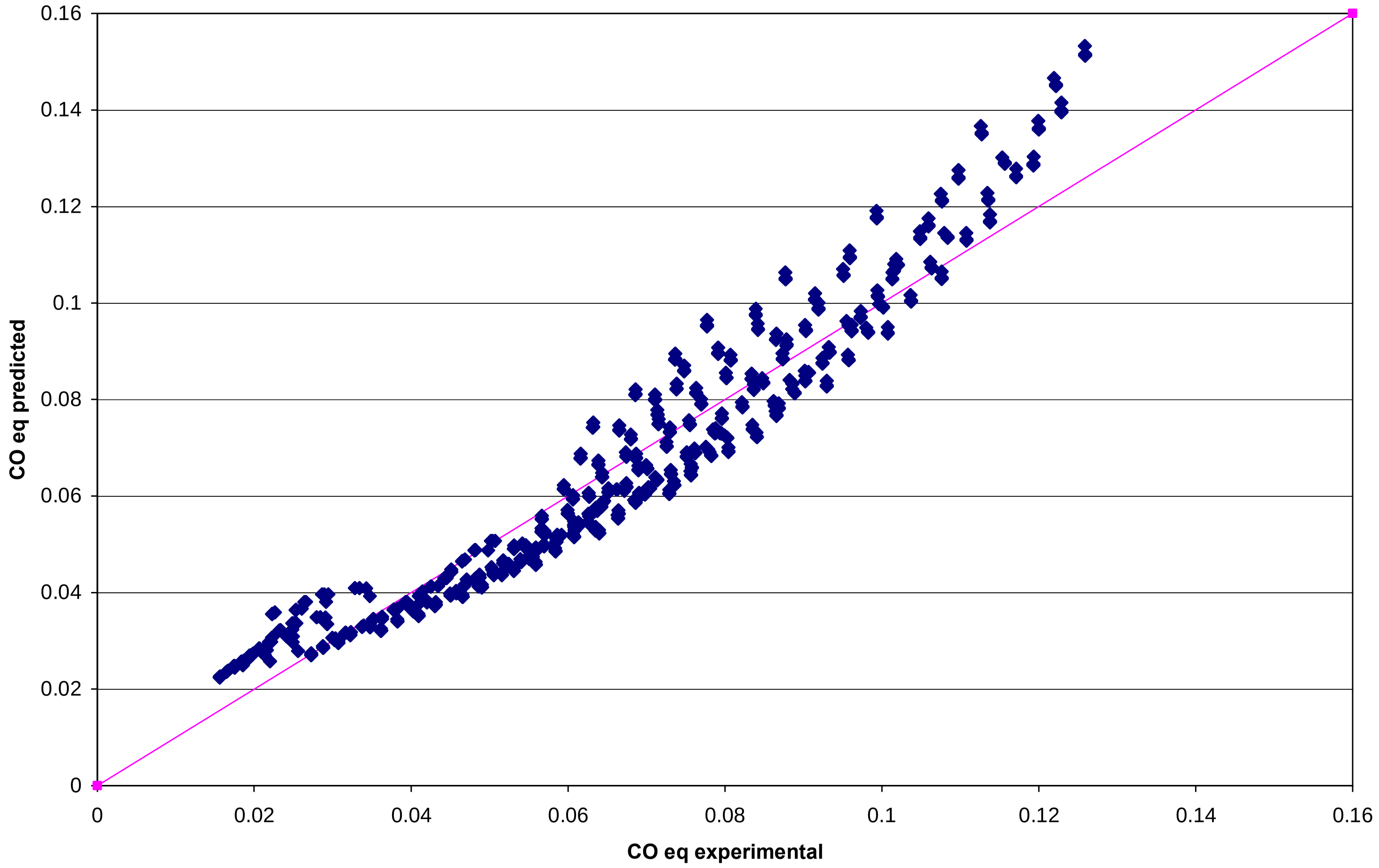


Figure 11
Kinetic Methane Fuel Tau Parity
Step One
(lean)

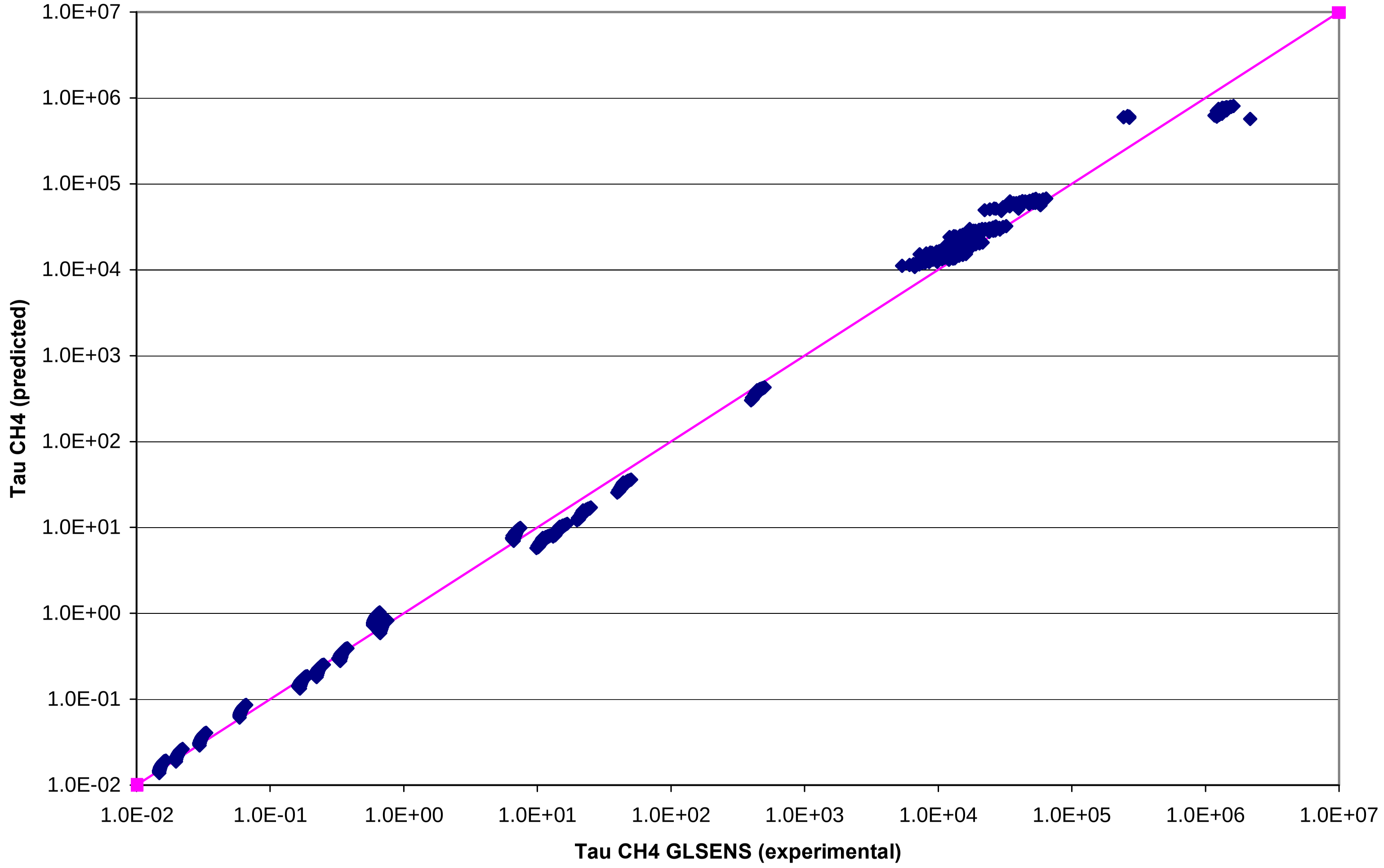


Figure 12
Kinetic Methane CO Tau Parity
Step One
(lean)

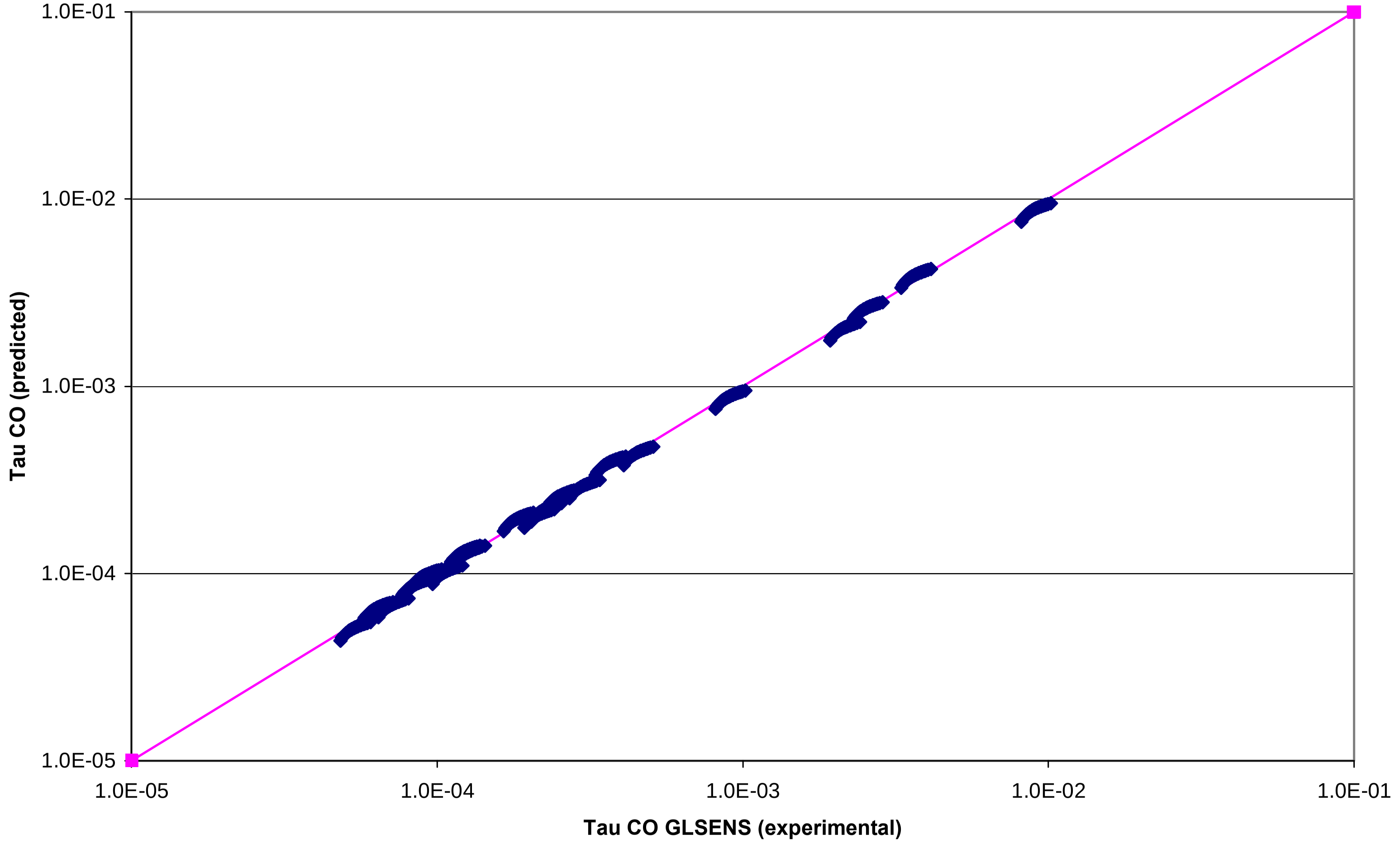


Figure 13
Kinetic Methane NOx Tau Parity
Step One
(lean)

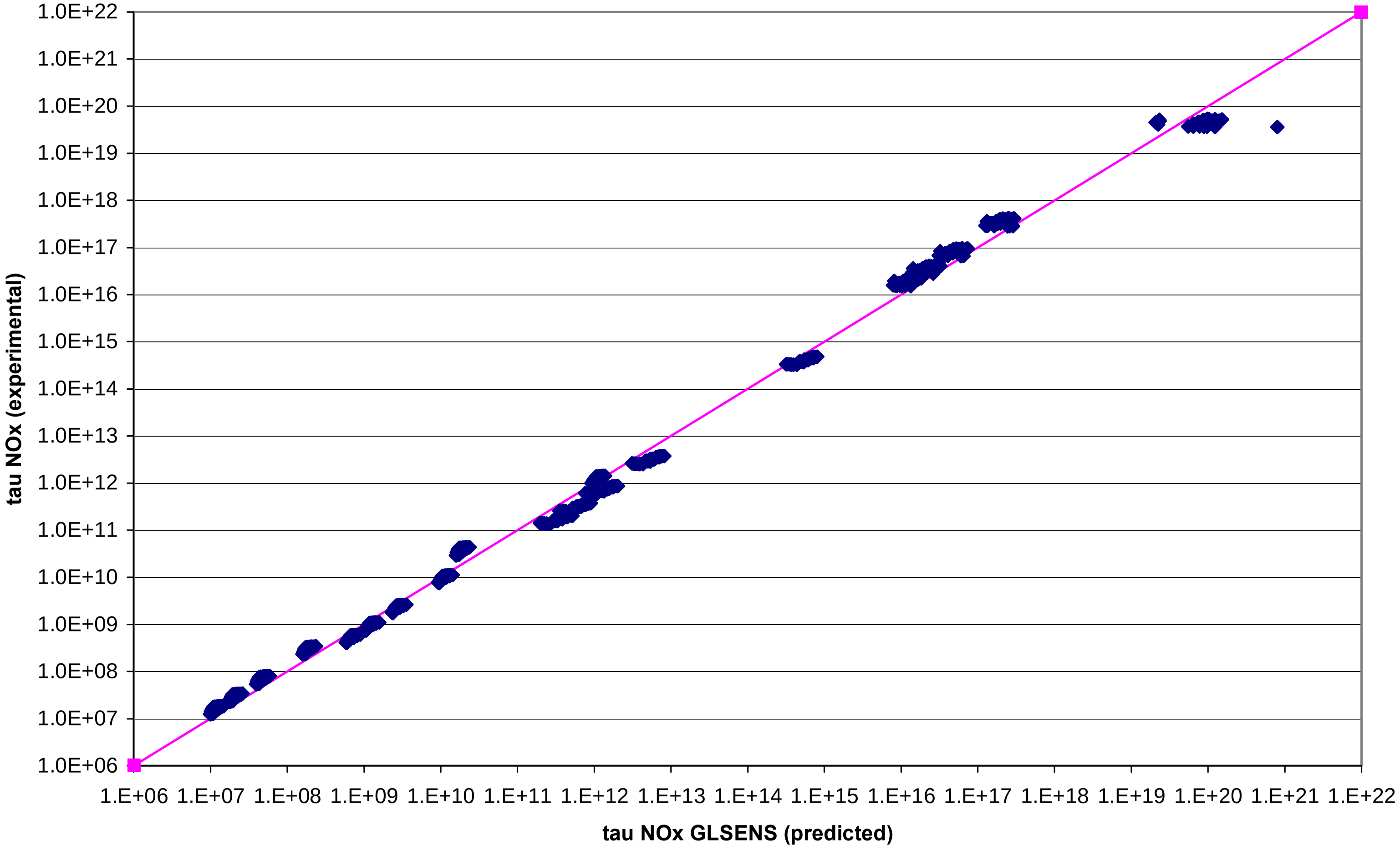


Figure 14
Methane Fuel Simple Step One Lean Model

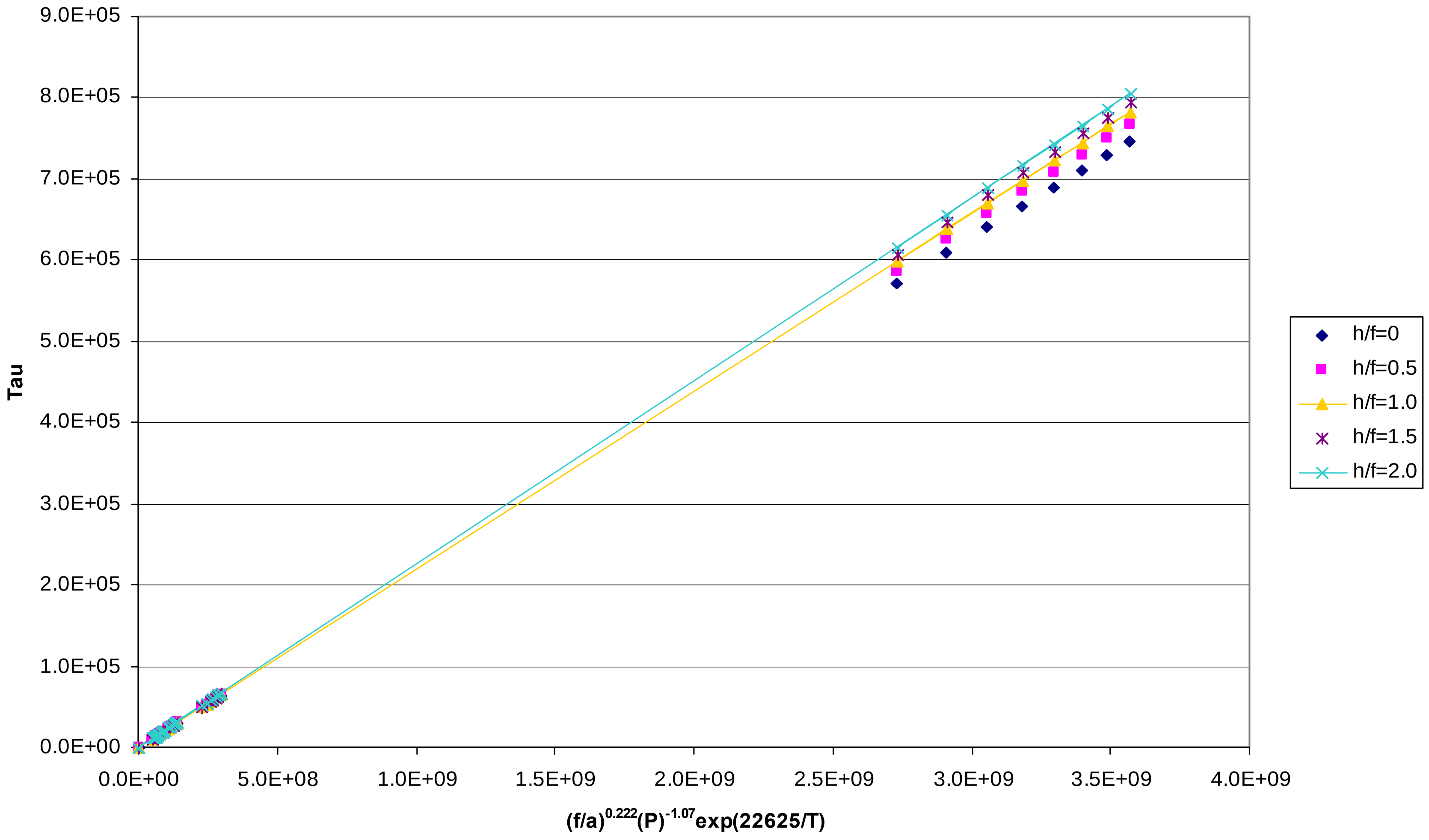


Figure 15
Kinetic Methane Tau Fuel Parity
Step Two
(lean)

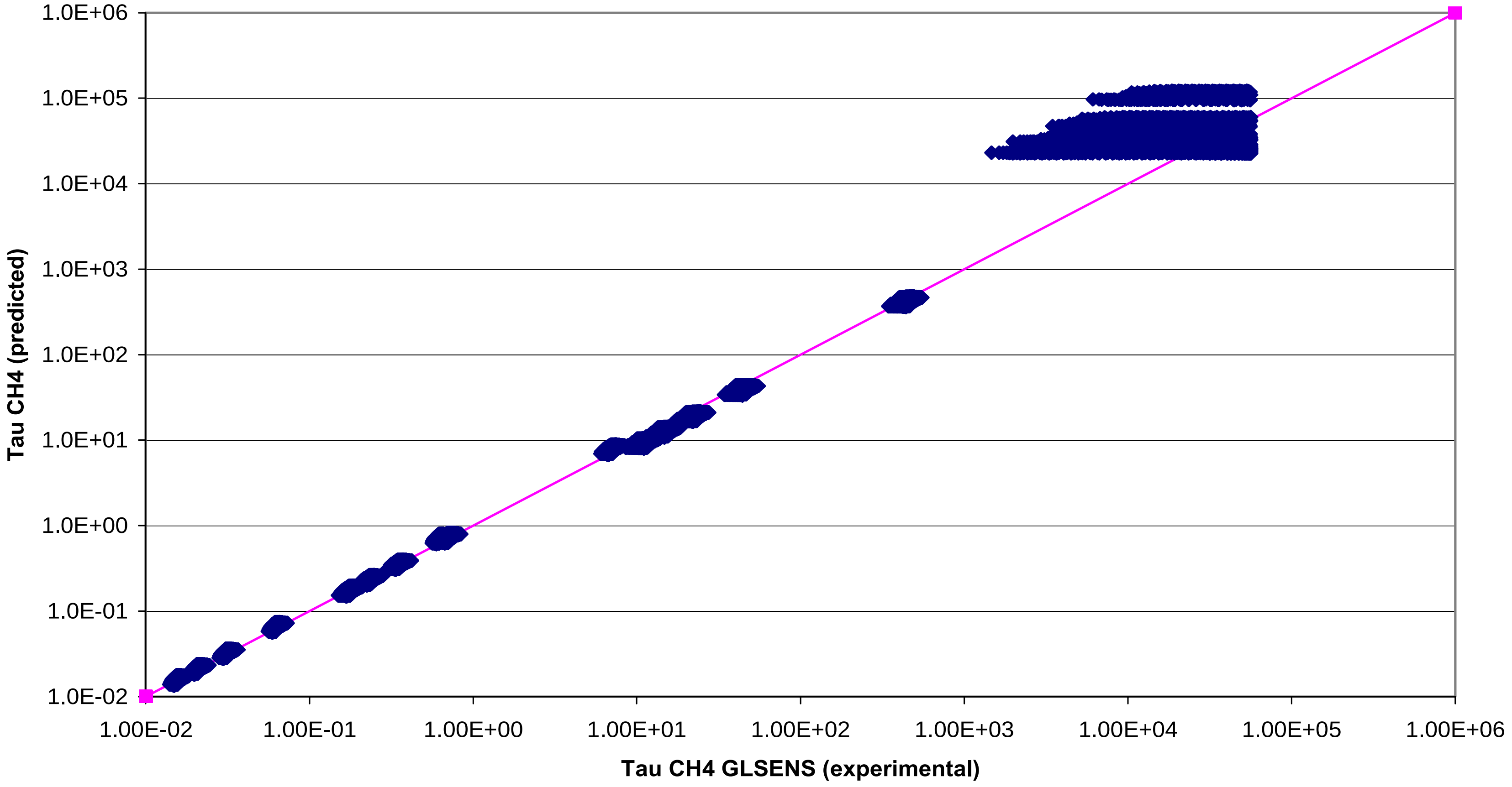


Figure 16
Kinetic Methane CO Tau Parity
Step Two
(lean)

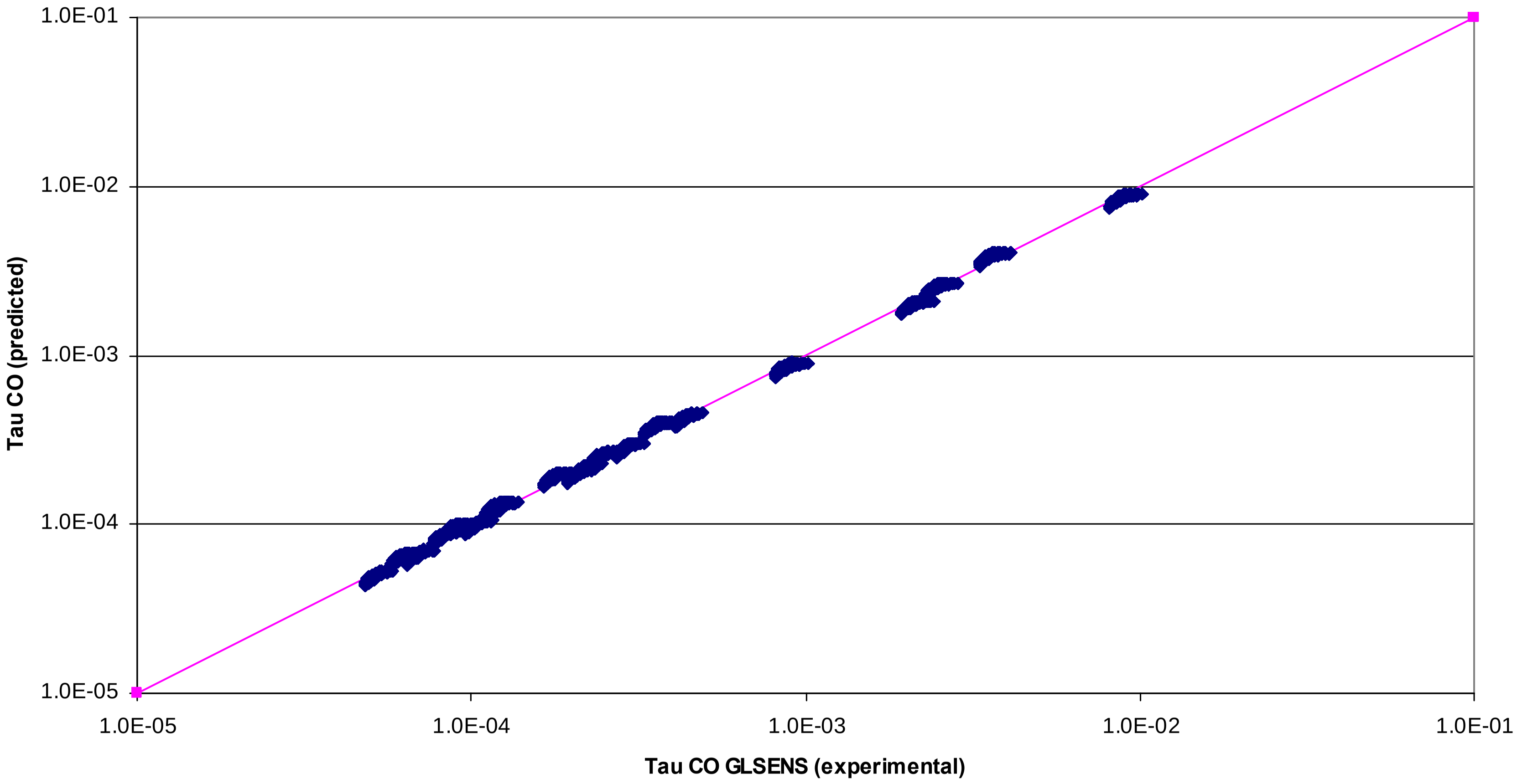


Figure 17
Kinetic Methane NOx Tau Parity
Step Two
(lean)

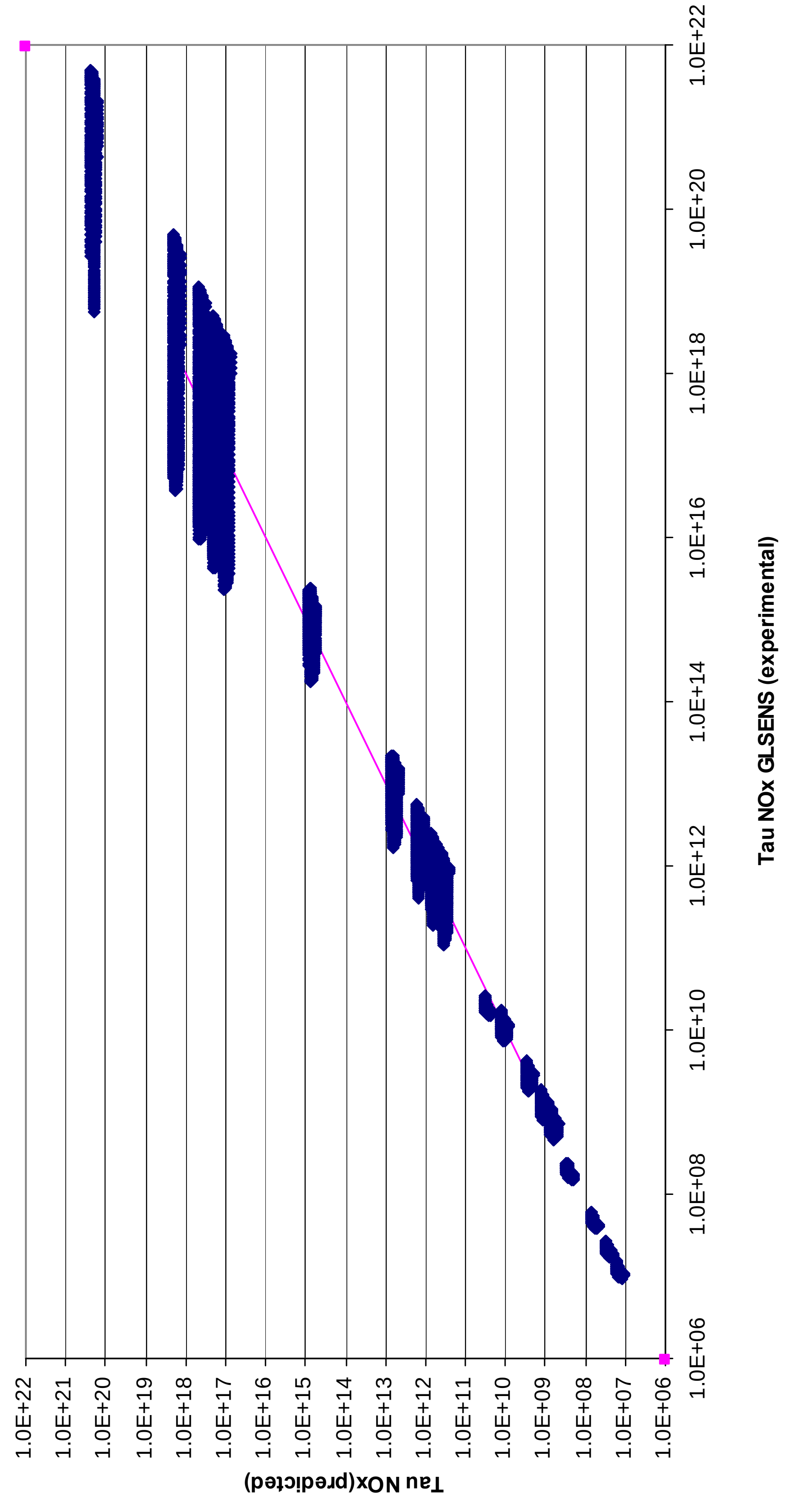


Figure 18
NOx water/NOx no water for Jet-A at f/a=0.06

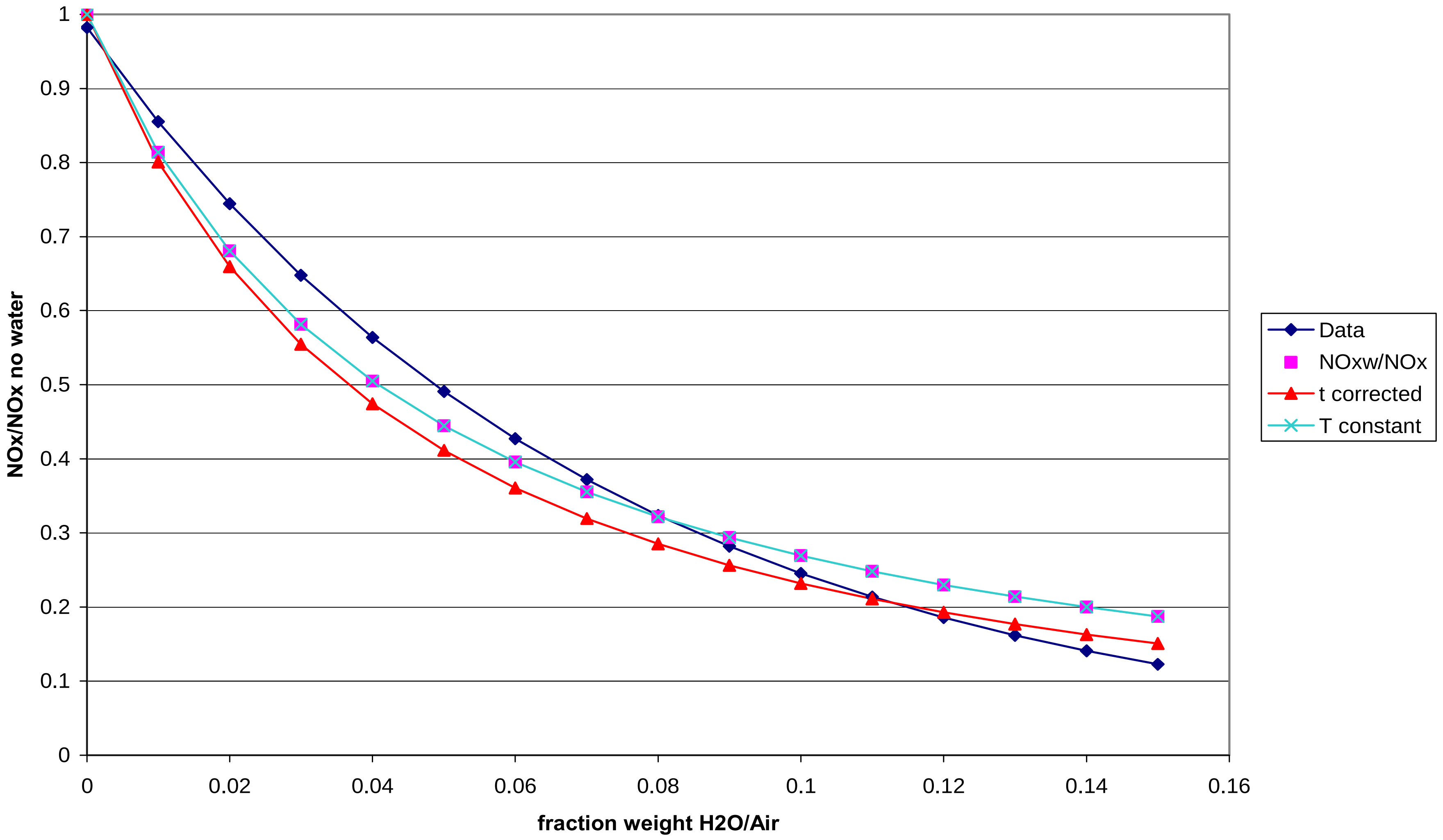


Figure 19
Methane Data Comparison (f/a=0.055)

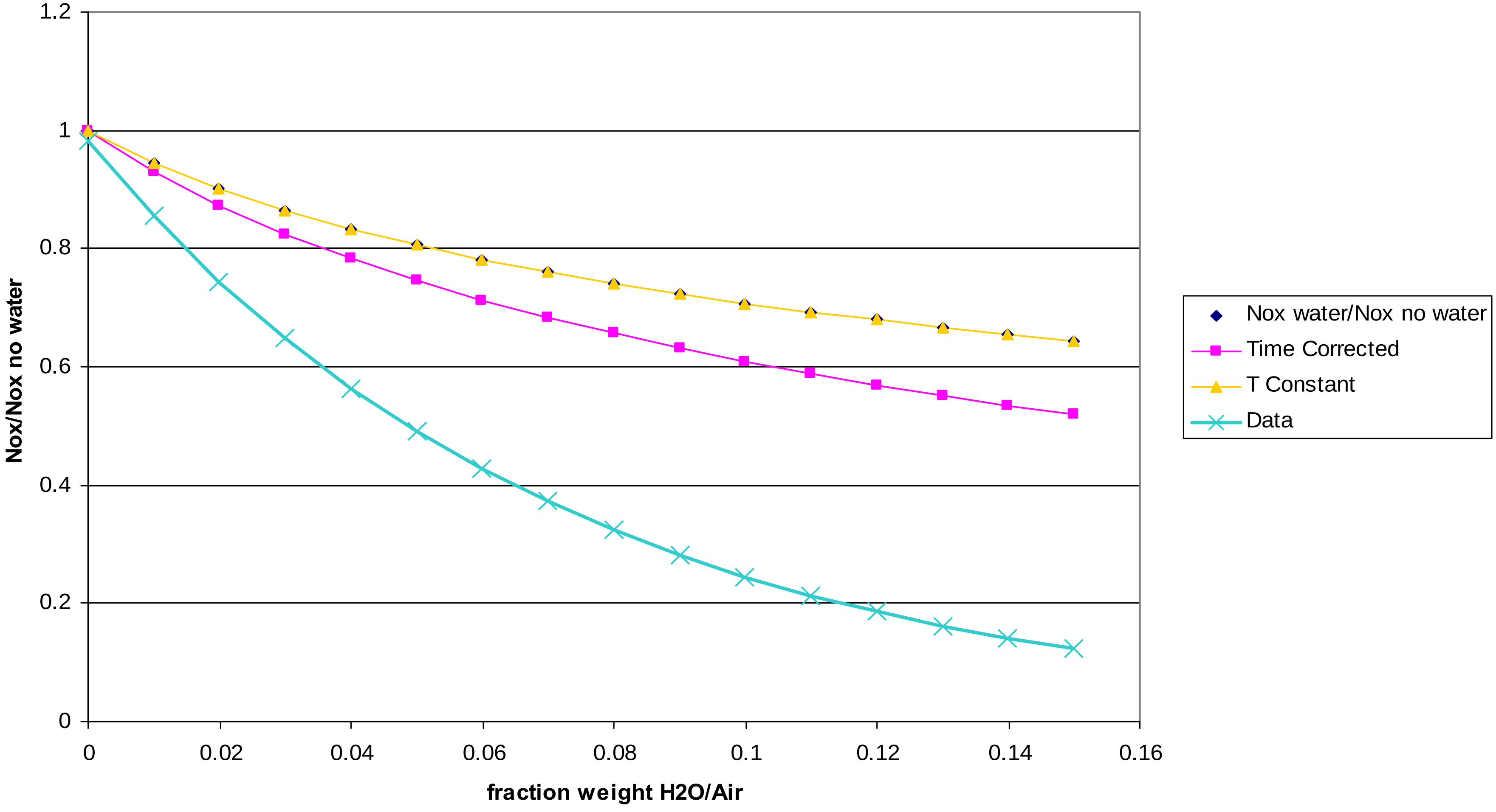


Figure 20 Methane
Tanks in Series, fa < 0.059

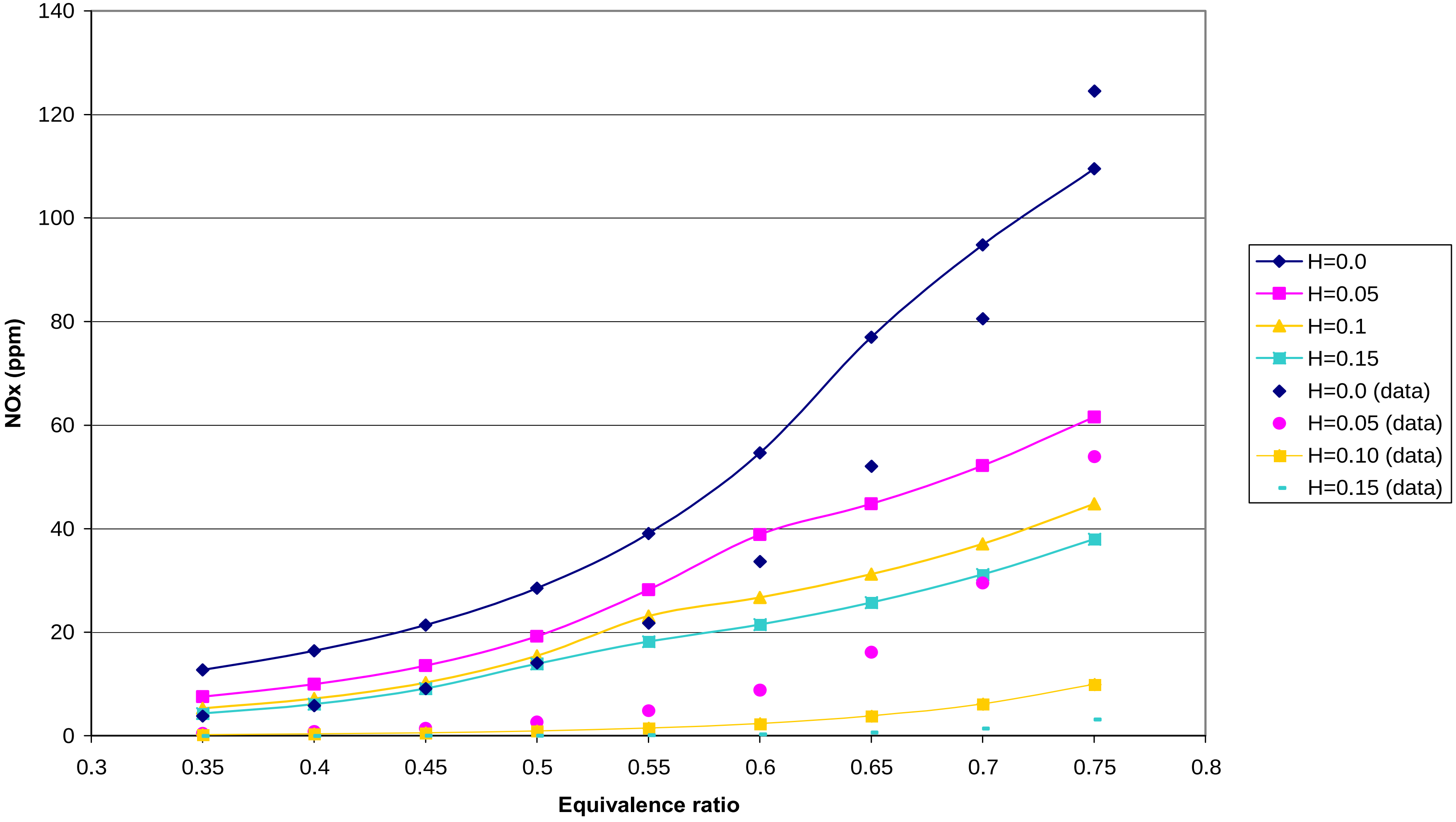


Figure 21

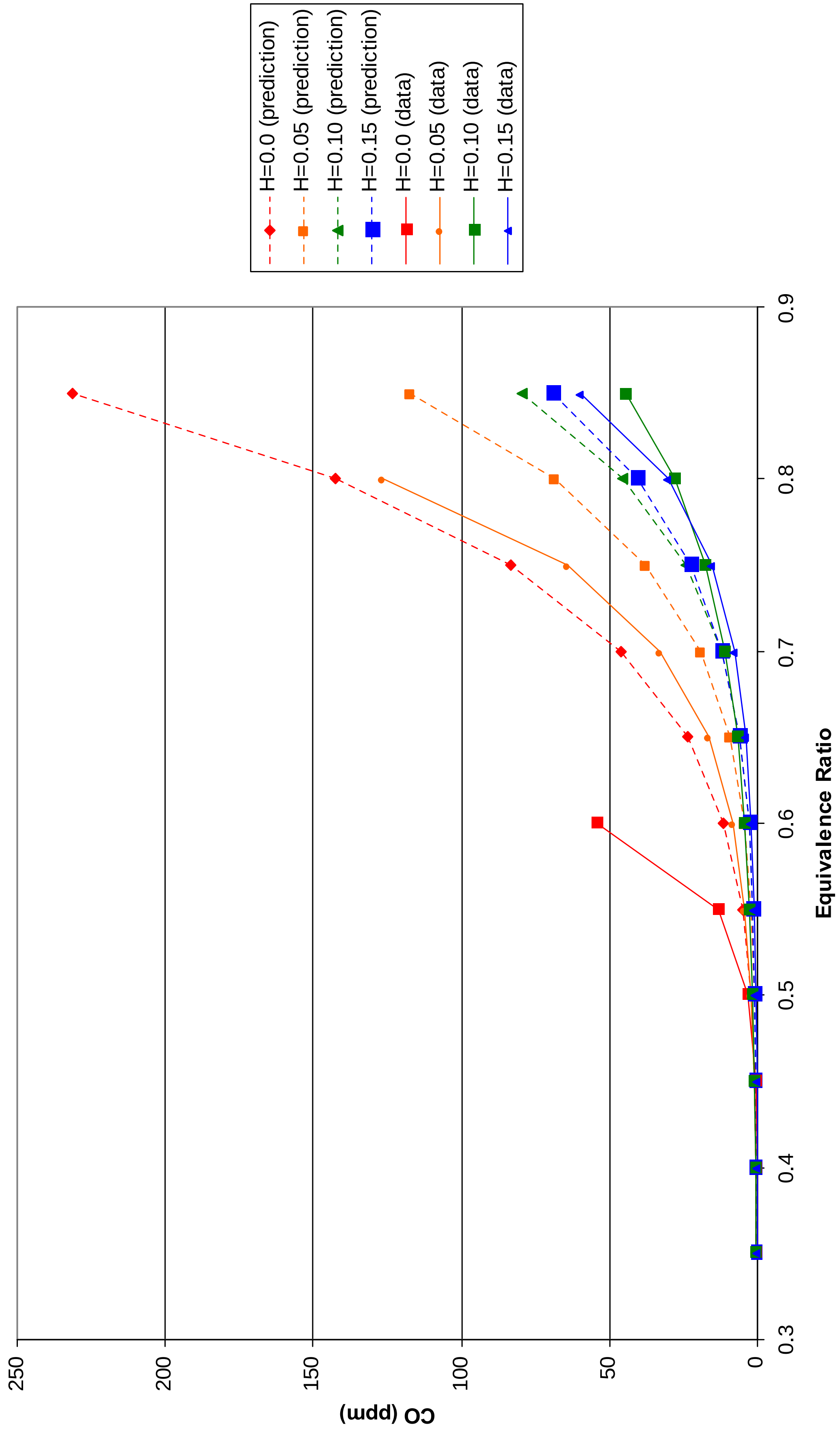

CO (ppm)
0
50
100
150
200
250
Equivalence Ratio
0.3
0.4
0.5
0.6
0.7
0.8
0.9
H=0.0 (prediction)
H=0.05 (prediction)
H=0.10 (prediction)
H=0.15 (prediction)
H=0.0 (data)
H=0.05 (data)
H=0.10 (data)
H=0.15 (data)

Figure 22 Methane
Nox versus Temperature

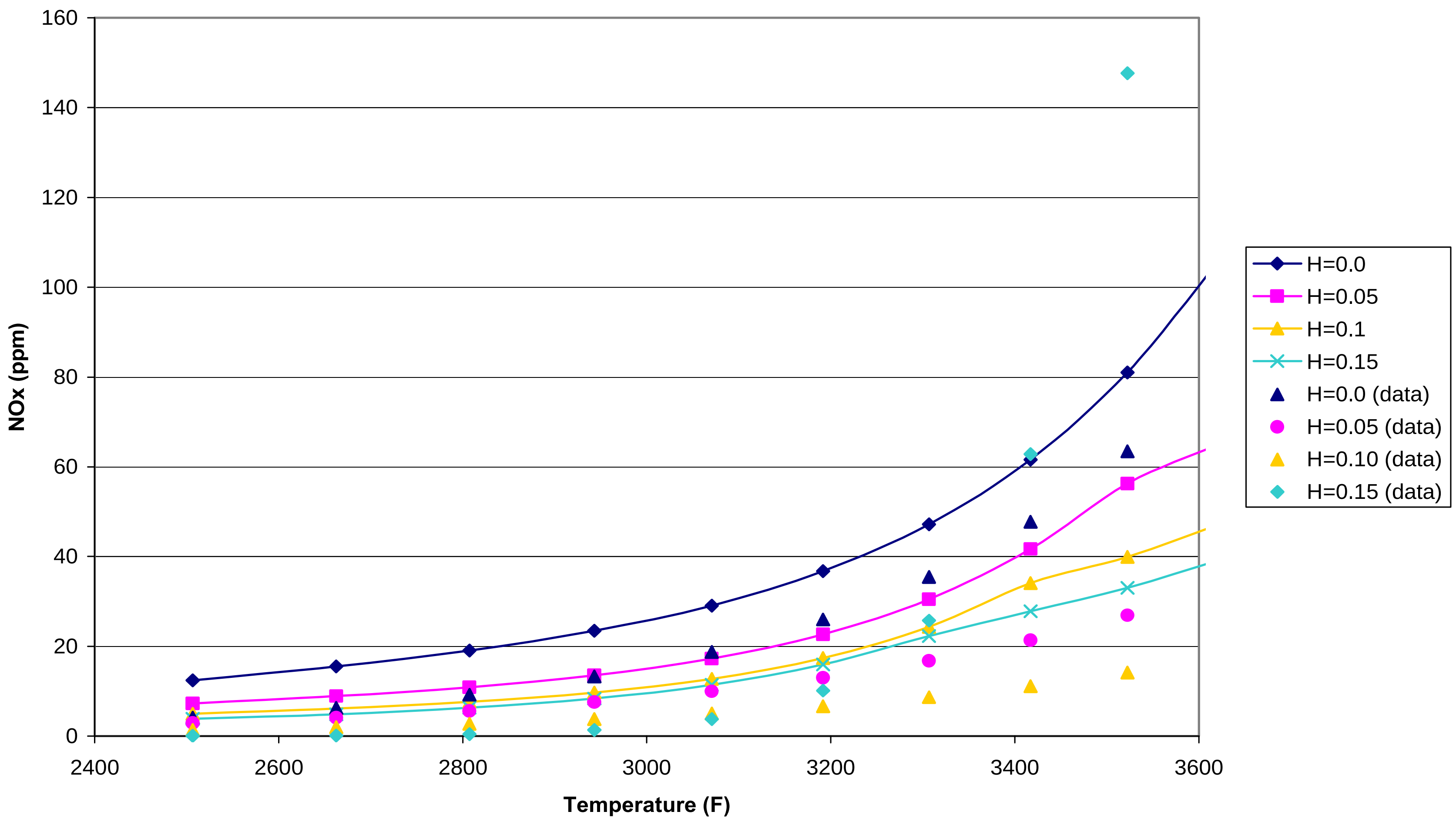


Figure 23

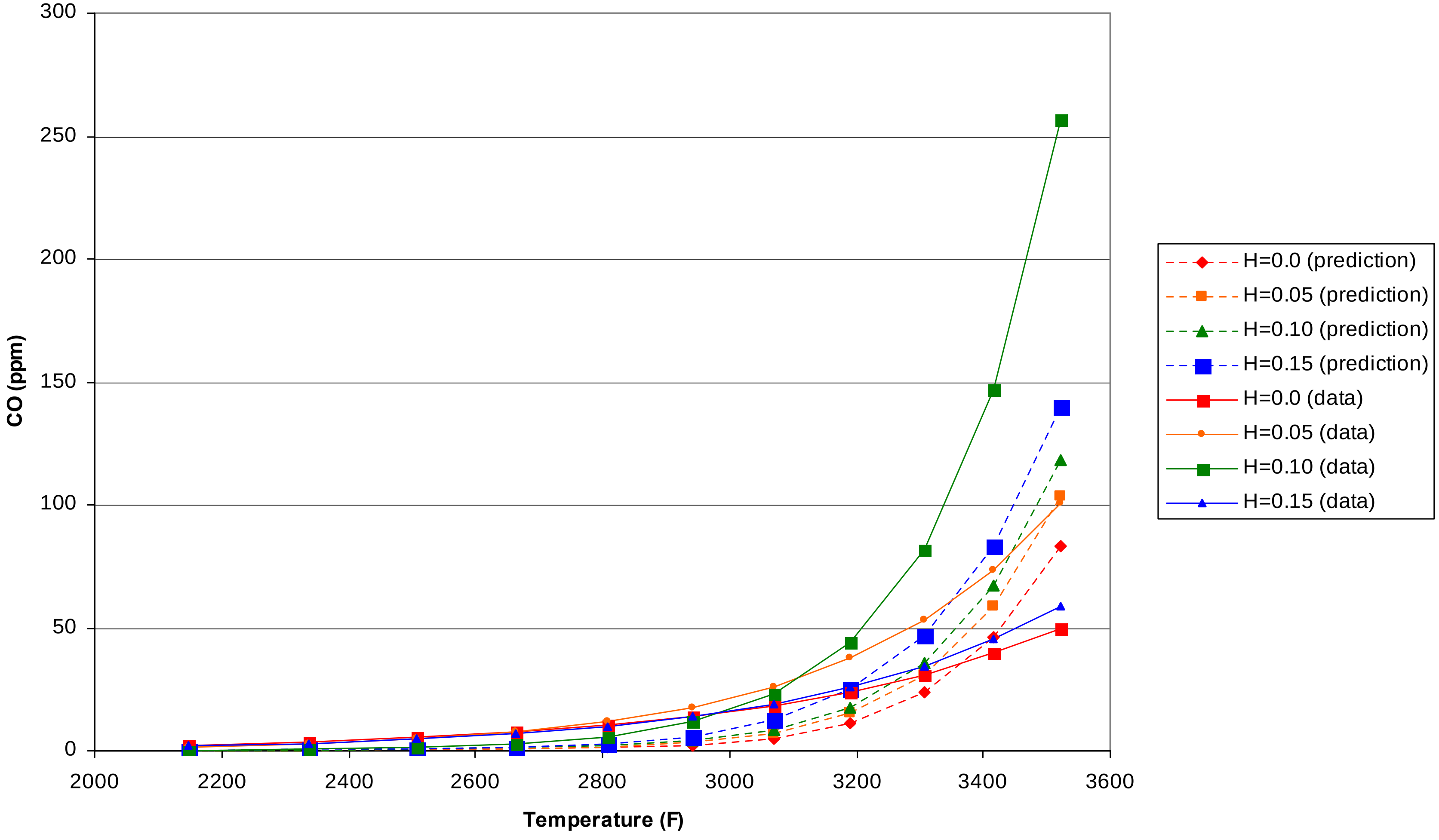

CO (ppm)
300
250
200
150
100
50
0
2000
2200
2400
2600
2800
3000
3200
3400
3600
Temperature (F)
H=0.0 (prediction)
H=0.05 (prediction)
H=0.10 (prediction)
H=0.15 (prediction)
H=0.0 (data)
H=0.05 (data)
H=0.10 (data)
H=0.15 (data)

Figure 24
tauf millisec for lean ch4

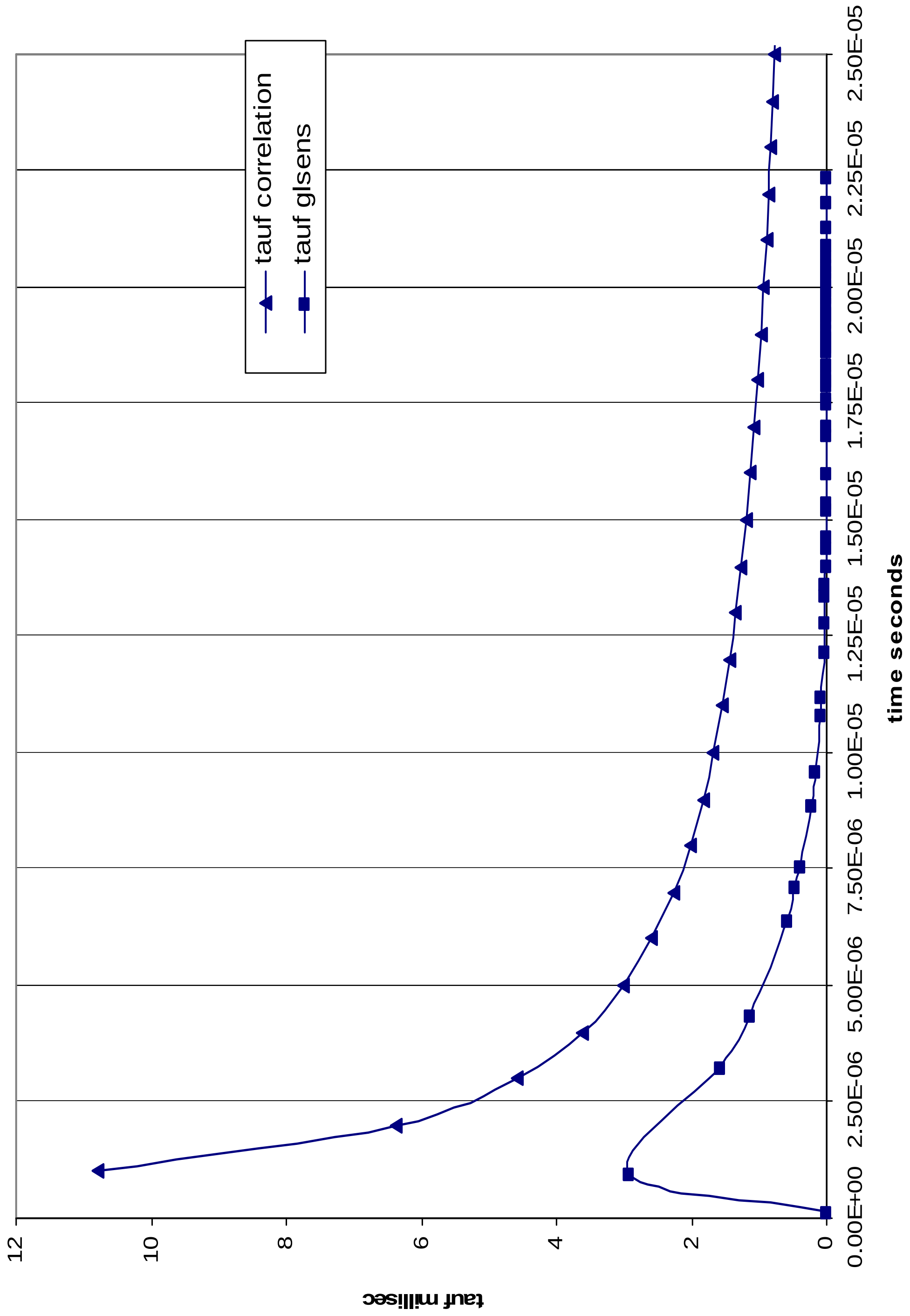
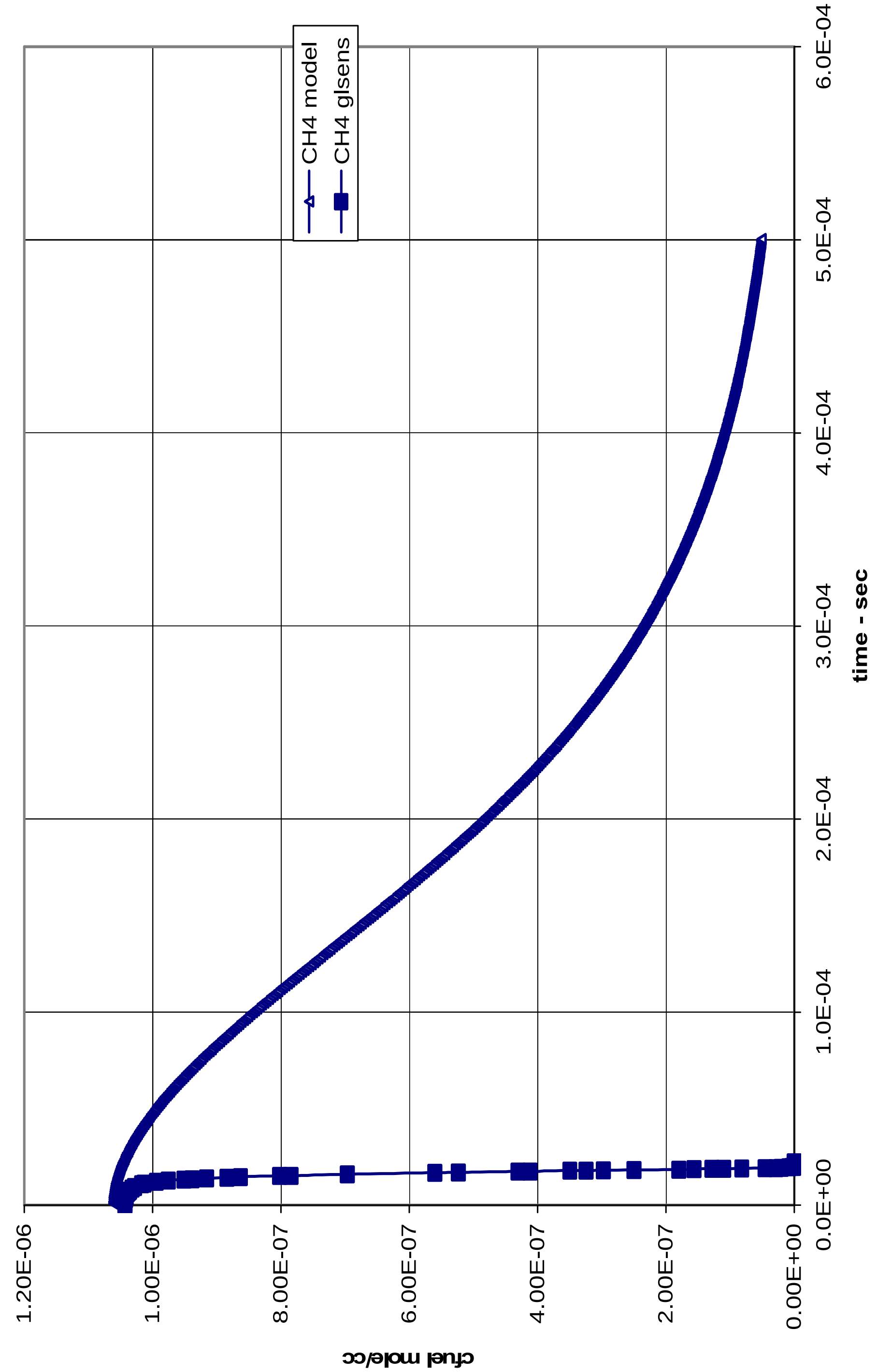


Figure 25

CH4 T=2000 P=2 atm Phi=0.8915 Gri-mech viet



REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (*Leave blank*)	**2. REPORT DATE** April 2004	**3. REPORT TYPE AND DATES COVERED** Technical Memorandum

4. TITLE AND SUBTITLE

New Reduced Two-Time Step Method for Calculating Combustion and Emission Rates of Jet-A and Methane Fuel With and Without Water Injection

5. FUNDING NUMBERS

WBS–22–714–20–10

6. AUTHOR(S)

Melissa Molnar and C. John Marek

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

National Aeronautics and Space Administration
John H. Glenn Research Center at Lewis Field
Cleveland, Ohio 44135–3191

8. PERFORMING ORGANIZATION REPORT NUMBER

E–14483

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

National Aeronautics and Space Administration
Washington, DC 20546–0001

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

NASA TM—2004-213046

11. SUPPLEMENTARY NOTES

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Unclassified - Unlimited
Subject Category: 07 Distribution: Nonstandard

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13. ABSTRACT ***(Maximum 200 words)***

A simplified kinetic scheme for Jet-A, and methane fuels with water injection was developed to be used in numerical combustion codes, such as the National Combustor Code (NCC) or even simple FORTRAN codes that are being developed at Glenn. The two time step method is either an initial time averaged value (step one) or an instantaneous value (step two). The switch is based on the water concentration in moles/cc of 1×10^{-20}. The results presented here results in a correlation that gives the chemical kinetic time as two separate functions. This two step method is used as opposed to a one step time averaged method previously developed to determine the chemical kinetic time with increased accuracy. The first time averaged step is used at the initial times for smaller water concentrations. This gives the average chemical kinetic time as a function of initial overall fuel air ratio, initial water to fuel mass ratio, temperature, and pressure. The second instantaneous step, to be used with higher water concentrations, gives the chemical kinetic time as a function of instantaneous fuel and water mole concentration, pressure and temperature (T4). The simple correlations would then be compared to the turbulent mixing times to determine the limiting properties of the reaction. The NASA Glenn GLSENS kinetics code calculates the reaction rates and rate constants for each species in a kinetic scheme for finite kinetic rates. These reaction rates were then used to calculate the necessary chemical kinetic times. Chemical kinetic time equations for fuel, carbon monoxide and NO_x were obtained for Jet-A fuel and methane with and without water injection to water mass loadings of 2/1 water to fuel. A similar correlation was also developed using data from NASA's Chemical Equilibrium Applications (CEA) code to determine the equilibrium concentrations of carbon monoxide and nitrogen oxide as functions of overall equivalence ratio, water to fuel mass ratio, pressure and temperature (T3). The temperature of the gas entering the turbine (T4) was also correlated as a function of the initial combustor temperature (T3), equivalence ratio, water to fuel mass ratio, and pressure.

14. SUBJECT TERMS

Combustion; Chemical kinetic times; Jet-A; Methane; Nitrogen oxides; Carbon monoxide

15. NUMBER OF PAGES

71

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT Unclassified	**18. SECURITY CLASSIFICATION OF THIS PAGE** Unclassified	**19. SECURITY CLASSIFICATION OF ABSTRACT** Unclassified	**20. LIMITATION OF ABSTRACT**