Simplified 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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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 time 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 rates 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 are used to calculate the necessary chemical kinetic times. Chemical kinetic time equations for fuel, carbon monoxide and NO_x are 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.

I.   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 time step kinetic scheme presented here results in a correlation that gives the chemical kinetic time as two separate functions. Instead of performing the detailed calculation over

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and over, one can quickly compute the overall progress of the reaction by using the correlation results. This method is also described in Reference 1 with other examples. The two time step method is used as opposed to a one step time averaged method[2] to determine the chemical kinetic time with increased accuracy. The first time averaged step is used at initial times with 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. 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.[3] 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,[4] 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 contain 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. Some chemistry models in the current version of NCC require 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.[5,6] The methane combustion was represented using the GRI-mech version 2.1 mechanism.[11]

GLSENS,[7] the NASA detailed kinetics code, 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 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[2] and the NO_x produced by the chemical kinetic time correlations will then be given.

II.   Mixing and Kinetics

The Magnussen model[4] 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.

$$\text{Net rate } \varpi_r = \min\left(\frac{A\varepsilon}{k} y_{\text{fuel}}, \frac{A\varepsilon}{k} \frac{y_{\text{oxygen}}}{r_f}, \varpi_{\text{kinetic}} \right) \tag{1}$$
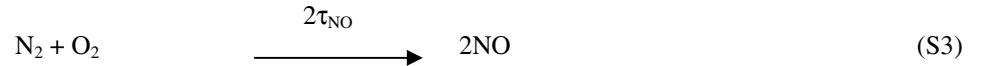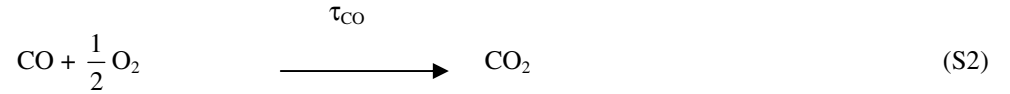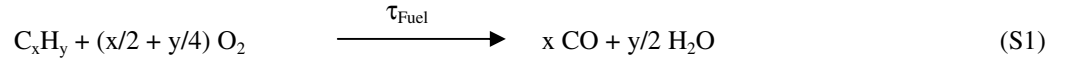
where $\frac{k}{A\varepsilon}$ equals the turbulent mixing time, τ_m, with k being the turbulent kinetic energy, ε is the dissipation rate, y is the mass fraction, and r_f, is the stoichiometric coefficient written on a mass fraction basis. The mixing constant, A, is usually given as 4.0. The factor $\frac{y_{\text{fuel}}}{\varpi_{\text{kinetic}}}$ 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 Fig. 1. This may also be represented by the following relationship:

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

III.   Model Equations

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

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

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

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

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 $\frac{\text{ms} \cdot \text{cc}}{\text{gmol}}$, while concentrations are given in gmoles/cc):

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

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.

$$\text{Fuel} = F_0 e^{\left(\frac{-t}{\tau_F} \right)} \tag{4}$$

The carbon monoxide reaction rate was represented by Eqs. (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.

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

and

$$\frac{d\text{CO}_2}{dt} = \frac{\text{CO}}{\tau_{\text{CO}}}$$

(5a)

$$\text{CO} - \text{CO}_{\text{eq}} = e^{\frac{-t}{\tau_{\text{CO}}}} \left[\text{CO}(t=0) - \text{CO}_{\text{eq}} - \frac{12F_0\tau_{\text{CO}}}{\tau_f - \tau_{\text{CO}}} \right] + \frac{12F_0\tau_{\text{CO}}}{\tau_f - \tau_{\text{CO}}} e^{-\frac{t}{\tau_f}}$$

(6)

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

$$\text{NO}_x = \frac{t}{\tau_{\text{NO}_x}}$$

(7)

or

$$\frac{d\text{NO}_x}{dt} = \frac{1}{\tau_{\text{NO}_x}}$$

(8)

$^*\tau_{\text{NO}_x}$ has units of $\dfrac{\text{ms} \cdot \text{cc}}{\text{gmol}}$

IV.   H₂O 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.[8] This procedure is described in detail below. The mixture is completely specified by fixing the equivalence ratio, Eratio, and the water to fuel ratio, H_2OF (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 Jet-A fuel and 0.059 for methane fuel, for all water to fuel ratios. The following H_2O mass balance was used for both Jet-A and methane fuels, where the term MWF represents the molecular weight of either fuel.

$$\text{Let} \quad y_i = \frac{\text{moles} \quad i}{\text{mole} \quad \text{mixture}}$$

(9)

$$\text{let} \quad x_i = \frac{\text{moles} \quad i}{\text{moles } O_2 \text{ in air}}$$

(10)

For the general chemical equation:

$$C_{n_c} H_{n_h} O_{n_o} + \frac{4n_c + n_n - 2n_o}{4} O_2 = n_c \text{CO}_2 + \frac{n_h}{2} H_2O$$

(11)

let

$$\phi = \frac{f/O_2}{\left(f/O_2\right)_{\text{stoich}}}$$

(12)

$$\frac{y_f}{y_{O_2}} = \frac{4\phi}{4n_c + n_h - 2n_o}$$

(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.

$$y_f + y_{H_2O} + y_{O_2} + y_{N_2} + y_{Ar} + y_{CO} = 1.0 \qquad (14)$$

let H$_2$OF = $\quad\quad\quad \dfrac{\text{lbs H}_2\text{O}}{\text{lb fuel}}$; $\text{H}_2\text{O}M = \dfrac{\text{moles H}_2\text{O}}{\text{mole fuel}} = \dfrac{\text{H2O}F * MWF}{18}$ \qquad (15)

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

$$y_{H_2O} = y_f \left(\frac{\text{H}_2\text{O}F * MWF}{18} \right) \qquad (16)$$

$$y_f = \frac{4\phi}{4n_c + n_h + 2n_o} y_{O_2} \qquad (17)$$

or

$$y_{O_2} = \frac{4n_C + n_H - 2n_O}{4\phi\left(1 + \dfrac{\text{H}_2\text{O}F * MW}{18}\right) + (4n_C + n_H - 2n_O)(1 + x_{N_2} + x_{Ar} + x_{CO_2})} \qquad (18)$$

(See the computer code modifications in Reference 1.)

V. 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 Fig. 1. The integration was performed for 2160 cases shown below for Jet-A and methane fuels with water injection.
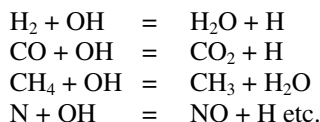
Table Input

Input Parameter	Range
Pressure	1 to 40 atmospheres (increments of 10 atm)
Temperature	1000 to 2500 K (increments of 500 K)
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 integration	From 1×10^{-6} to 2 ms
Step Two times between	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 Eq. (3) the chemical kinetic time is given as

$$\tau_f = -\frac{\text{Fuel}}{\left(\dfrac{d\text{Fuel}}{dt}\right)} \qquad (19)$$

This simple calculation was done using additional steps in Subroutine Out2 in the GLSENS code.[1] 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 time period 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

$$
\begin{aligned}
H_2 + OH &= H_2O + H \\
CO + OH &= CO_2 + H \\
CH_4 + OH &= CH_3 + H_2O \\
N + OH &= NO + H \text{ etc.}
\end{aligned}
$$

the radicals (OH, H) could be correlated with H_2O because of the first reaction.

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

VI. 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 create 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. The 23 step mechanism in the format used by LSENS[8] is given as follows:

```
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 $2.5 \times 10^{10} \, T^0 e^{-30000/RT} \, N_2^{0.8} C_{12}H_{23}^{0.8}$ in an irreversible step.

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

Note, some reactions are bimolecular and some are trimolecular expressions.

VII.   Partial Methane Kinetics Scheme

Whereas Jet-A is broken down by two irreversible steps with known rates in the reduced mechanism used here, methane, CH_4, 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 time step method to predict the chemical time constants. We list only the CH_4 reactions to illustrate this process. The complete GRI-mech mechanism is listed in References 1 and 2. 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).

CH_4 partial mechanism showing free radical attack

OH	CH_4	$= CH_3$	H_2O	1.000E+08	1.600	3120.00
OH	CO	= H	CO_2	4.760E+07	1.228	70.00
N	OH	= NO	H	7.333E+13	.000	1120.00
2.0	O	$= O_2$	M	1.200E+17	−1.000	.00
H	H	$= H_2$	M	1.000E+18	−1.000	.00
O	H_2	= H	OH	5.000E+04	2.670	6290.00
H	O_2	= O	OH	8.300E+13	.000	14413.00
H	HO_2	$= O_2$	H_2	2.800E+13	.000	1068.0
OH	H_2	= H	H_2O	2.160E+08	1.510	3430.00
O	CH_4	= OH	CH_3	1.020E+09	1.500	8600.00
OH	CH_2	= CH	H_2O	1.130E+07	2.000	3000.00
OH	CH_3	$= CH_3OH$	M	6.300E+13	.000	.00
CH	CH_4	= H	C_2H_4	6.000E+13	.000	.00
CH_2	CH_4	= 2.0	CH_3	2.460E+06	2.000	8270.00
CH_3	CH_2O	= HCO	CH_4	3.320E+03	2.810	5860.00
CH_3	CH_3OH	$= CH_2OH$	CH_4	3.000E+07	1.500	9940.00
CH_3	CH_3OH	$= CH_3O$	CH_4	1.000E+07	1.500	9940.00
CH_3	C_2H_4	$= C_2H_3$	CH_4	2.270E+05	2.000	9200.00
CH_3	C_2H_6	$= C_2H_5$	CH_4	6.140E+06	1.740	10450.00
N	O_2	= NO	O	2.650E+12	.000	6400.00
NO	O	$= NO_2$	M	1.060E+20	−1.410	.00

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VIII.   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 9. (A detailed procedure describing the regression used for both equilibrium and finite rate chemical times can be found in the Appendix). CEA has a plot f option for direct tabulation of the output data, for 'f/a, P, T H_2O, 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. Figure 2 is a parity plot showing the accuracy 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 over the complete range of independent variables listed in the Table Input.

Table 1. Equilibrium lean Jet-A with water injection correlations

Species	Lean (f/a ≤ 0.068)	R-squared	
T4	$T4 = 1725\,(T3)^{0.241}\left(f/a\right)^{0.442}\left(1 + H_2O/f\right)^{(-0.151)} P^{0.00301}$	0.949	(20)
CO	$CO_{eq} = 226\left(f/a\right)^{2.22}\left(1 + H_2O/f\right)^{0.0658} P^{0.524} \exp\left[\dfrac{-31647}{T}\right]$	0.995	(21)
NO_x	$NO_{x_{eq}} = 2.65e^{-8}\left(f/a\right)^{(-1.52)}\left(1 + H_2O/f\right)^{(-0.133)} P^{0.980} \exp\left[\dfrac{-9953}{T}\right]$	0.958	(22)

Table 2. Equilibrium rich Jet-A with water injection correlations

Species	Rich (f/a > 0.068)	R-squared	
T4	$T4 = 163(T3)^{0.186}\left(f/a\right)^{(-0.613)}\left(1 + H_2O/f\right)^{(-0.296)} P^{0.00231}$	0.959	(23)
CO	$CO_{eq} = 3.85e^{-4}\left(f/a\right)^{2.86}\left(1 + H_2O/f\right)^{(-0.369)} P^{0.995} \exp\left[\dfrac{185}{T}\right]$	0.990	(24)
NO_x	$NO_{x_{eq}} = 1.80e^{-8}\left(f/a\right)^{(-6.08)}\left(1 + H_2O/f\right)^{0.418} P^{0.530} \exp\left[\dfrac{-38952}{T}\right]$	0.993	(25)

IX.   Chemical Kinetic Times for Jet-A With and Without Water Injection

A. Step One Equations for Jet-A

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

$$\tau = A(P)^a\left(f/a\right)^b\left(1 + \frac{H_2O}{fuel}\right)^c \exp\frac{D}{T} \tag{26}$$

where τ s 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, $\dfrac{H_2O}{fuel}$ 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:

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

where fuel, CO, CO_2, and N_2 represent mole fractions.

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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 range of conditions listed in Table Input. Parity plots for the lean step one correlations have been created and may be found in Figs. 3 to 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.

B. 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

$$\tau = A(P)^a\,(c\text{fuel})^b\,(cO_2)^c\,(cH_2O)^d\,\exp\frac{E}{T} \tag{34}$$

and for the Jet-A step two CO correlation

$$\tau = A(P)^a\,(\text{cfuel})^b\,(cCO)^c\,(cO_2)^d\,(cH_2O)^e\,\exp\frac{F}{T} \tag{35}$$

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 CO_2 is the instantaneous molar concentration of O_2, cH_2O 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 Figs. 6 to 8. 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	cO_2	cH_2O	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)

X. 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 Fig. 9.

Table 5. Equilibrium lean methane with water injection correlations

Species	Lean (f/a ≤ 0.058)	R-Squared	
T4	$T4 = 1565 \left(f/a \right)^{0.435} (1 + \frac{H_2O}{f})^{-0.069} (T3)^{0.258} (P)^{0.00284}$	0.944	(42)
CO	$COeq = 3.37 \times 10^6 \left(f/a \right)^{1.90} (1 + \frac{H_2O}{f})^{0.00705} (P)^{-0.477} \exp\frac{-33388}{T}$	0.998	(43)
NO_x	$NOxeq = 2.44 \times 10^{-2} \left(f/a \right)^{-1.13} (1 + \frac{H_2O}{f})^{-1.07} (P)^{-0.017} \exp\frac{-11415}{T}$	0.953	(44)

Table 6. Equilibrium rich methane with water injection correlations

Species	Rich (f/a > 0.058)	R-Squared	
T4	$T4 = 177 \left(f/a \right)^{-0.559} (1 + \frac{H_2O}{f})^{-0.146} (T3)^{0.176} (P)^{0.00167}$	0.976	(45)
CO	$COeq = 72.2 \left(f/a \right)^{2.55} (1 + \frac{H_2O}{f})^{-0..358} (P)^{-0.00393} \exp\frac{-31365}{T}$	0.911	(46)
NO_x	$NOxeq = 0.218 \left(f/a \right)^{-4.43} (1 + \frac{H_2O}{f})^{0.427} (P)^{-0.493} \exp\frac{-41408}{T}$	0.998	(47)

XI. Chemical Kinetic Times for Methane With and Without Water Injection

A. Step One Equations for Methane

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

$$\tau = A(P)^a \left(f/a \right)^b (1 + \frac{H_2O}{fuel})^c \exp\left[\frac{D}{T} \right]$$ (48)

where P is pressure in atm, f/a is the initial or overall fuel air ratio, $\frac{H_2O}{fuel}$ 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:

$$f/a = (fuel + (CO + CO_2)) * 16 / \frac{0.79}{28N_2}$$ (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 Figs. 10 to 12. These parity plots show minimal scatter, which is consistent with the high R-squared values of the lean correlations. Figure 13 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	2.09×10^{-4}	−1.07	22625	0.222	0.0675	0.996	(50)
Co	Lean	9.99×10^{-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	1.30×10^{-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)

B. Step Two Equations for Methane

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

$$\tau = A(P)^a\,(\text{cfuel})^b\,(\text{cH}_2\text{O})^c\,(1+\frac{\text{cH}_2\text{O}}{\text{cfuel}})^d\,\exp\left[\frac{E}{T}\right] \tag{56}$$

The following form of equation was used for the rich Methane step two correlations for fuel and NO$_x$:

$$\tau = A(P)^a\,(\text{cfuel})^b\,(\text{cO}_2)^c\,(\text{cH}_2\text{O})^d\,\exp\left[\frac{E}{T}\right] \tag{57}$$

and for the rich Methane step two CO correlation:

$$\tau = A(P)^a\,(\text{cfuel})^b\,(\text{cCO})^c\,(\text{cO}_2)^d\,(\text{cH}_2\text{O})^e\,\exp\left[\frac{F}{T}\right] \tag{58}$$

Table 8 provides a summary of these correlations, and lean parity plots can be found in Figs. 14 to 16.

Table 8. Step Two methane with water injection chemical kinetic time correlations

Component	A	Pressure	1/T	cfuel	cCO	cO$_2$	cH$_2$O	$1+\dfrac{\text{cH}_2\text{O}}{\text{cfuel}}$	R-squared	
Fuel (lean)	3.50×10^{-9}	−0.0713	14149	−0.307	---	---	−0.465	−0.221	0.416	(59)
CO (lean)	3.07×10^{-3}	−1.09	2291	0.0957	---	---	-9.82×10^{-4}	0.131	0.999	(60)
NO$_x$ (lean)	1.48×10^{5}	−2.28	37437	0.239	---	---	−0.0206	0.778	0.986	(61)
Fuel (rich)	9.99×10^{-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)

XII. Two Time 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

Component	A	Pressure	1/T	cfuel	cCO	cO_2	cH_2O	$1+\dfrac{cH_2O}{cfuel}$	R-squared	
Fuel (lean)	1.86×10^{-9}	0.479	13446	0.182	---	0.0528	–0.704	0.349	0.767	(65)
CO (lean)	1.43×10^{-3}	–1.04	2371	0.0461	---	---	-5.7×10^{-4}	---	0.999	(66)
NO_x (lean)	10.0	–1.92	38229	0.0389	---	---	–0.200	---	0.992	(67)
Fuel (rich)	2.02×10^{-14}	0.498	14860	0.252	---	–0.776	–0.756	0.254	0.995	(68)
CO (rich)	6.73×10^{-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)

XIII.   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:

$$\tau = A(P)^a\,(\text{cfuel})^b\,(cO_2)^c\,(cH_2O)^d\,\exp\!\left[\frac{E}{T}\right] \tag{71}$$

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

$$\tau = A(P)^a\,(\text{cfuel})^b\,(cH_2O)^c\,(1+\frac{cH_2O}{\text{cfuel}})^d\,\exp\!\left[\frac{E}{T}\right] \tag{72}$$

Table 10. Combined Step Two methane with water injection chemical kinetic time correlations

Component	A	Pressure	1/T	cfuel	cO_2	cH_2O	$1+\dfrac{cH_2O}{cfuel}$	R-squared	
Fuel	6.20×10^{-9}	–0.290	14259	–0.0532	–0.332	–0.429	---	0.433	(73)
CO	1.18×10^{26}	–5.37	–1877	4.68	---	–0.106	4.90	0.627	(74)
NO_x	2.42×10^{-14}	0.585	37951	–2.92	---	0.0539	–2.98	0.879	(75)

XIV.   Comparison of the Model With the Full Mechanism Kinetics

The predictions of the full mechanism (FUEL, H, O, OH, H_2O, CO, etc.) are plotted in Figs. 17(a) and (b), and then our model predictions are superimposed on the calculations. The model predictions are close to the full mechanism predictions. We used a simple backward differencing scheme in Microsoft® Excel with a time step of 1.E-6. After the first time step, the water concentration was at 1.E-13, so we used Step 2 for the calculations. We used the inefficiency as the primary variable given by:

$$\text{INEFF} = \frac{cFuel_n}{cFuel_{n-1}} = \exp\!\left(-\frac{t_n - t_{n-1}}{\tau_F}\right) \tag{76}$$

where τ_F is given by Eqs. (36) and (59).

$$cFuel_n = cFuel_{n-1}*\text{INEFF} \tag{77}$$

The mass balances for O_2 and H_2O are

$$C_{12}H_{23} + 11.75 O_2 = 12\ CO + 11.5\ H_2O \tag{78}$$

$$CH_4 + 1.5\ O_2 = CO + 2\ H_2O \tag{79}$$
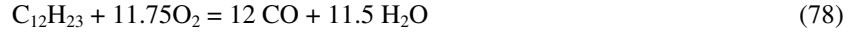
So for Jet-A

$$cH_2O = (cFuel^o - cFuel)*11.5 \tag{80}$$

$$cO_2 = cO_2{}^o - (cFuel^o - cFuel)*11.75 - 0.5\ CO_2 \tag{81}$$

$$cCO_n = (cFuel^o - cFueln)*12 - cCO_{2n}; \quad cCO_{2n} = cCO_{2n-1} + cCO_n * \exp\left(-\frac{(tn - tn - 1)}{\tau_{CO}}\right) \tag{82}$$

The agreement between the simple model predictions and the full mechanism results are quite good. The fuel falls off slightly slower for the model (235 vs. 50 microseconds for Jet-A). Some of the difference may be the result of using the full mechanism concentrations in generating the correlations rather than using the model concentrations to correlate the kinetic times. In other words the water for the full mechanism was somewhat different than assuming that water is the only H/O species. The comparison for the O_2 and H_2O is good. The increase in CO compares well, but the burnout has not been predicted, i.e. τ_{CO} is too large. The correlation for CO is not as good, $R^2 = 0.578$. Finally the model is used for comparison to the mixing times, so if the kinetics are very fast one would switch to the mixing rate limits. Also, as expected the OH, H, and O increases at almost the same rate as the H_2O, so the H_2O concentration is a good indicator of the reaction rate.

XV.   Chemical Kinetic Times for Jet-A and CH4

Chemical kinetic times versus equivalence ratio are plotted in Figs. 18 to 20 at 2000 K and 10 atm. Correlation Step 1 and 2 are shown with Step 2 computed at the 50 percent INEFF value. For step 1 (18a), Jet-A was about 100 times faster than methane. The Jet-A mechanism includes a forward irreversible breakup of the fuel to CH and C_2H_2. For correlation Step 2, methane is faster. Addition of 0.5 gm H_2O/gm fuel does not change the rates much. It does accelerate the fuel kinetic times by 30 percent for Jet-A on the rich side. The CO reaction (19a) was much slower for Jet-A than for methane. The time for correlation Step 1 was long for methane being 1 millisecond for the lean conditions and 10 milliseconds for the rich conditions. For step 2, the CO burnout rates were 1.E-4 milliseconds for methane and 1.E-3 to 1.E-1 milliseconds for Jet-A. Additional water increased the kinetic times from 7.E-5 to 2.E-4 milliseconds. The times are still very small.

Instead of τ_{NOX} as ms-cc/mole, we chose to plot τ as ms/ppp.

$$\tau\ {}^{ms}\!/_{ppm} = \tau\left(\frac{ms \cdot cc}{mole\ NO_x}\right)*\rho\left(\frac{moles\ mix}{cc}\right)*1.e^{-6}\left(\frac{mole\ fraction}{ppm}\right) \tag{83}$$

The predicted NO_x production rates for correlation Step 2 are about two orders of magnitude faster than for Step 1, probably because of the large concentration of radicals. The kinetic times are surprisingly constant with equivalence ratios for the lean and rich cases indicating a relatively low value for the cFuel correlation exponent.

XVI.   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 3. This reduction is with constant T4. So the equations from Table 1 Lean T4 are solved for the increased f/a with an increase in, H_2O/F, then the NO_x value Table 3 Step One Lean is solved for the new NO_x value.

Figures 21 and 22 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 3. 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).
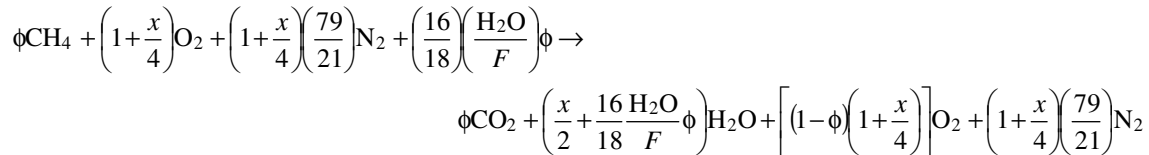
XVII.   Tanks in Series Model for Predicting Emissions

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 10. This model accounts for the increase in fuel/air ratio in the initial fuel injection and mixing process. Figures 23 to 26 show the results of this comparison.
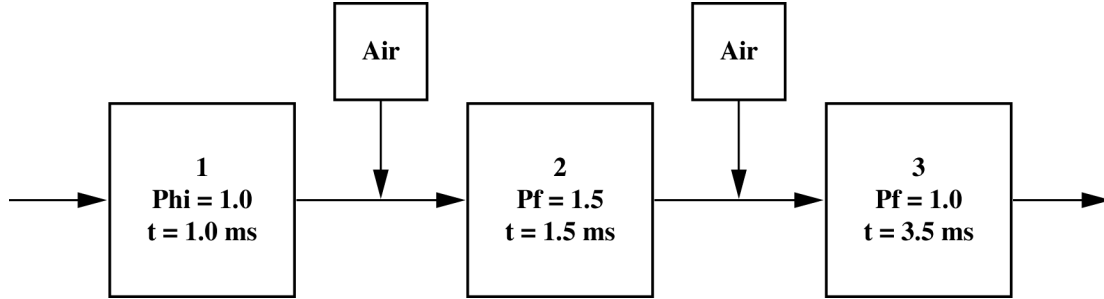
Pf is the ratio of the tank f/a to the exit f/a. The primary zone (tank 1 was set at stoichiometric conditions, Phi = 1.) for all computations. This prevented it from going overstoichiometric as the exit f/a was increased. Then T4 was computed from Eq. (23) and all of the concentrations computed. Reference 10 used 15 reactors with two recycle loops and 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 of the NO_x (Figs. 23 and 25) and the CO (Figs. 24 and 26) are not quite as close to the Reference 10 predictions, but these equations are simple to use and the trends and magnitudes of the predictions are correct.

The Fortran computer code is given in Reference 1. 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:

$$\phi CH_4 + \left(1+\frac{x}{4}\right)O_2 + \left(1+\frac{x}{4}\right)\left(\frac{79}{21}\right)N_2 + \left(\frac{16}{18}\right)\left(\frac{H_2O}{F}\right)\phi \rightarrow$$

$$\phi CO_2 + \left(\frac{x}{2}+\frac{16}{18}\frac{H_2O}{F}\phi\right)H_2O + \left[(1-\phi)\left(1+\frac{x}{4}\right)\right]O_2 + \left(1+\frac{x}{4}\right)\left(\frac{79}{21}\right)N_2$$

where x is the ratio of hydrogen to carbon, and is equal to 4 for methane. The $\frac{H_2O}{F}$ 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 percent O_2.

XVIII.   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. Accurate step one Jet-A correlations were developed ($R^2 > 0.9$). The Jet-A step two correlations for CO and NO_x are slightly less accurate, but still thought to be effective. The Methane step one correlations were all very accurate, 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—Multiple Linear Regression With Microsoft® Excel

A. 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.

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

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

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 Microsoft® 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 Microsoft® 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 Microsoft® Excel 2003 and was used for all equations given in this report. Microsoft® Excel has the capability to handle one dependent variable and multiple independent variables. As many as 42,000 points were used in the regressions.

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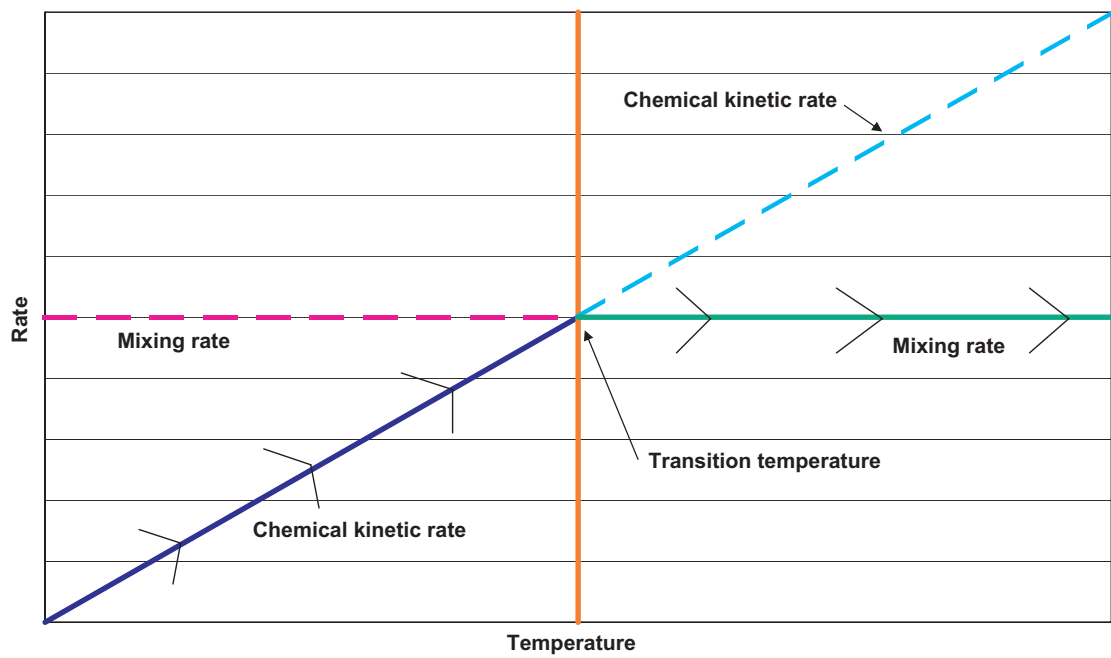11. GRI-Mech Version 2.1 released 9/6/95 http://www.me.berkeley.edu/gri_mech/
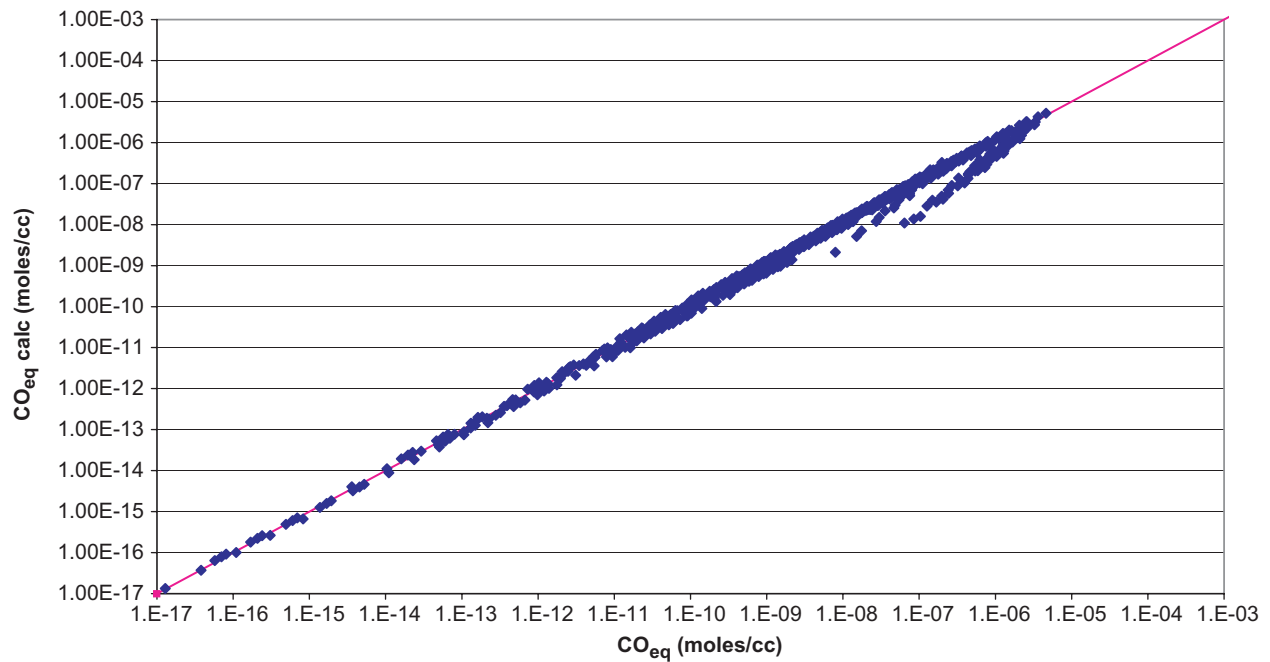
Figure 1. Magnussen mixing model.

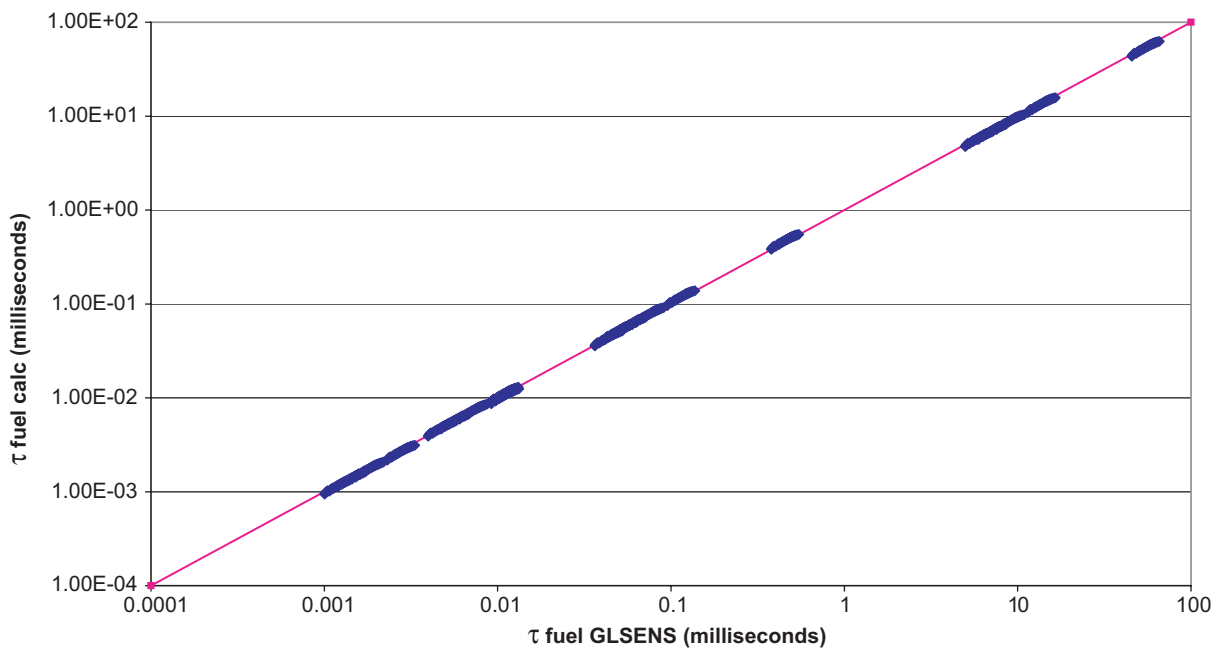**Figure 2. Equilibrium Jet-A water injection CO_{eq} parity, $0.2 <$ Eratio $ 1.0$ (lean).**

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Figure 3. Kinetic Jet-A water injection fuel τ parity, step one (lean).
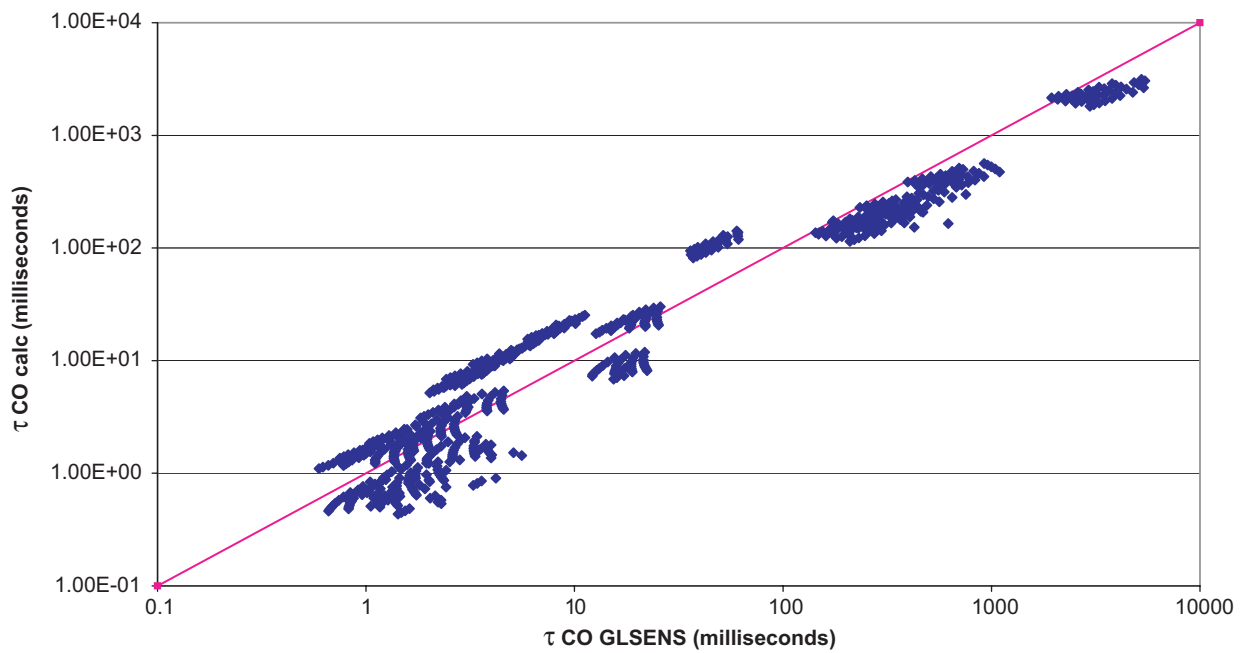
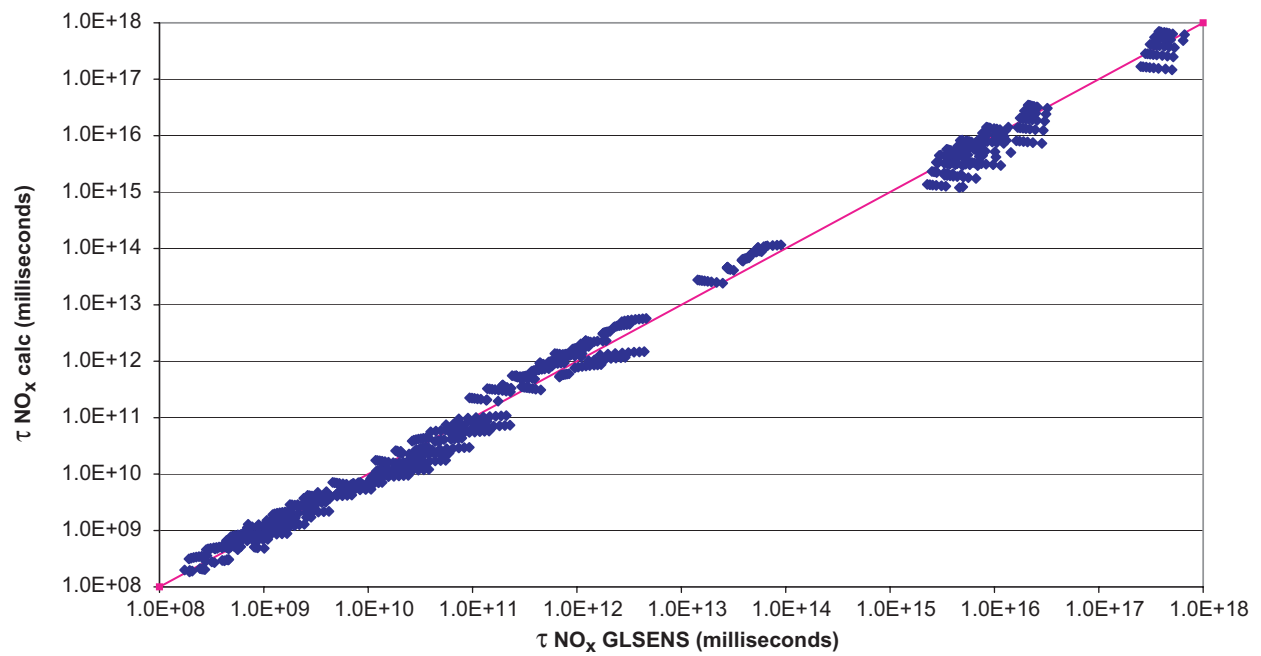**Figure 4. Kinetic Jet-A water injection CO τ parity, step one (lean).**

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Figure 5. Kinetic Jet-A water injection NO$_x$ τ parity, step one (lean).
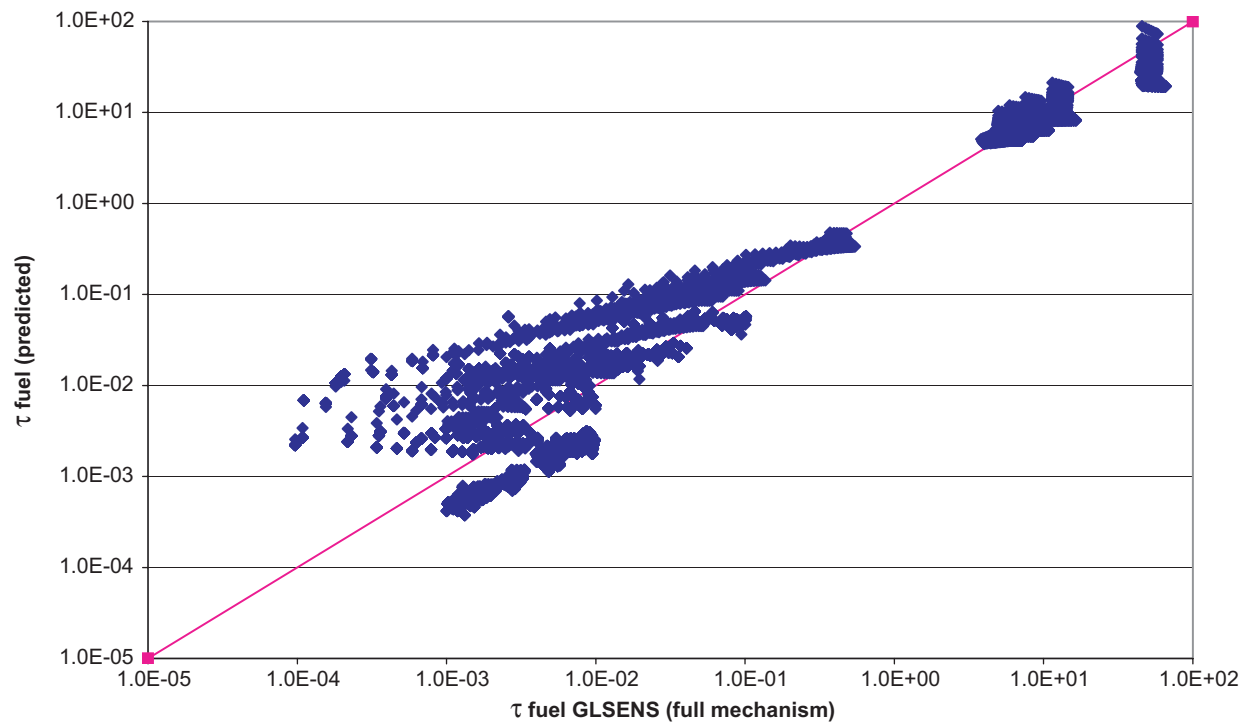
Figure 6. Kinetic Jet-A fuel τ parity, step two (lean).

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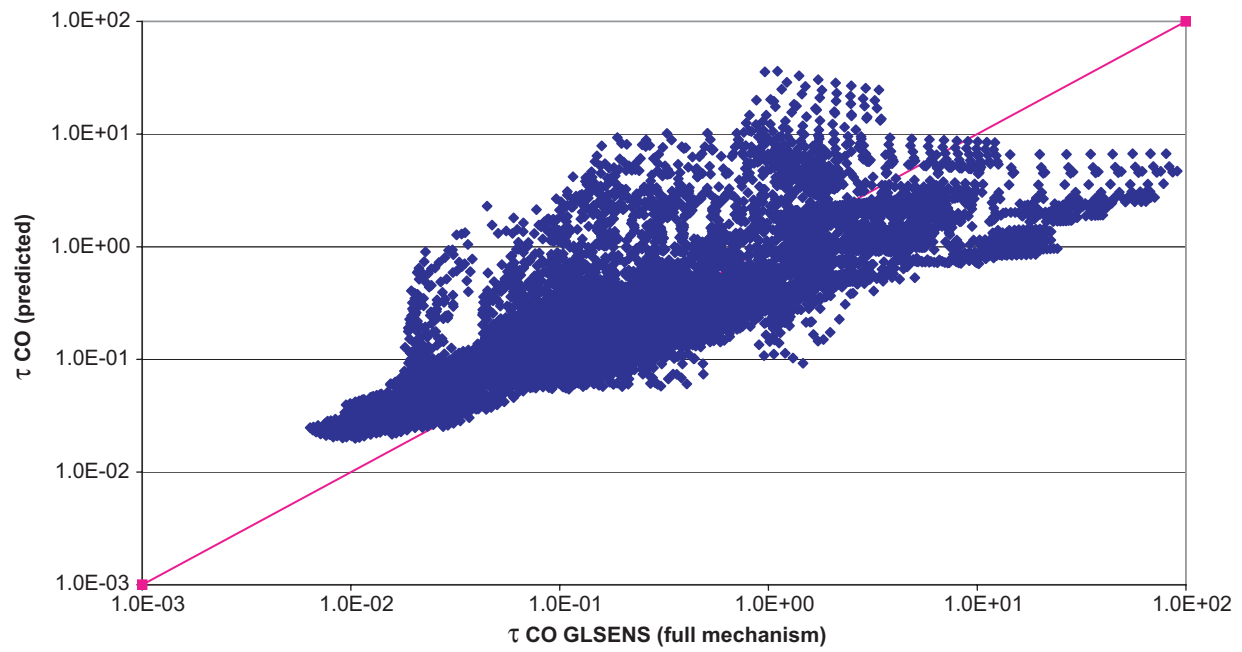
Figure 7. Kinetic Jet-A CO τ parity, step two (lean).
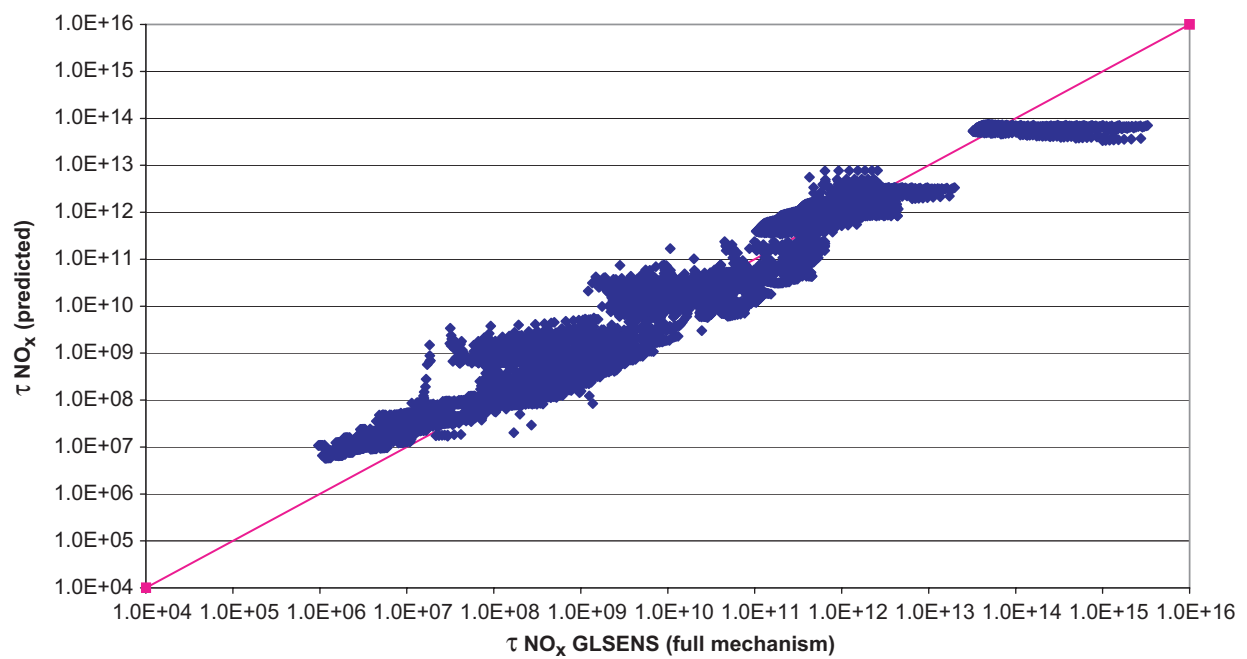
Figure 8. Kinetic Jet-A NO_x τ parity, step two (lean).

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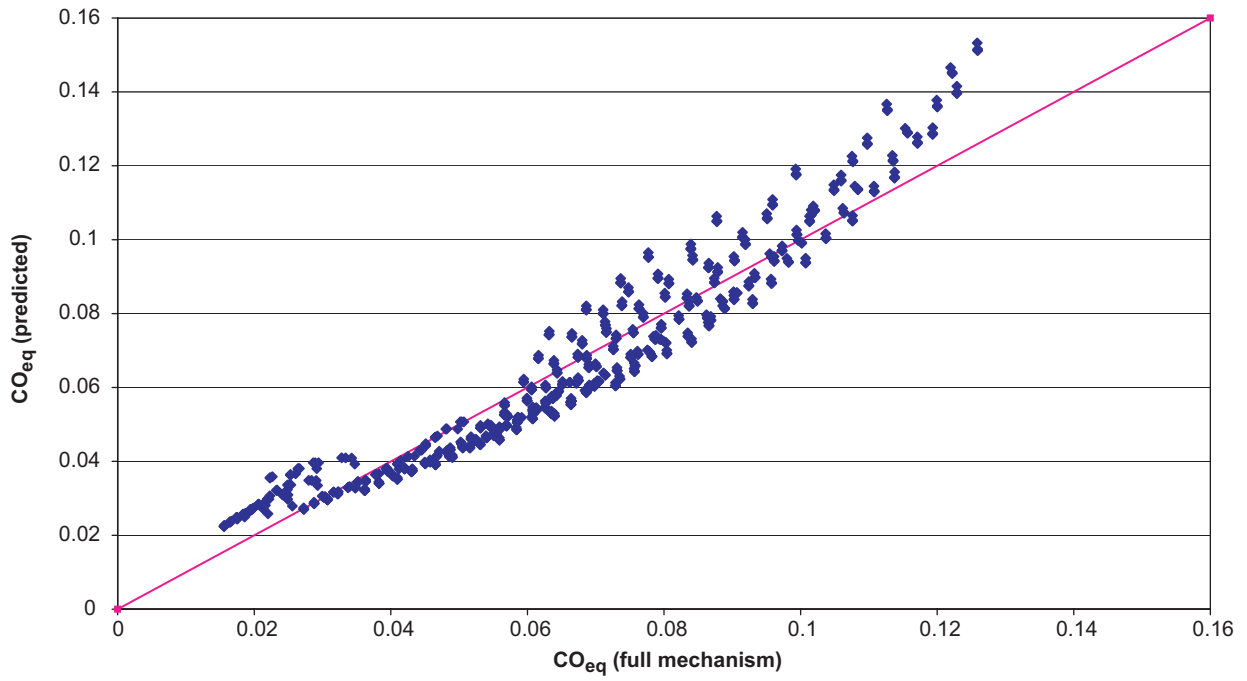
Figure 9. Equilibrium methane CO parity (rich).
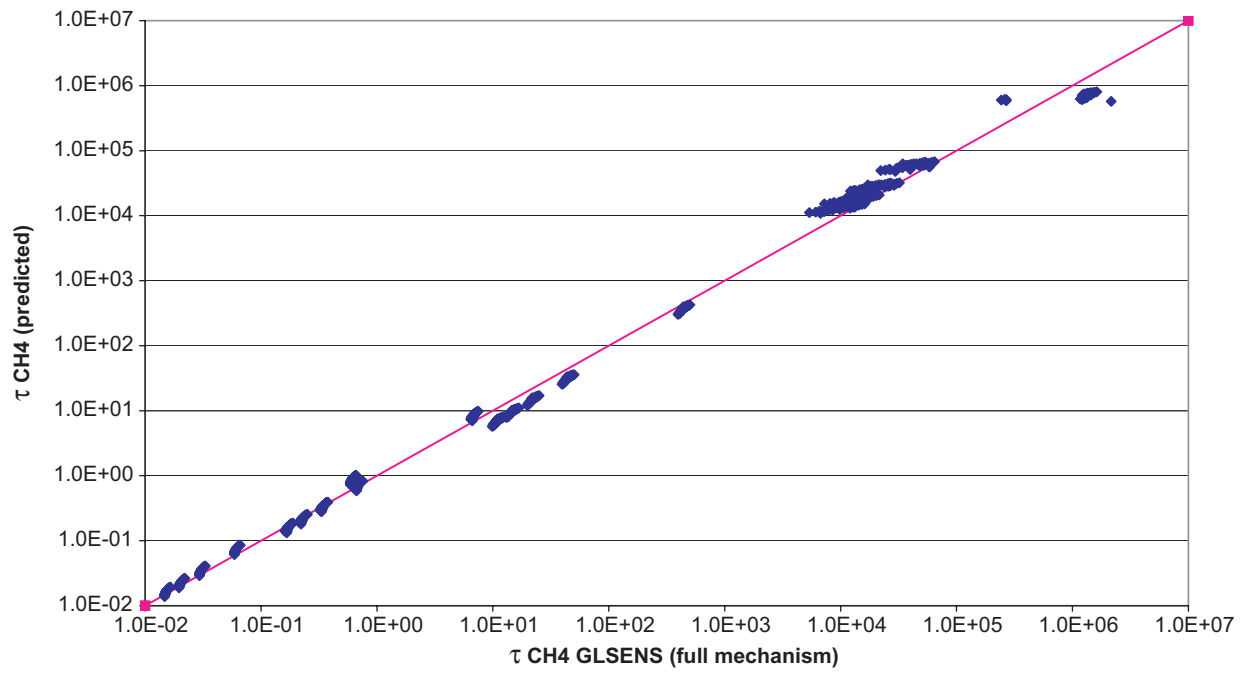
Figure 10. Kinetic methane fuel τ parity, step one (lean).

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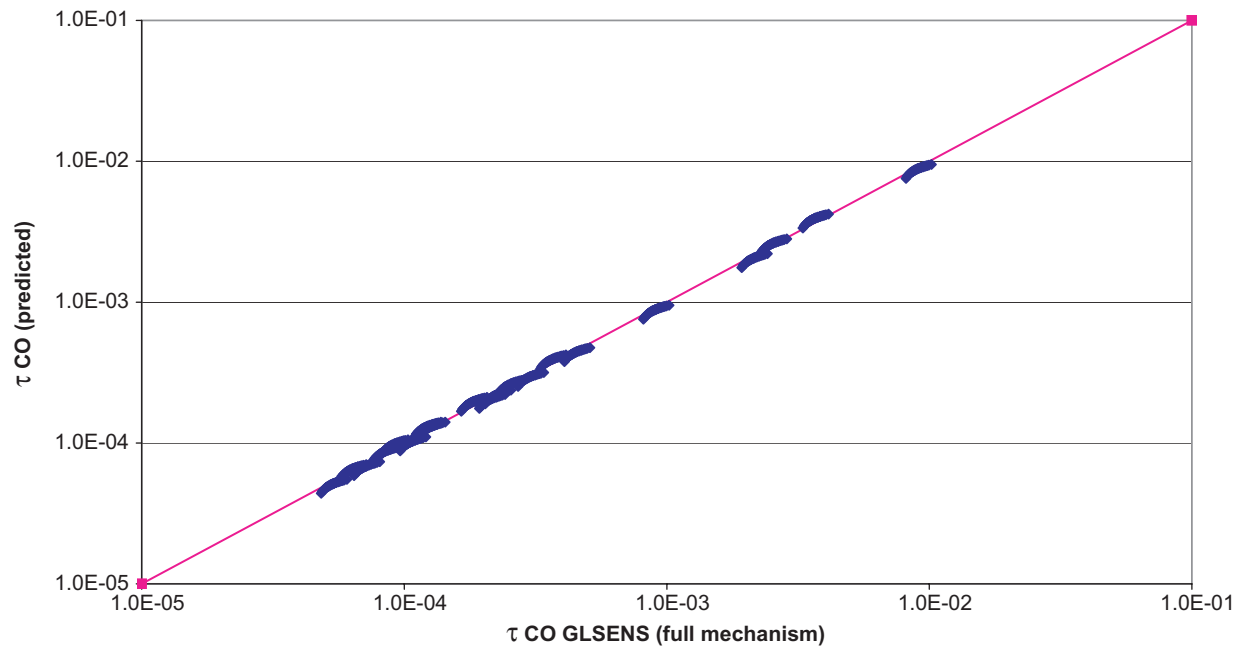
Figure 11. Kinetic methane CO τ parity, step one (lean).
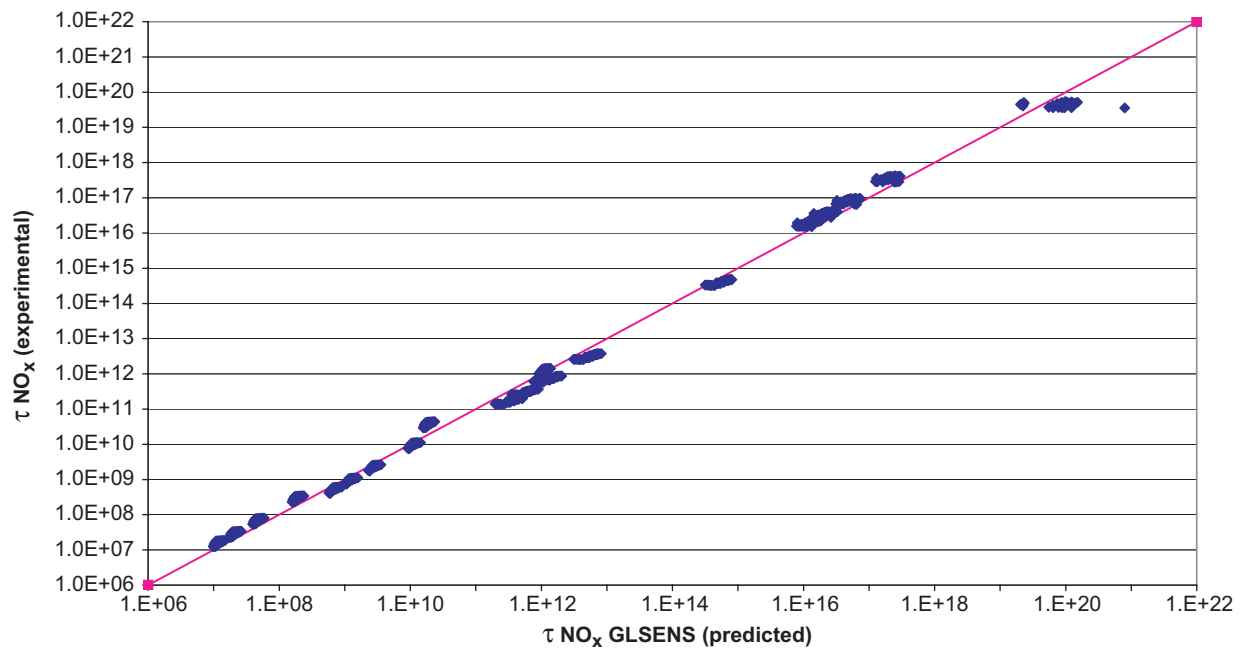
Figure 12. Kinetic methane NO$_X$ τ parity, step one (lean).

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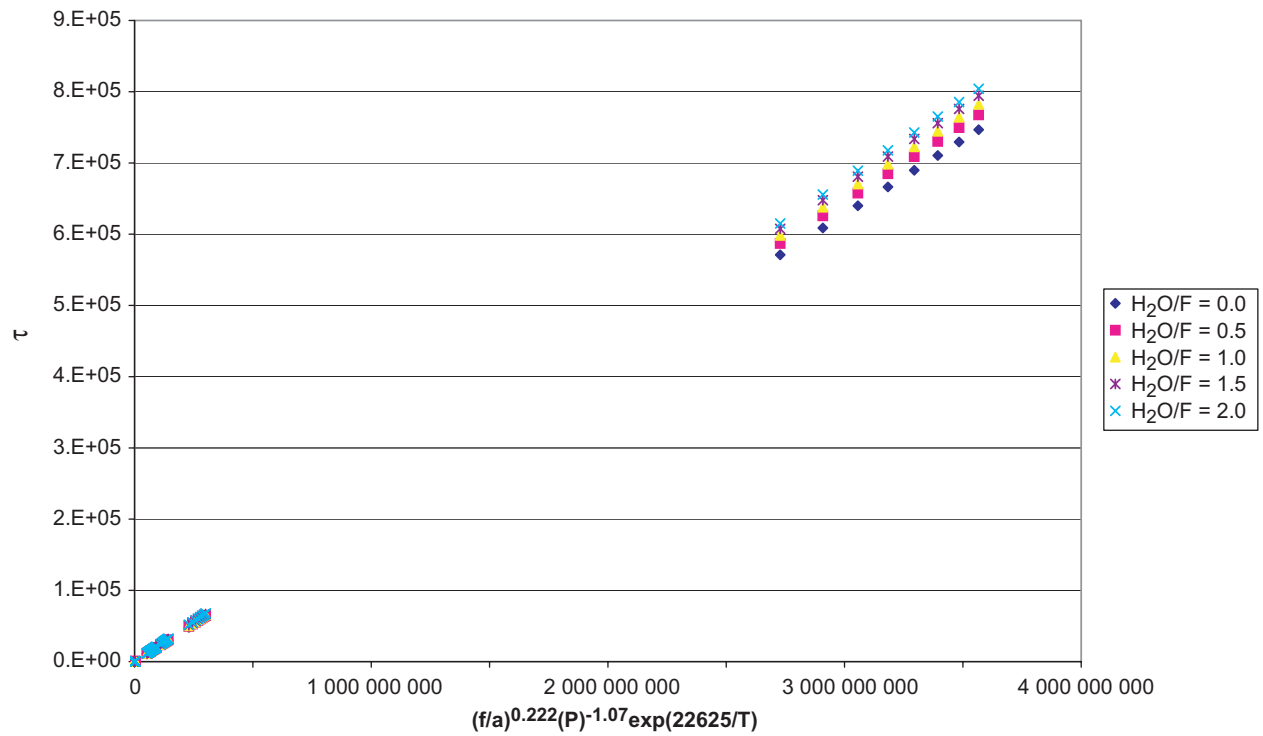
Figure 13. Methane fuel simple step one lean model.
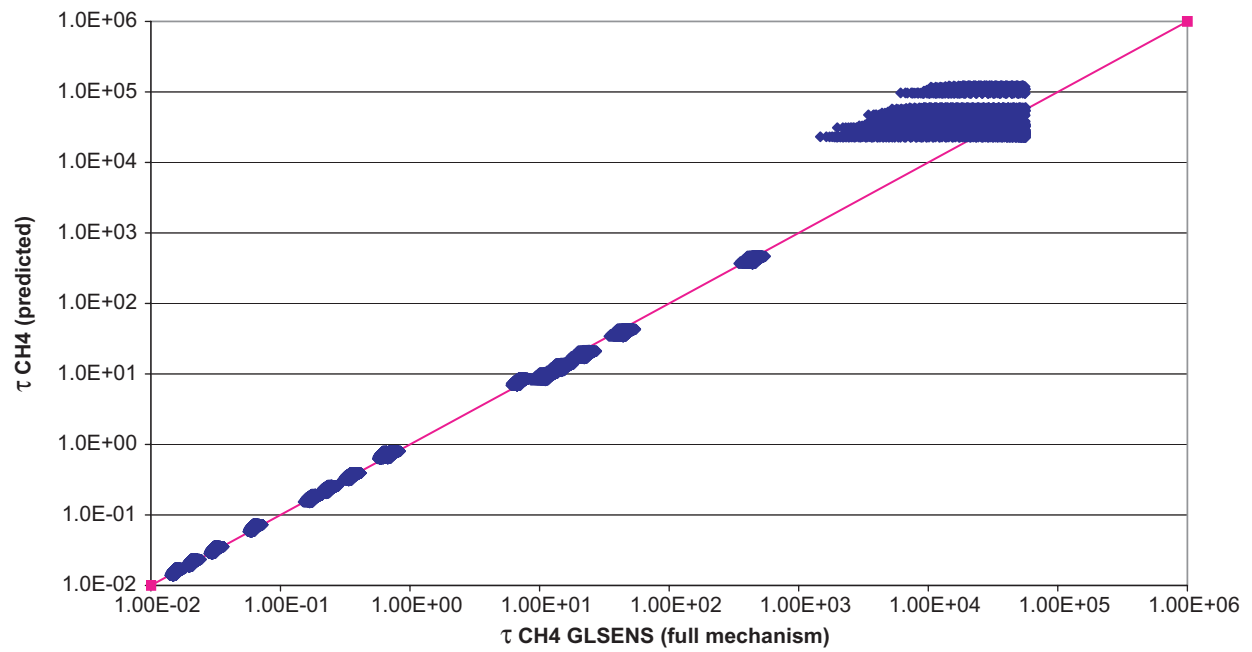
Figure 14. Kinetic methane τ fuel parity, step two (lean).
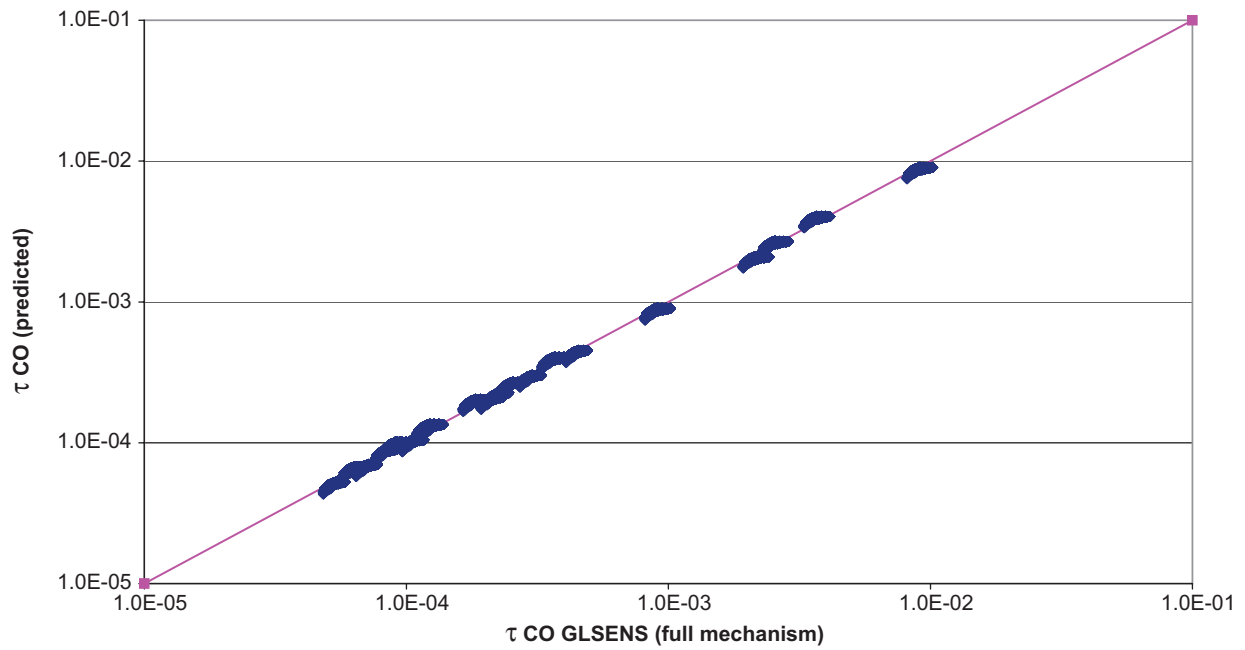
Figure 15. Kinetic methane CO τ parity, step two (lean).
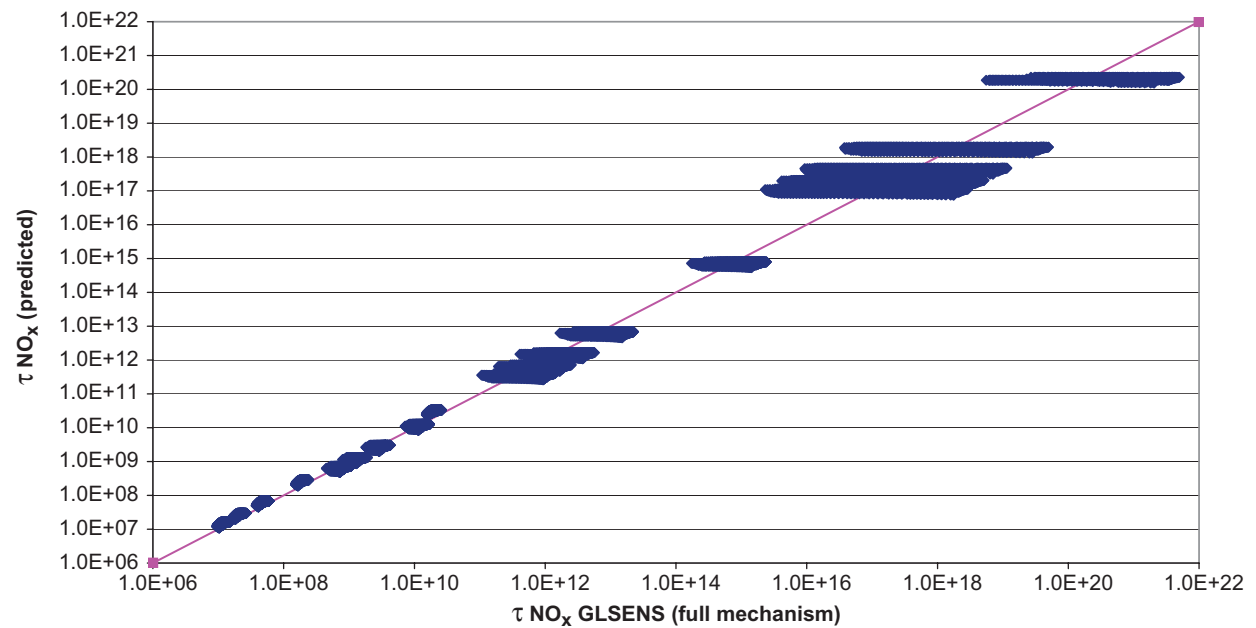
Figure 16. Kinetic methane NO$_X$ τ parity, step two (lean).

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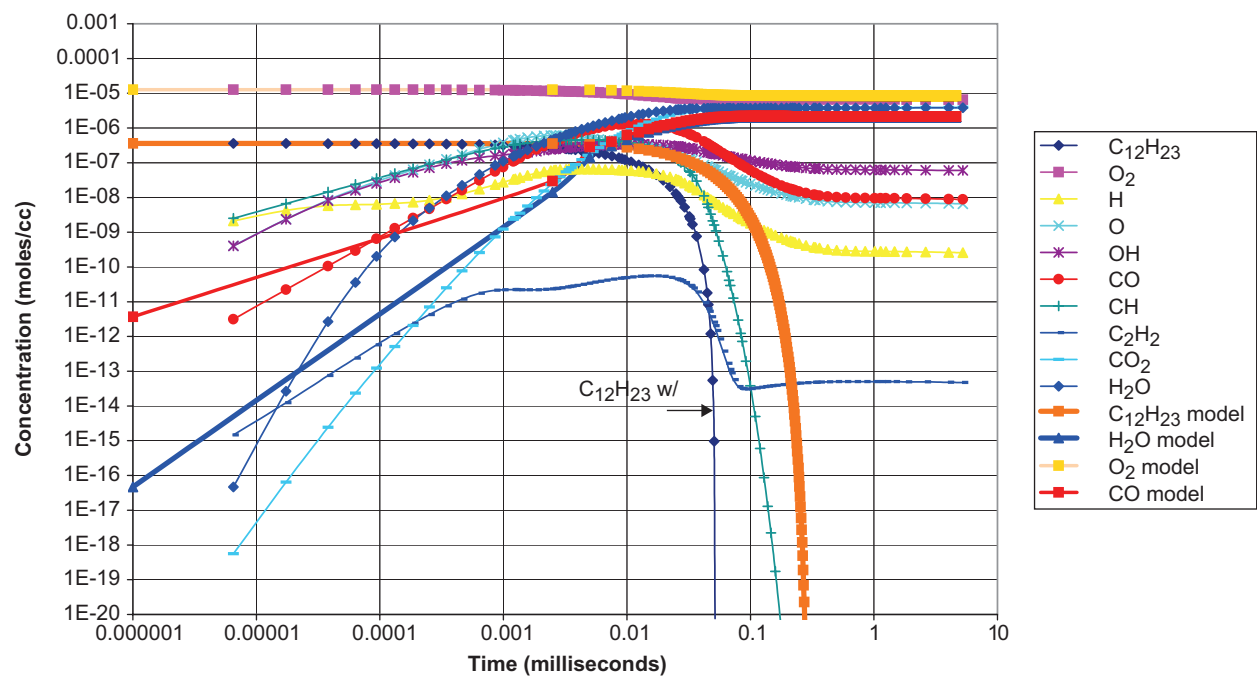
Figure 17a. Comparison of new one step model with full mechanism for Jet-A. T = 2000 K, P = 10 atm, Phi = 0.5. No water injection.
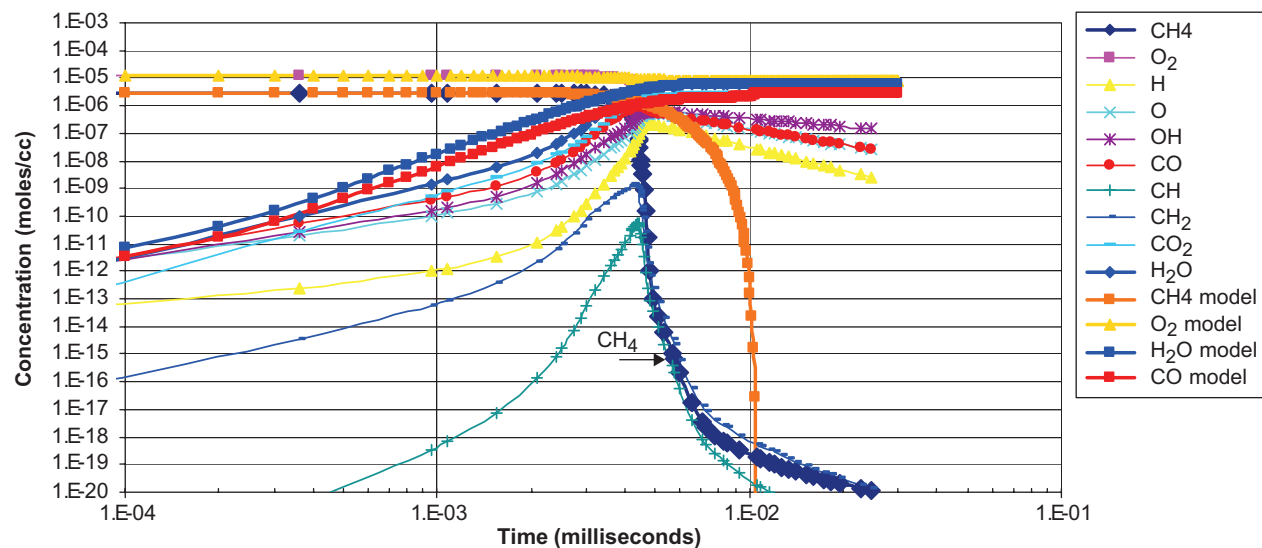
Figure 17b. Comparison of new two time step model with full mechanism for methane at 2000 K and 10 atm. Phi = 0.5. No water injection.

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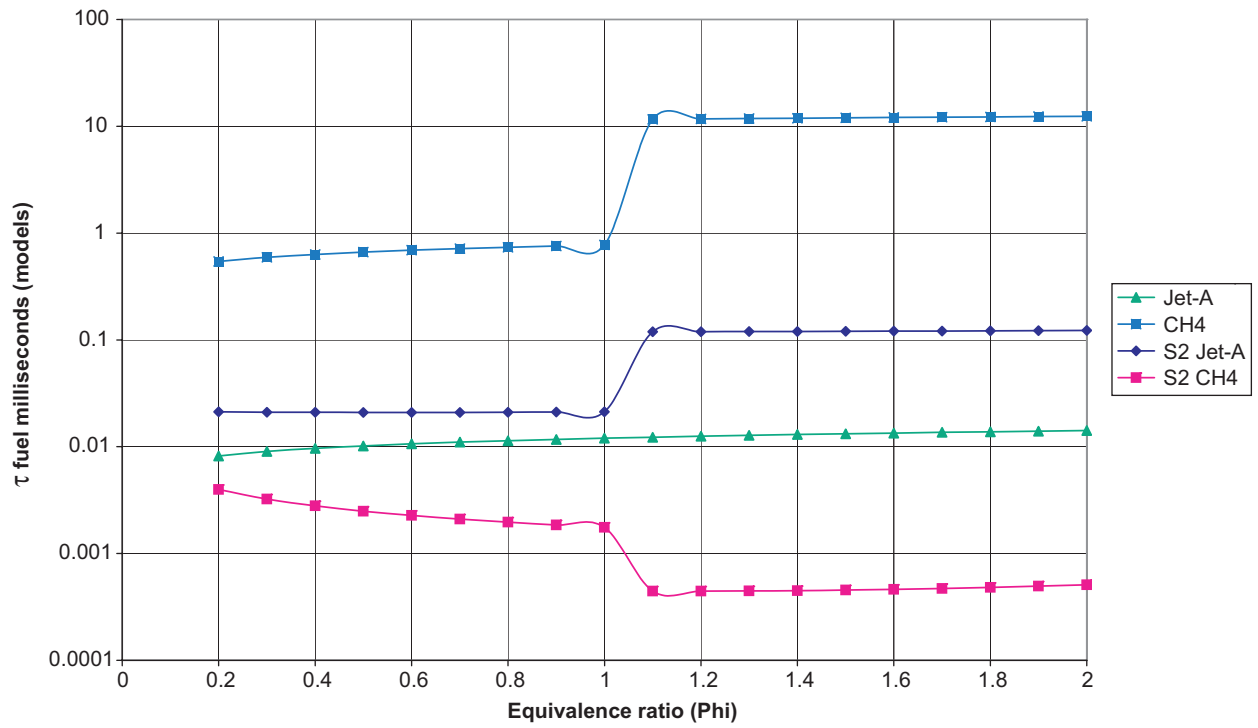
Figure 18a. Kinetic τ fuel at 10 atm and 2000 K for fuel reactions step one and two (lean and rich) without water injection.
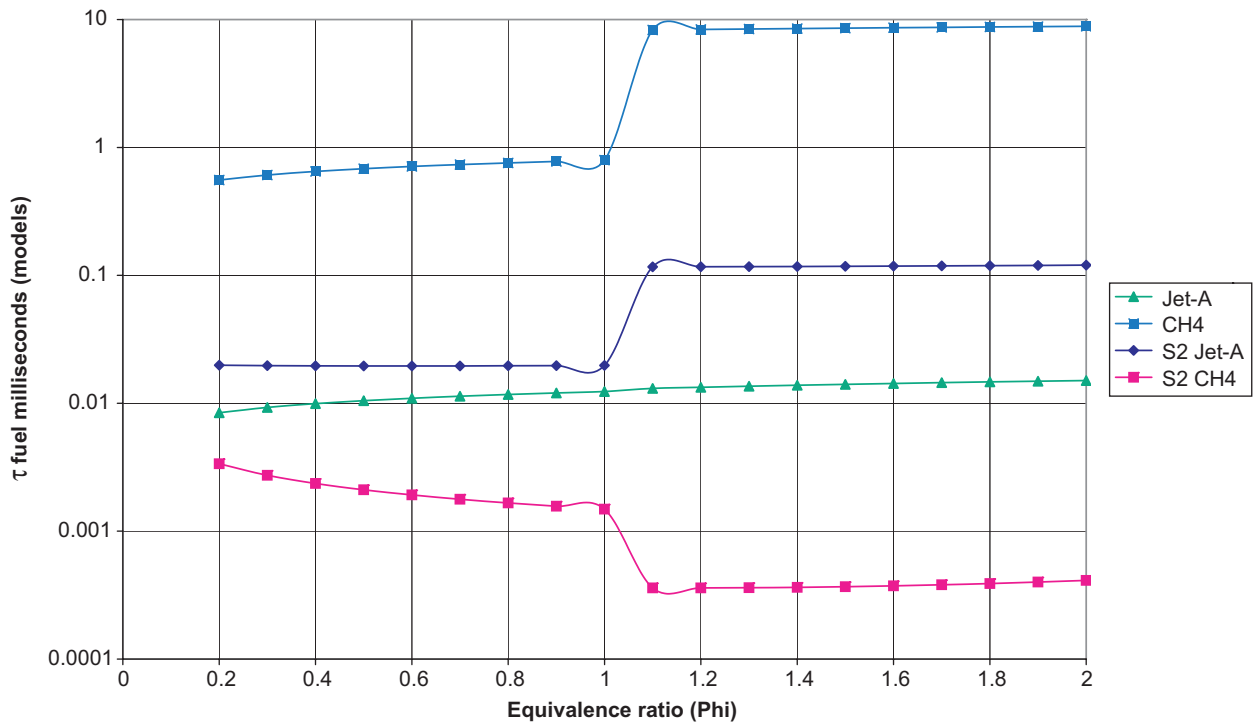
Figure 18b. Kinetic τ fuel at 10 atm and 2000 K for fuel reactions step one and two (lean and rich) with water/fuel 0.5 gm H_2O/gm fuel.
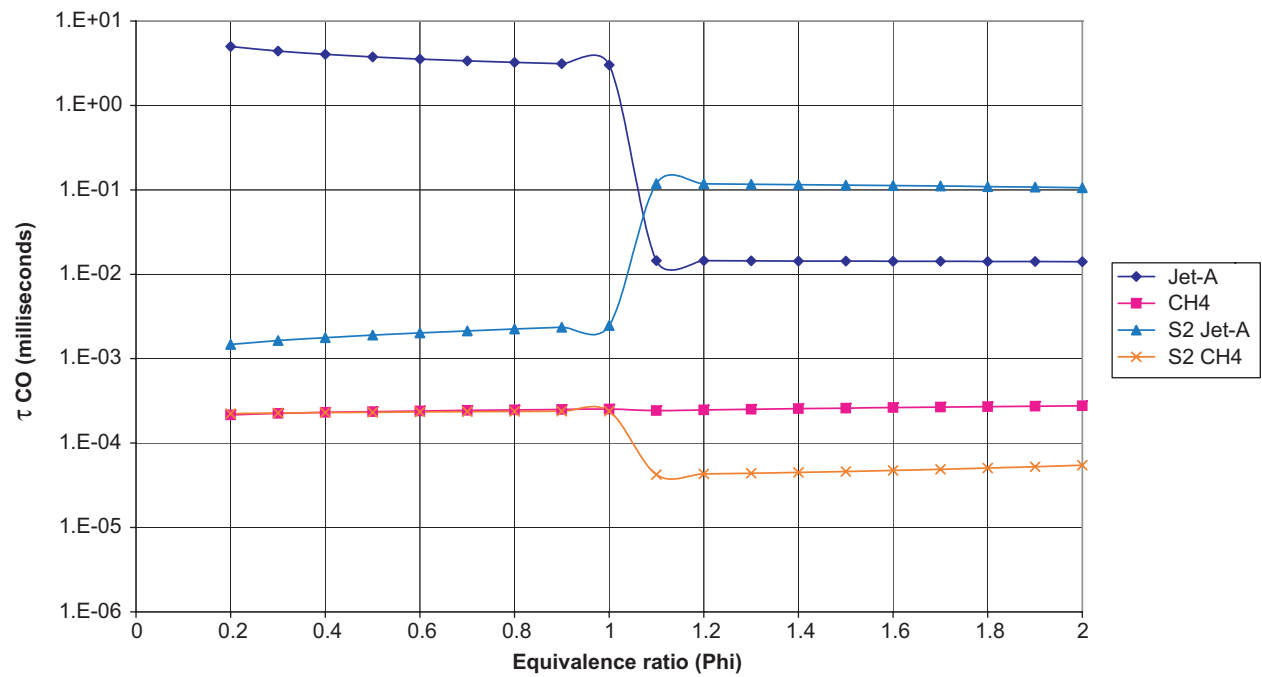
Figure 19a. Kinetic τ CO at 10 atm and 2000 K for CO step one and two (lean and rich) without water injection.
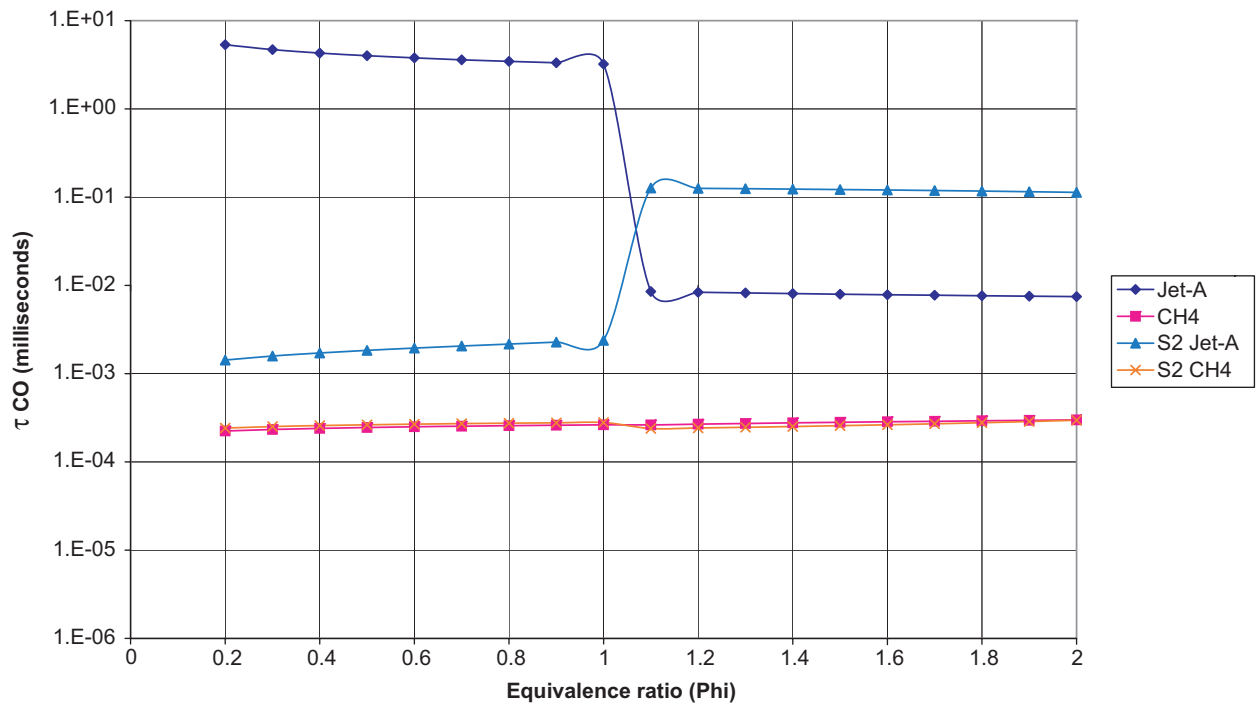
Figure 19b. Kinetic τ CO at 10 atm and 2000 K for step one and two (lean and rich) with water/fuel of 0.5 gm H_2O/gm fuel.

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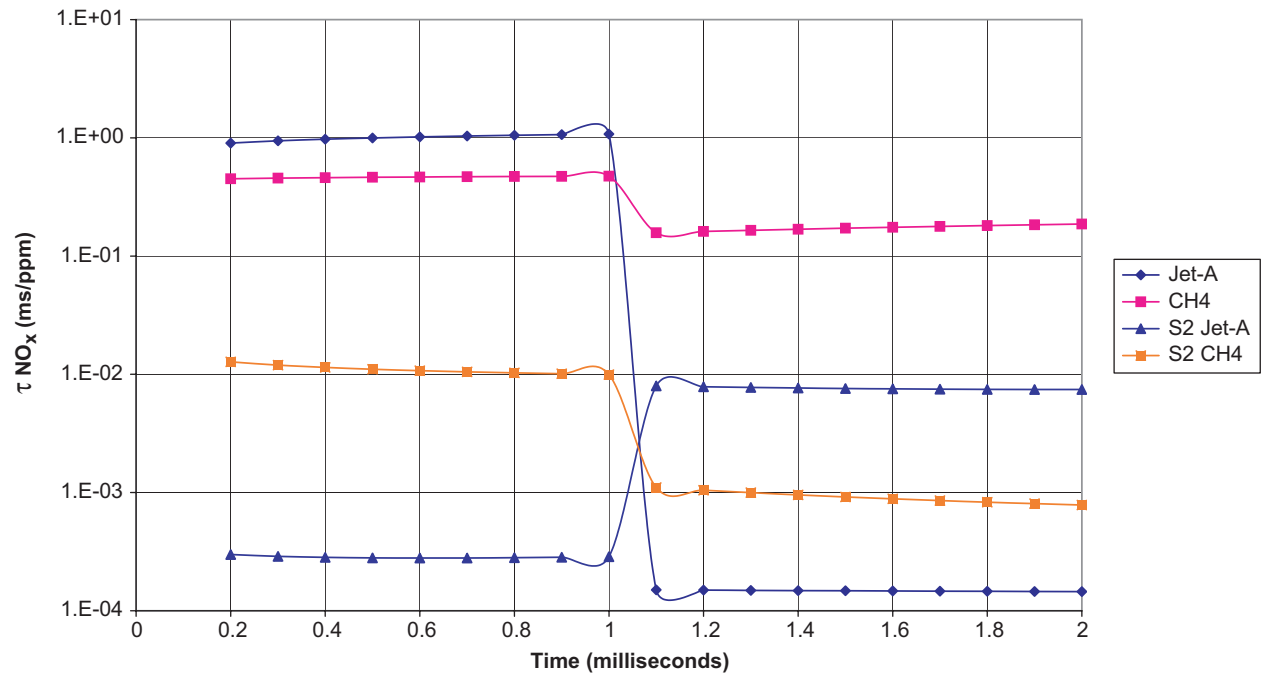
Figure 20a. Kinetic τ NO$_x$ milliseconds/ppm at 10 atm and 2000 K for NO$_x$ reaction step one and two (lean and rich) without water injection.

Figure 20b. Kinetic τ NO$_x$ milliseconds/ppm at 10 atm and 2000 K for NO$_x$ reaction step one and two (lean and rich) with water/fuel of 0.5 gm H$_2$O/gm fuel.

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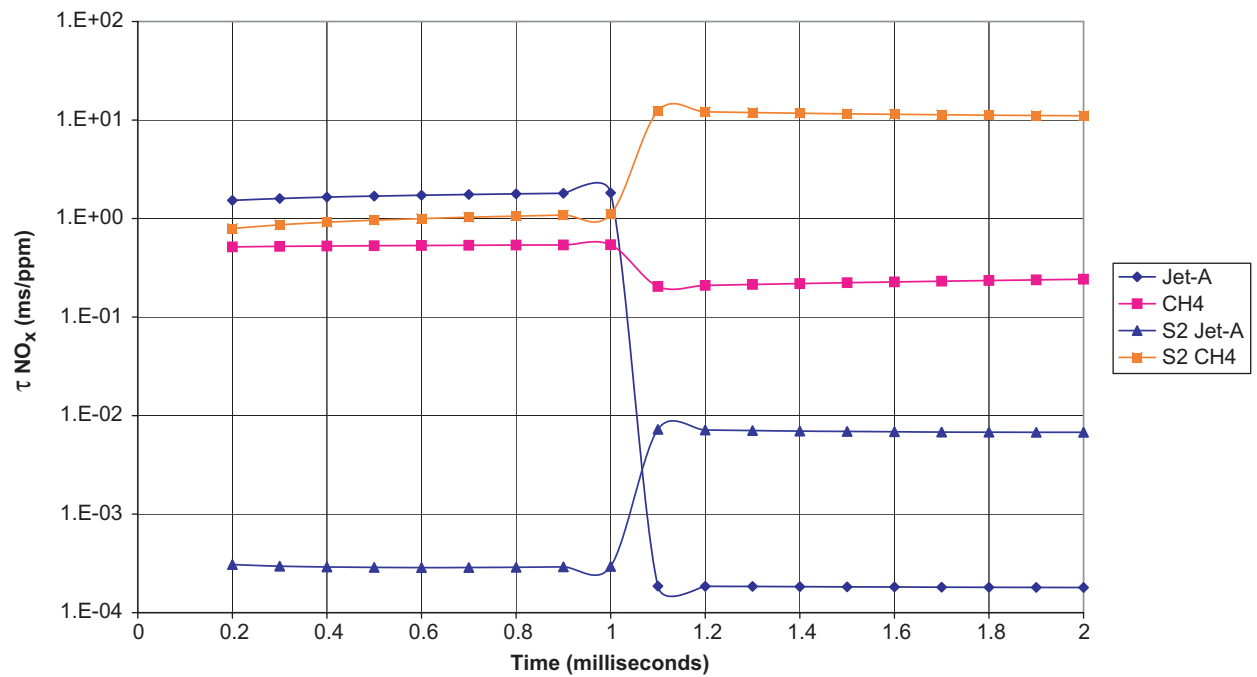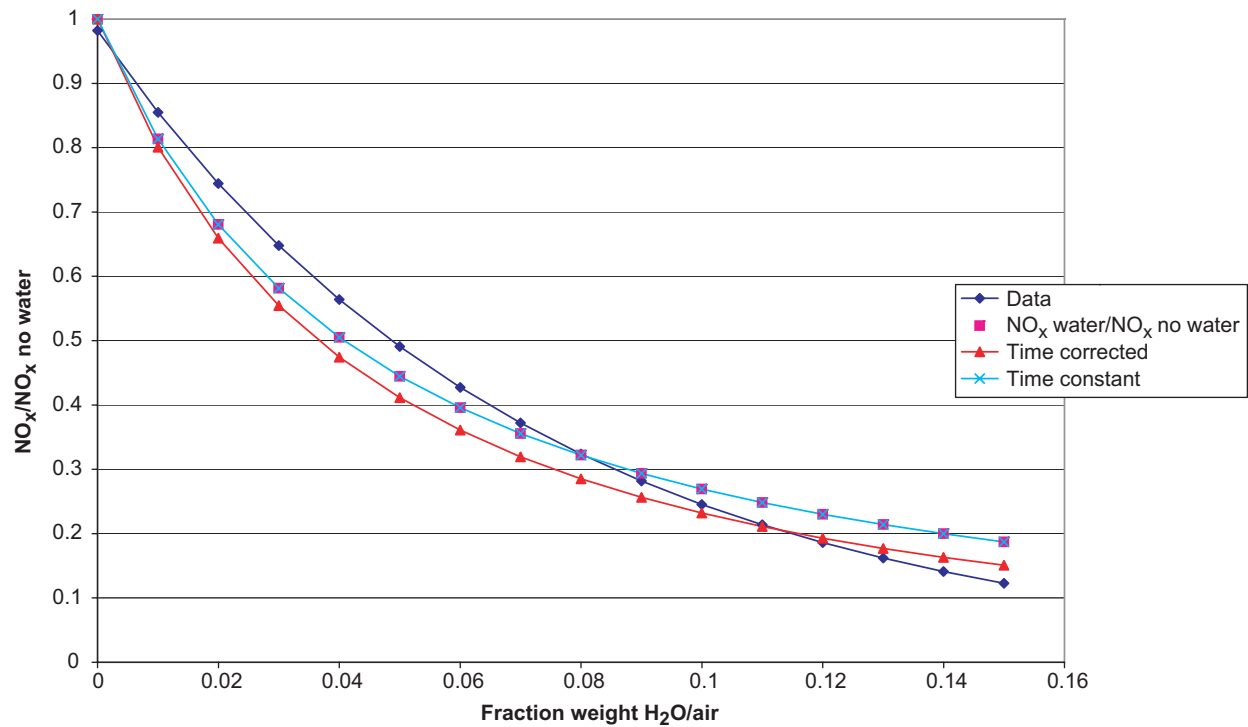
Figure 21. NO$_X$ water/NO$_X$ no water for Jet-A at f/a = 0.06.
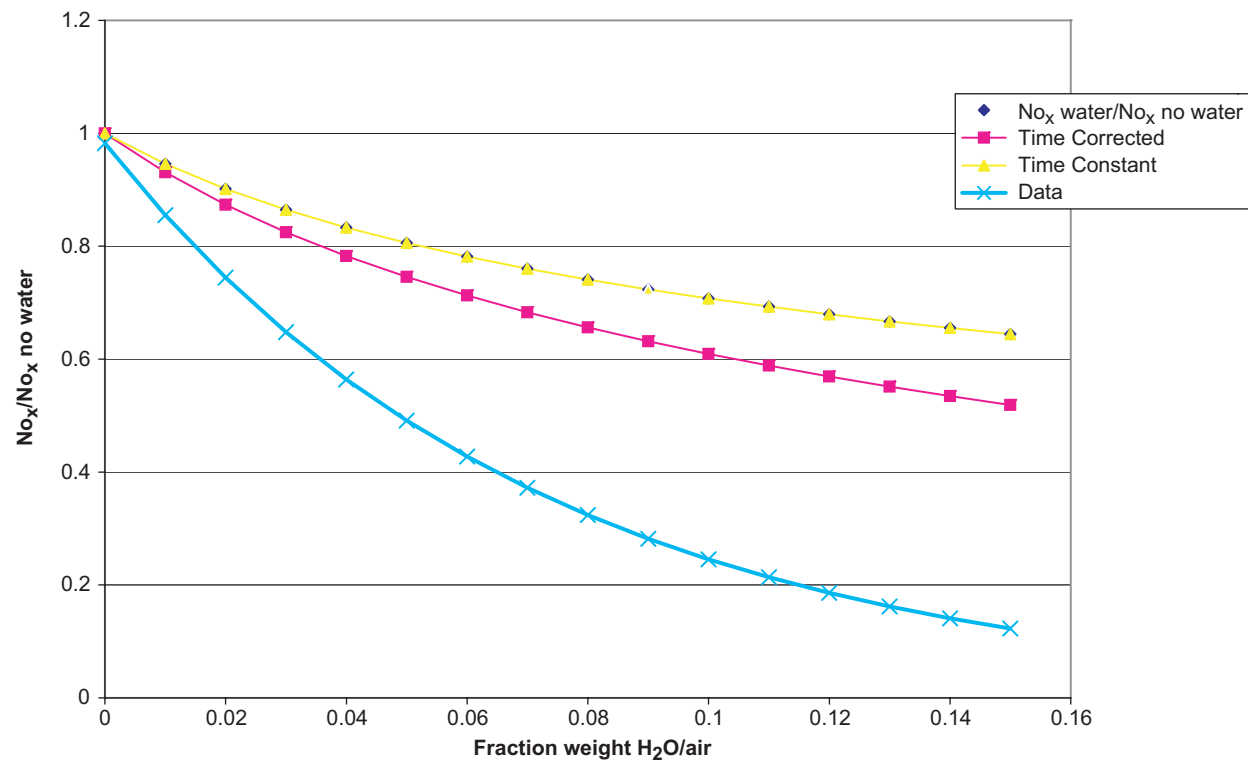
Figure 22. Methane data comparison (f/a = 0.055).

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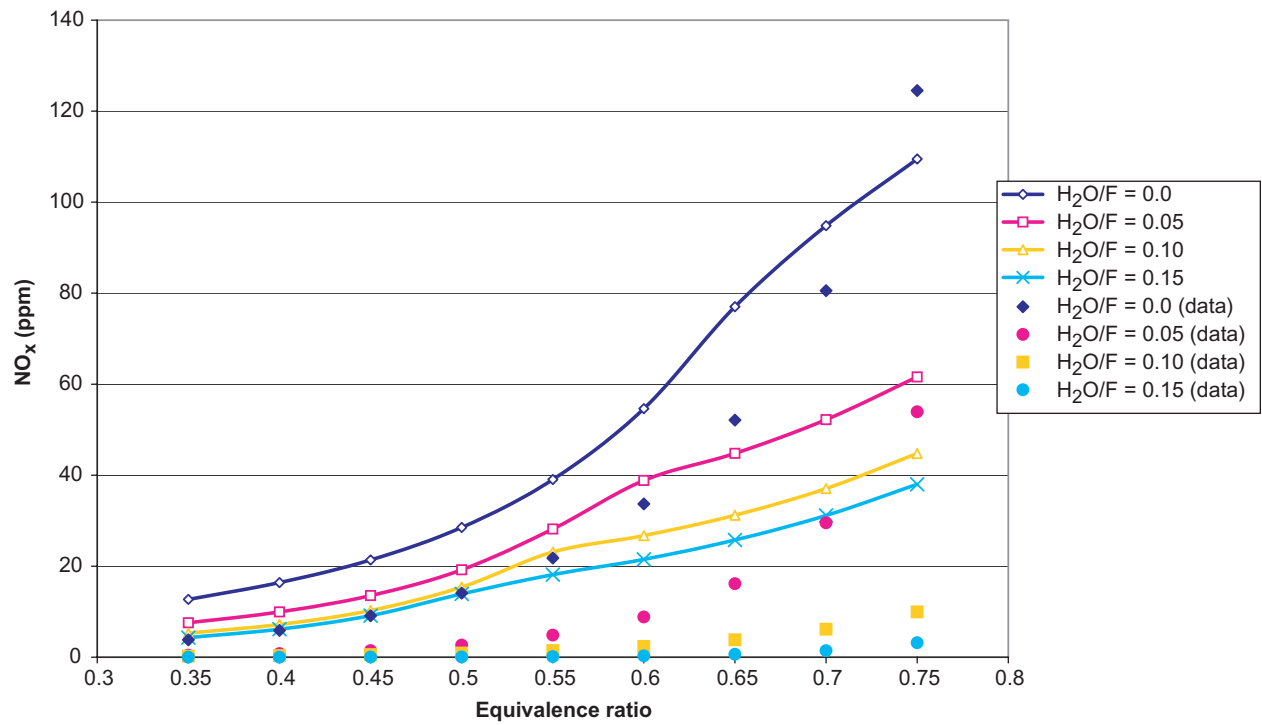
Figure 23. Methane tanks in series, fa < 0.059.
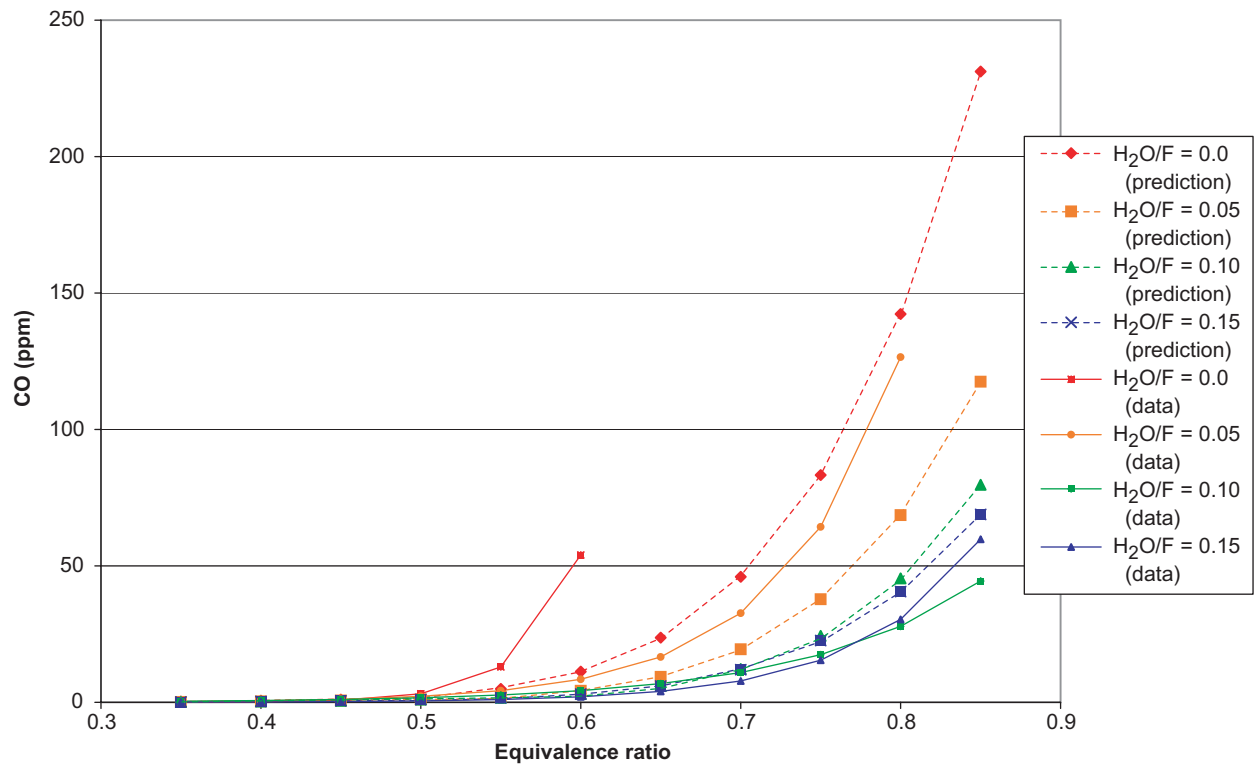
Figure 24. Methane CO versus equivalence ratio, f/a < 0.059.

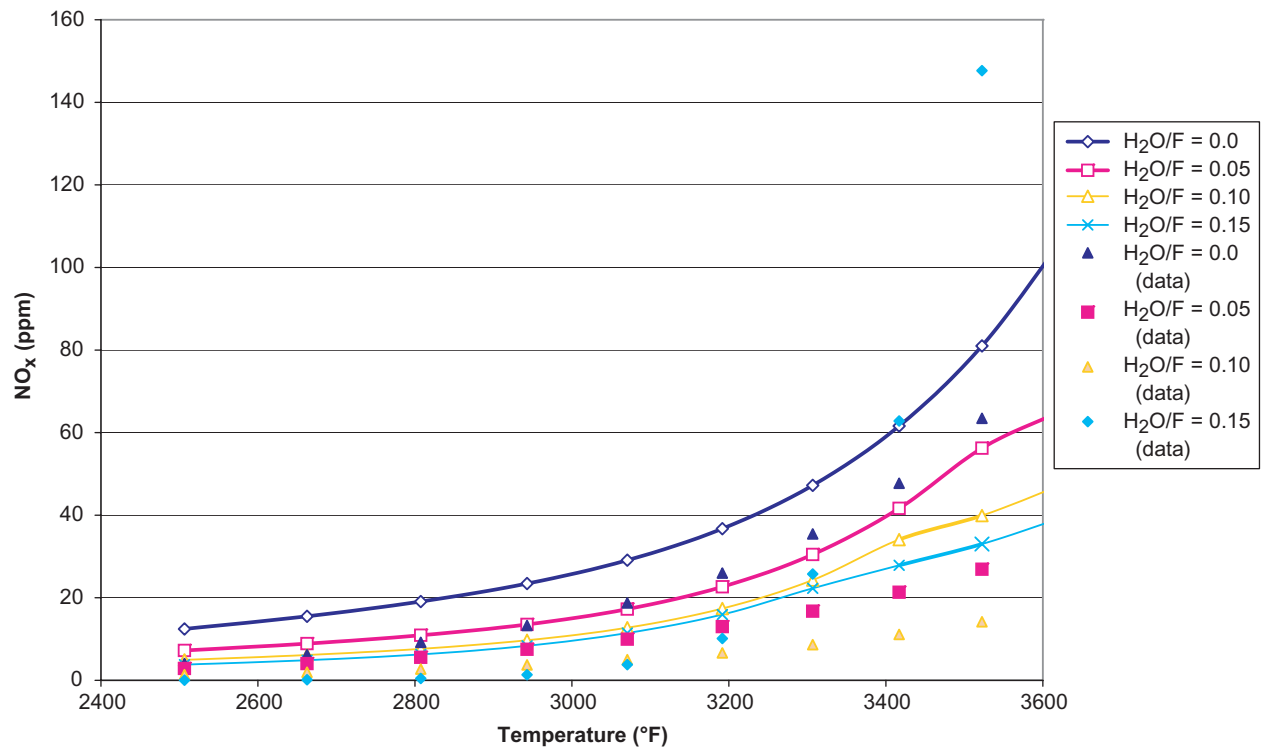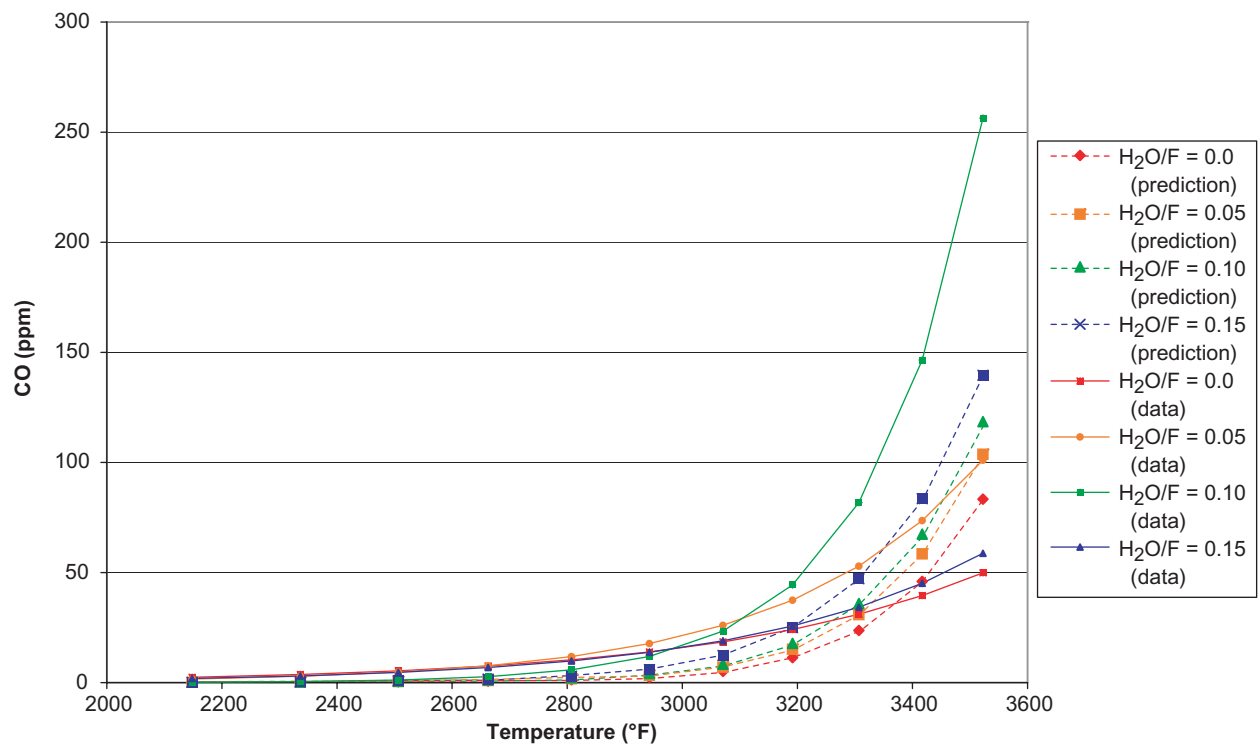American Institute of Aeronautics and Astronautics

Figure 25. Methane NO$_X$ versus temperature.

Figure 26. Methane CO versus temperature, f/a < 0.059.

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