EVALUATION OF POLLUTANTS IN COMBUSTION
OF AN INDIAN COAL

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ABSTRACT

Kinetic modelling of NO_x, CO_x and hydrocarbons is carried out incorporating 107 reactions pertaining to the combustion of coal in order to evaluate the concentration of pollutants at a given temperature and fuel/air ratio during the combustion of an indian variety of coal, called Sangrauli coal, in a particular power plant. The results, obtained for the concentration of pollutants in the emission of combustion of this variety of coal, have been presented in the form of graphs.

Key words : Combustion, Sangrauli coal, Pollutants

INTRODUCTION

The continuously increasing air pollution in the atmosphere and health risks associated with it, has attracted the attention of many scientists and engineers towards this area of study. Combustion of different types of fossil fuels is one of the major sources of air pollution. It is known that chemical kinetics deal with changes in chemical reactions with time. Equations of chemical kinetics are found to be useful in investigating the process of combustion of fossil fuels in the power plants.[1-4] For this, non-linear differential equations representing the non-equilibrium time behaviour of chemical species covered in the combustion process are solved with a suitable numerical method taking into consideration the problems of stiffness and time-step control.

Mitchel and Tarbel[1] have studied the kinetic modelling of nitric oxide formation during pulverized coal combustion. The study on simultaneous reduction of SO_x and NO_x in an entrained-flow reactor has been conducted by Wang et al.[5]. Yossefi et al.[6] studied modelling of combined effects of detailed chemical kinetics and thermal properties on the early stages of combustion of methane and ethane with CO_2 replacing N_2 as a diluent. Reduction of nitrogen oxides from post-combustion gases utilizing molecular radial species has been studied by Boyle et al.[7]. Verma and Okazaki[8] have studied kinetics of nitrous oxide formation from pulverized coal combustion at low temperature. Devanathan and Saxena[9] have studied devolatilization modelling of large coal particles. The study on numerical simulations of axisymmetric stretched

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premixed laminar twin flame burning methane in air has been done by Yang and Puri[4] in order to understand the formation of NO_x.

In the present study, we have carried out the evaluation of the concentration of NO_x, CO_x and hydrocarbon pollutants during the combustion of an Indian variety of coal in a particular power plant using the method of kinetic modelling for 107 combustion reactions pertaining to this variety of coal.

EXPERIMENTAL

Analytical Technique for Chemical Kinetics

Let us consider a set of j chemical reactions involving i different chemical species. Let n_i (i = 1,2,3....I) be the time dependent molar density of the ith species. The jth reaction with forward rate constant K_f and backward rate constant K_b can be written as :

$$n_{j1} + n_{j2} = n_{j3} + n_{j4} \qquad ...(1)$$

where 1, 2, 3 and 4 are simply the specific values of the index i associated with the reactants and products of the jth reaction. Time-dependent forward and backward rates, R_{fj} and R_{bj}, respectively of the jth reaction can be written as :

$$R_{fj} = K_{fj} n_{j1} n_{j2} \qquad ...(2)$$

$$R_{bj} = K_{bj} n_{j3} n_{j4} \qquad ...(3)$$

Similar procedure is extended to the third-order reaction also. The molar density of the chemical species is calculated with the help of time dependent rate constant for the chemical reactions. Thus, we get a set of first-order, coupled non-linear ordinary differential equations of the form :

$$\frac{dn}{dt} = P_i (t, n_i) - n_i L_i (t, n_i) \qquad ...(4)$$

Production term $P_i(t,n_i)$ and loss term $L_i(t,n_i)$ are functions of time. The chemical production rates and loss rates, P_i and L_i in above first-order differential equation for chemical species can be written as :

$$P_i = K_{fij} n_j + K_{fijk} n_j n_k + Kfijkl \, n_j n_k n_l \qquad ...(5)$$

$$L_i = K_{bi} + K_{bij} n_j + K_{bijk} n_j n_k \qquad ...(6)$$

Let YM_i and WM_i denote the mass fraction and molecular weight of the ith chemical species in a reaction. The total density (PG) of the this species is then given by -

$$\text{Total density (PG)} = n_i (YM_i/WM_i) \qquad ...(7)$$

$$\text{and molar density } n_i = PG (YM_i/WM_i) \qquad ...(8)$$

If X_i (mole fraction) is given by $X_i = PG/WM_i$

then we can write $n_i = X_i \, YM$.

Thus, the differential equation of molar density in terms of mass fraction becomes -

$$\frac{d(YM_i)}{dt} = \left[\frac{WM_i}{PG}\right] \left\{P_i\,(t, n_i) - n_i L_i(t,n_i)\right\} \qquad ...(9)$$

Let $f(t, YM)$ represent -

$$f\,(t, YM_i) = \left[\frac{WM_i}{PG}\right] \left\{P_i\,(t, n_i) - n_i L_i(t,n_i)\right\} \qquad ...(10)$$

The system of i differential equations (i is the number of chemical species involved in the considered set of chemical reactions) can be written as -

$$\frac{d(YM_1)}{dt} = f_1\,(t, YM_1, YM_2, ...YM_i) \qquad ...(11)$$

$$\frac{d(YM_2)}{dt} = f_2\,(t, YM_1, YM_2, ...YM_i) \qquad ...(12)$$

$$\frac{d(YM_3)}{dt} = f_3\,(t, YM_1, YM_2, ...YM_i) \qquad ...(13)$$

These equations can be solved with help of explicit one-step or multi-step methods subject to the initial conditions $YM_1 = C_1$, $YM_2 = C_2$, ... The major problem associated with the simulantaneous integration of large sets of chemical kinetics rate equations is of a phenomenon called stiffness. Frequently the individual reactions proceed with vastly different characteristic time cosntants. These widely varying time constants present classifical numerical methods (such as explicit Runge-Kutta method) with difficulties like ensuring stability of the numerical solution, which requries using very short time for all the chemical species to reach near equilibrium values. Therefore, classical methods require enormous amount of computer time for solving stiff system of ordinary differential equations (ODEs). To deal with the problem of stiffness of ordinary differential equations, a number of integration methods with various advantages have been put forward by many researchers in this field (e.g., Lomax and Bailey[10]). In the present study, a time step of 0.1 µs is taken in order to simulate the results with the experimental findings.

(i) Evaluation of backward rate constants

Since our investigations involve non-equilibrium reactions, it is important to have a knowledge of the forward rate constant and backward rate constant of various reactions involving combustion of coal. The data of the chemical reactions occurring in the combustion process of various types of fossil fuels collected from various sources contains only forward rate constant[1,5-8]. In order to evaluate the backward rate constant of a chemical reaction, let us consider a general combustion reaction of a hydrocarbon A as -

$$A + B = C + D \qquad ...(14)$$

where B is the oxidant, and C and D are the combustion products.

The equilibrium constant K_p, in terms of the partial pressures of the reactants and products of such reaction is given by,

$$K_P = \frac{K_p [C] \, K_P [D]}{K_p [A] \, K_p [B]} \qquad \qquad ...(15)$$

It is well known that the equilibrium constant K_c of a reaction in terms of concentration of reactants and products can be written as :

$$K_C = K_p (RT)^{(n_r - n_p)} \qquad \qquad ...(16)$$

where, R is the universal gas constant = 82.056 cm^3 atm./g mol K, n_r and n_p are the stoichiometric numbers of reactants and products of chemical reaction. The relation connecting the backward rate constant (K_b) and forward rate constant (K_f) to equilibrium constant (K_c) is given by,

$$K_b = \frac{K_f}{K_c} \qquad \qquad ...(17)$$

(ii) Calculation of equilibrium constants at different temperatures in Arrhenius form

In the analysis of dynamic reactions, it is usual to evaluate and employ the backward rate constant of the above chemical reactions in the Arrhenius form. The values of log of equilibrium constant, log K_p, at different temperatures (T) for different species participating in various combustion reactions of coal have been collected from JANAF Thermochemical Tables[11]. The equilibrium constant K_p of a reaction at a temperature T is given by

$$K_p = A \exp (-E_a/kT) \qquad \qquad ...(18)$$

where A, E_a and k respectively are Arrhenius constant, activation energy of reaction and Boltzmann's constant. Taking log of both sides and putting the value of Boltzman's constant k, we get

$$\log K_p = \log A - (E_a/4.575 \, T) \qquad \qquad ...(19)$$

Substituting 1/T by X and log K_p by Y, the above equation becomes

$$Y = \log A - (E_a X/4.575) \qquad \qquad ...(20)$$

With the help of normal equations, the expressions for E_a and A are given by -

$$E_a = 4.575 \left[\frac{\Sigma X \, \Sigma Y - N \, \Sigma \, XY}{N \, \Sigma X^2 - (\Sigma X)^2} \right] \qquad \qquad ...(21)$$

and

$$\log A = \frac{\Sigma X^2 \, \Sigma Y - \Sigma \, XY}{N \, \Sigma X^2 - (\Sigma X)^2} \qquad \qquad ...(22)$$

The chemical reactions with their forward rate constants pertaining to the combustion process have been collected from various journals for the kinetic study. We have been able to collect the data for forward rate constants of 107 chemical reactions. The backward rate constants of the respective reactions have been calculated with the help of a programme developed on the basis of the method described earlier. All the reactions of coal combustion

included in this study are given in Table 1 with their forward and backward rate constants. A computer code, based on the method described above, has been developed to evaluate equilibrium constants of various chemical species as function of temperature in the Arrhenius form. Their respective values have been presented in Table 2 for temperature range 1000-2300 K.

Table 1. Chemical reactions with their backward and forward rate constants in Arrhenius form

1	$CH_4+M = CH_3+H+M$	1.995E+17	0.00	88000	4.052E+11	1.00	-19918.6
2	$CH_4+OH = CH_3+H_2O$	1.600E+06	2.10	2460	2.847E+05	2.10	17389.5
3	$CH_4+O = CH_3+OH$	1.020E+09	1.50	8604	1.847E+07	1.50	6741.4
4	$CH_4+H = CH_3+H_2$	2.200E+04	3.00	8750	9.160E+03	3.00	8839.4
5	$CH_3+O_2 = CH_2O+OH$	5.200E+13	0.00	34570	5.237E+13	0.00	88127.6
6	$CH_3+O = CH_2O+H$	8.000E+13	0.00	0	9.908E+14	0.00	69289.2
7	$CH_3+OH = CH_2OH+H_2$	4.000E+12	0.00	0	1.139E+14	0.00	71241.2
8	$CH_2O+O = CHO+OH$	5.012E+13	0.00	4600	1.832E+12	0.00	17716.8
9	$CH_2O+OH = CHO+H_2O$	7.586E+12	0.00	170	2.724E+12	0.00	30078.9
10	$CH_2O+H = CHO+H_2$	3.311E+14	0.00	10500	2.781E+13	0.00	25568.8
11	$CH_2O+M = CHO+H+M$	3.310E+16	0.00	81000	1.361E+11	1.00	-11939.2
12	$CHO+O = CO+OH$	1.000E+14	0.00	0	2.982E+14	0.00	88393.9
13	$CHO+H = CO+H_2$	1.995E+14	0.00	0	1.368E+15	0.00	90345.9
14	$CHO+O_2 = CO+HO$	3.310E+12	0.00	7000	7.519E+12	0.00	39421.9
15	$CHO+OH = CO+H_2O$	1.000E+14	0.00	0	2.930E+15	0.00	105186.0
16	$CHO+M = CO+H+M$	1.445E+14	0.00	19000	4.832E+10	1.00	1337.9
17	$CO+OH = CO_2+M$	1.510E+07	1.30	-770	1.561E+09	1.30	20749.0
18	$CO+O+M = CO_2+M$	6.170E+14	0.00	3000	5.687E+20	-1.00	130575.0
19	$H+O_2 = O+OH$	5.129E+16	-0.82	16510	4.170E+15	-0.82	778.4
20	$O+H_2 = H+OH$	5.060E+04	2.67	6290	2.201E+04	2.67	4338.0
21	$O+H_2O = OH+OH$	6.760E+13	0.00	18360	6.880E+12	0.00	1567.9
22	$H+H_2O = H_2+OH$	9.550E+13	0.00	20300	2.234E+13	0.00	5459.9
23	$H+OH+M = H_2O+M$	1.600E+22	-2.00	0	3.243E+27	-3.00	129737.9
24	$O+O+M = O_2+M$	1.890E+13	0.00	-1788	2.073E+18	-1.00	119999.6
25	$H+H+M = H_2+M$	1.000E+18	-1.00	0	2.050E+22	-2.00	108008.0
26	$H+HO_2 = OH+OH$	1.400E+14	0.00	1073	1.495E+13	0.00	41313.4
27	$H+O_2+M = HO_2+M$	3.610E+17	-0.72	0	2.452E+21	-1.72	50084.0
28	$O+N_2 = NO+N$	6.630E+13	0.00	75050	1.449E+13	0.00	-220.0
29	$N+O_2 = NO+O$	6.400E+09	1.00	6280	1.371E+09	1.00	38290.4
30	$N+OH = NO+H_2$	3.800E+13	0.00	0	1.001E+14	0.00	47742.0
31	$CH_3+H = CH_2+H_2$	9.000E+13	0.00	15100	1.807E+13	0.00	10567.4
32	$CH_3+OH = CH_2+H_2O$	7.500E+06	2.00	5000	6.435E+06	2.00	15307.5

33	$CH_2+O = CH+OH$	2.000E+11	0.68	25000	6.403E+10	0.68	26275.7
34	$CH_2+H = CH+H_2$	1.000E+18	-1.56	0	7.360E+17	-1.56	3227.7
35	$CH_2+OH = CH+H_2O$	1.130E+07	2.00	3000	3.55E+07	2.00	21067.8
36	$CH+NO = HCN+O$	1.100E+17	0.00	0	2.238E+15	0.00	70399.2
37	$CH_2+NO = HCN+OH$	2.000E+13	0.00	0	1.303E+14	0.00	71674.9
38	$CH_3+NO = HCN+H_2O$	1.000E+11	0.00	15000	5.590E+11	0.00	96982.4
39	$CH+N_2 = HCN+N$	3.000E+11	0.00	13600	1.334E+12	0.00	8729.2
40	$CH_2+N_2 = HCN+NH$	1.000E+13	0.00	74000	6.812E+12	0.00	42895.9
41	$CH+NH_2 = HCN+H+H$	3.000E+13	0.00	0	1.210E+11	1.00	45621.6
42	$CH+NH = HCN+H$	5.000E+13	0.00	0	5.600E+15	0.00	145650.2
43	$CH_2+NH = HCN+H+H$	3.000E+13	0.00	0	1.206E+12	1.00	40869.9
44	$CH+N = CN+H$	1.300E+13	0.00	0	1.193E+14	0.00	98805.6
45	$CH_2+N = HCN+H$	5.000E+13	0.00	0	8.579E+14	0.00	119416.9
46	$CH_3+N = HCN+H+H$	5.000E+13	0.00	0	8.401E+09	1.00	6876.3
47	$CH_4+N = NH+CH_3$	1.000E+13	0.00	24000	8.667E+10	0.00	-5371.6
48	$HNCO+H = NH_2+CO$	2.000E+13	0.00	3000	1.642E+12	0.00	12008.5
49	$HCN+M = CN+H+M$	5.700E+16	0.00	117034	1.095E+12	1.00	-8357.6
50	$CN+H_2 = HCN+H$	2.950E+05	2.45	2237	7.493E+05	2.45	19620.6
51	$HCN+CN = C_2N_2+H$	2.000E+13	0.00	0	4.500E+15	0.00	6682.1
52	$HCN+O = CN+OH$	2.700E+09	1.58	26600	4.624E+08	1.58	7264.4
53	$HCN+O = NCO+H$	1.380E+04	2.64	4980	2.007E+04	2.64	3732.0
54	$HCN+O = NH+CO$	3.450E+03	2.64	4980	1.487E+03	2.64	35338.6
55	$HCN+OH = H_2O+CN$	1.450E+13	0.00	10929	2.440E+12	0.00	8385.5
56	$HCN+H = HNCO+H$	4.800E+11	0.00	11000	7.850E+12	0.00	26322.7
57	$NH_3+M = NH_2+H+M$	1.400E+16	0.00	90600	1.058E+11	1.00	-20603.6
58	$NH_3+OH = NH_2+H_2O$	2.040E+06	2.04	566	1.351E+05	2.04	12210.5
59	$NH_3+O = NH_2+OH$	2.100E+13	0.00	9000	1.416E+12	0.00	3852.4
60	$NH_3+H = NH_2+H_2$	6.360E+05	2.39	10171	9.855E+04	2.39	6975.4
61	$NH_2+OH = NH+H_2O$	4.000E+06	2.00	1000	1.251E+06	2.00	23819.5
62	$NH_2+O = NH+OH$	6.750E+12	0.00	0	2.148E+12	0.00	6027.4
63	$NH_2+O = HNO+H$	6.630E+14	-0.50	0	3.517E+15	-0.50	27741.6
64	$NH_2+H = NH+H_2$	6.920E+13	0.00	3650	5.063E+14	0.00	11629.4
65	$NH_2+O_2 = HNO+OH$	4.500E+12	0.00	25000	1.941E+12	0.00	37010.0
66	$NH+OH = HNO+H$	2.000E+13	0.00	0	3.334E+14	0.00	21714.2
67	$NH+OH = N+H_2O$	5.000E+11	0.50	2000	1.036E+12	0.50	46300.6
68	$NH+O = NO+H$	2.000E+13	0.00	0	1.111E+14	0.00	75251.0
69	$NH+O = N+OH$	6.300E+11	0.50	7948	1.329E+12	0.50	35456.5
70	$NH+H = N+H_2$	1.000E+14	0.00	0	4.847E+14	0.00	29460.5

71	$NH+O_2 = HNO+O$	1.000E+13	0.00	12000	1.355E+13	0.00	17982.6
72	$NH+NH_2 = N_2H_2+H$	5.000E+13	0.00	0	3.089E+15	0.00	30135.3
73	$HNO+OH = NO+H_2O$	3.600E+13	0.00	0	1.179E+13	0.00	70328.9
74	$HNO+O = NO+OH$	5.000E+11	0.50	1987	1.666E+11	0.50	55523.8
75	$HNO+H = NO+H_2$	5.000E+12	0.00	0	3.830E+12	0.00	55488.8
76	$HNO+M = NO+H+M$	1.500E+16	0.00	48680	5.604E+11	1.00	-3839.2
77	$NH_2+NO = N_2+H_2O$	6.200E+15	-1.25	0	1.871E+16	-1.25	125598.5
78	$NH_2+NO = N_2+H+OH$	6.300E+19	-2.5	1888	2.170E+16	-1.50	4638.4
79	$NO+HO_2 = NO_2+OH$	2.110E+12	0.00	-479	8.414E+12	0.00	8382.0
80	$NO_2+OH = NO+O_2$	1.000E+13	0.00	600	3.293E+12	0.00	47711.0
81	$NO_2+H = NO+OH$	3.500E+14	0.00	1500	9.371E+12	0.00	32879.4
82	$CN+O = CO+N$	1.800E+13	0.00	0	9.468E+13	0.00	77202.7
83	$CN+OH = NCO+H$	6.000E+13	0.00	0	5.096E+14	0.00	18087.6
84	$CN+O_2 = NCO+O$	5.600E+12	0.00	0	3.867E+12	0.00	2356.0
85	$CN+NO_2 = NCO+NO$	3.000E+13	0.00	0	6.821E+12	0.00	49467.0
86	$NCO+M = N+CO+M$	3.100E+16	-0.50	48000	2.153E+12	0.50	1059.1
87	$NCO+H = NH+CO$	5.000E+13	0.00	0	1.469E+13	0.00	31606.6
88	$NCO+O = NO+CO$	2.000E+13	0.00	0	3.262E+13	0.00	106857.6
89	$NCO+OH = NO+CN$	1.000E+13	0.00	0	1.829E+09	1.00	801.6
90	$C_2N_2+O = NCO+CN$	4.570E+12	0.00	8880	2.954E+11	0.00	950.9
91	$NCO+NO = N_2O+CO$	1.000E+13	0.00	-390	5.321E+14	0.00	67963.2
92	$NO+NH = N_2O+H$	2.400E+15	-0.80	0	4.348E+17	-0.80	36746.6
93	$NO+NH_2 = N_2O+H_2$	5.000E+13	0.00	24640	6.627E+15	0.00	69366.0
94	$NO_2+NH_2 = N_2O+H_2O$	1.900E+20	-3.00	0	2.882E+20	-3.00	90945.5
95	$HNO+HNO = N_2O+H_2O$	3.950E+12	0.00	5000	1.405+13	0.00	90361.3
96	$HNO+NO = N_2O+OH$	2.000E+12	0.00	26000	2.174E+13	0.00	41032.4
97	$N_2H_2+NO = N_2O+NH_2$	3.000E+12	0.00	0	8.798E+12	0.00	6611.3
98	$N_2O+M = N_2+O+M$	1.620E+14	0.00	51600	9.677E+08	1.00	11576.4
99	$N_2O+H = N_2+OH$	7.600E+13	0.00	15200	4.049E+12	0.00	81232.4
100	$N_2O+OH = N_2+HO_2$	2.000E+12	0.00	10000	9.981E+11	0.00	35792.0
101	$N_2O+O = NO+NO$	1.000E+14	0.00	28200	3.066E+12	0.00	66704.4
102	$N_2O+O = N_2+O_2$	1.000E+14	0.00	28200	6.552E+13	0.00	109964.0
103	$N_2O+CO = N_2+CO_2$	5.000E+13	0.00	44000	2.753E+14	0.00	131551.4
104	$N_2O+CN = NCO+N_2$	1.000E+13	0.00	0	4.524E+12	0.00	84120.0
105	$CO+O_2 = CO_2+O$	2.512E+12	0.00	47690	2.111E+13	0.00	53477.4
106	$CO+HO_2 = CO_2+OH$	5.754E+13	0.00	22930	6.349E+14	0.00	84689.4
107	$CH_4+O_2 = CH_3+HO_2$	7.900E+13	0.00	56000	1.0908+12	0.00	-1834.6

$M = N_2$

Table 2. Values of different constants for each of chemical species in Arrhenius form

S.No.	Chemical Species	A	E_a
1.	O	3.000E+03	60893.8
2.	OH	5.317E+00	8841.8
3.	H	1.297E+03	54004.0
4.	N	2.970E+03	114534.5
5.	CN	1.330E+05	102850.1
6.	NH	1.110E+01	89991.0
7.	CHO	1.350E+02	8348.6
8.	HO_2	2.327E-03	3920.0
9.	CH	5.331E+05	141125.7
10.	CH_2	3.025E+02	90349.4
11.	CH_3	4.682E-02	31812.8
12.	CH_4	1.503E-06	-22101.8
13.	O_2	1.000E+00	0.00
14.	HCN	4.037E+01	31462.5
15.	NO	4.623E+00	21629.8
16.	H_2	1.000E+00	0.00
17.	CH_2O	8.744E-03	-30586.6
18.	H_2O	9.591E-04	-60002.3
19.	CO_2	1.013E+00	-94674.5
20.	CO	2.554E+04	-27993.3
21.	N_2	1.000E+00	0.00
22.	C_2N_2	1.840E+02	73627.5
23.	N_2H_2	8.674E-07	49818.1
24.	HNCO	1.012E-02	-29022.4
25.	HNO	2.730E-03	23114.6
26.	NH_3	7.480E-07	-13233.2
27.	NH_2	6.261E-03	43966.4
28.	NCO	6.420E+01	39600.3
29.	NO_2	5.074E-04	6847.0
30.	N_2O	2.184E-04	20870.2

Evaluation of pollutants – A computer code, based on the analytical technique described above, has been developed to evaluate the concentration of various pollutants as a function of time during the combustion of coal. It was expected, right in the beginning, that the time-step for evaluation of combustion products would be fairly small and therefore, an ordinary computer like a good PC, would require an extremely long processing time to carry out the calculations even for short residence time for coal combustion in a furnace. An effort was therefore made to link PC with the Main Frame Computer of our Institute with a view to reduce the processing time. We were able to have an access to the machine DRS-6000 of our main frame computer for executing our programme. Eventually, the programme was executed on the main frame computer for an extremely short time-step of 10^{-8} second. It required approximately one and a half hour of the prcocessing time, even on the main frame computer, to carry out the calculation for a residence time of 1 ms. At this rate, it would have required over 300 hours of processing time on the main frame at a stretch to carry out the calculation for a residence time of 2.5 - 3.0 s, which is the usual time required for coal combustion in a furnace. Therefore, the results of evaluation of NO_X, CO_X and hydrocarbon pollutants for a residence time of 1 ms are presented in this communication.

RESULTS AND DISCUSSION

The computer programme was executed to evaluate the products of coal combustion for a combustion temperature of 1000 K and above for different residence times in a furnace of a power plant of National Thermal Power Corporation, India for combustion of coal found at a place in India, called Sangrauli. The particulars of the coal used and the specification of a furnace of Sangrauli Power Plant are mentioned in Table 3 and Table 4, respectively. The results in terms of concentration of various pollutants and combustion products have been plotted in terms of various graphs, given below, under various combustion conditions. Evaluation of all combustion products have been carried out, when the combustion takes place for an equivalence ratio, $\phi = 1$, fuel lean condition, $\phi = 0.95$ and fuel rich condition $\phi = 1.18$.

Table 3. Particulars of Sangrauli coal

S. No.	Proximate Analysis	Sangrauli Coal (in percentage)
1.	Moisture	7.65
2.	Ash	28.90
3.	Volatile Matters	23.75
4.	Fixed Carbon	39.70
5.	Calorific values (MJ/kg)	21.40

Table 4. Specification of Sangrauli Power Plant

S.No.	Properties	Description
1.	Capacity	200 MW
2.	Furnace dimensions	
	(i) Width	13.8 m
	(ii) Depth	10.5 m
	(iii) Volume	82 m^3
3.	Pressure	-10 mm water column
4.	Coal flow rate	120 T/h
5.	Air flow rate	790-800 T/h
6.	Excess of O$_2$ flow	3%

(i) Concentration of NO$_x$

Figure 1 shows the variation of N$_2$O in ppm with residence time t up to 1 ms for various values of ϕ. The N$_2$O concentration is found to increase with the residence time for all the conditions of combustion. However, its concentration is found to be larger in magnitude with increasing value of equivalence ratio of ϕ.
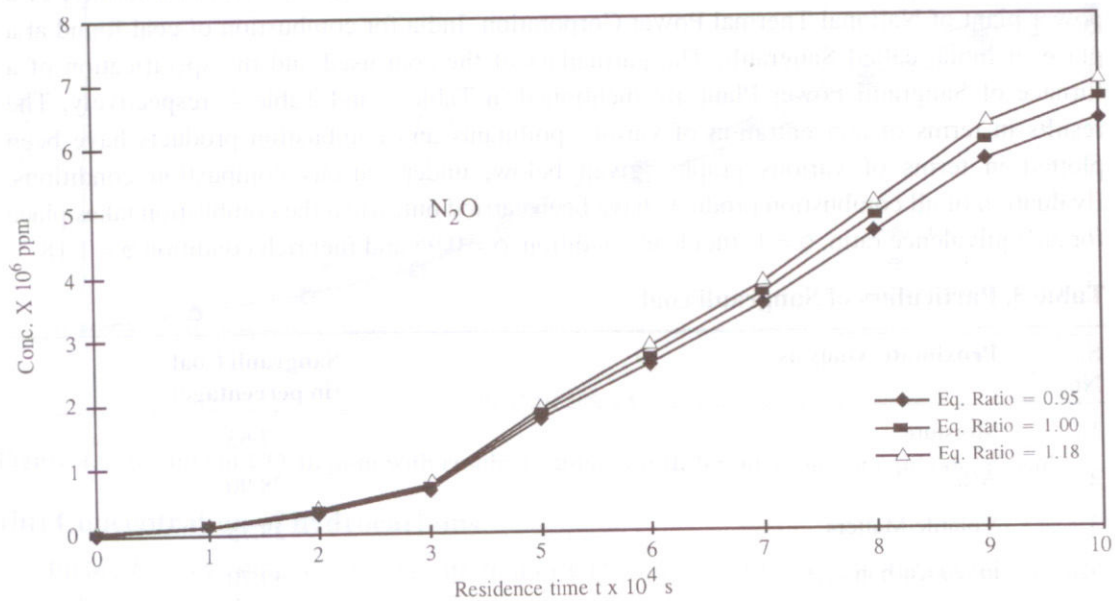
Figure 1. Variation of N₂O in ppm with residence time t for different values of equivalence ratio φ

Figure 2 shows the variation of the concentration of NO in ppm with residence time for various values of the equivalence ratio ϕ. The concentration of NO is found to increase with residence time for all values of ϕ. However, the numerical magnitude of NO is found to be same for all values of ϕ.
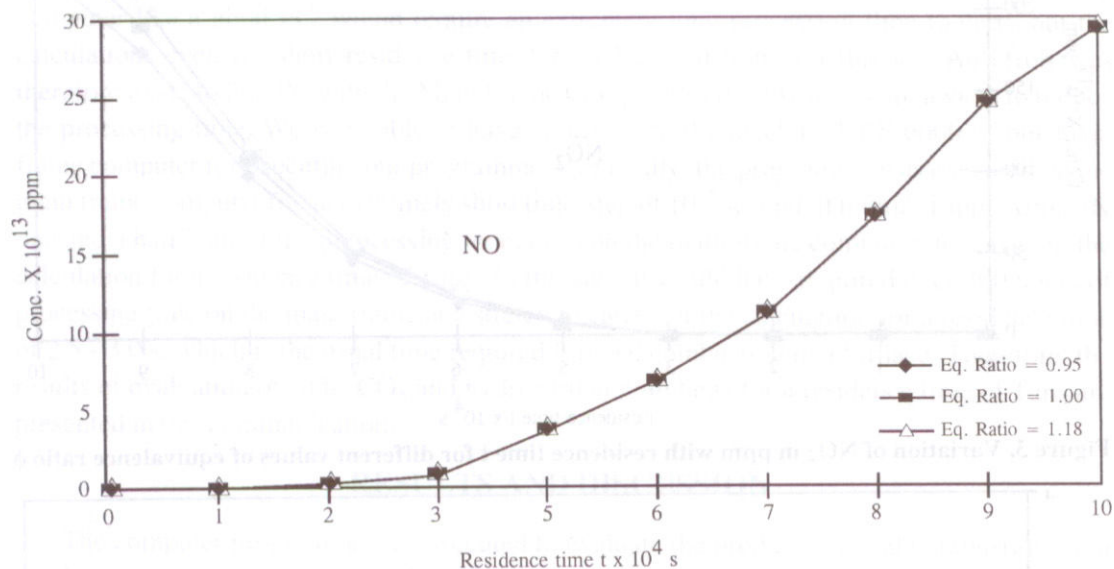

Figure 2. Variation of NO in ppm with residence time t for different values of equivalence ratio ϕ

Figure 3 shows the variation of NO_2 in ppm with residence time t at three different values of equivalence ratios mentioned above. The concentration of NO_2 is found to increase with residence time in all the three cases. However, the rate of increase in concentrations decreases with decrease in the ϕ values. The maximum rate of increase has been observed at $\phi = 1.18$, and the minimum at $\phi = 0.95$.

(ii) Concentration of CO_x

Figure 4 is a plot of concentration of CO in ppm versus residence time t. This figure shows that the concentration of CO increases with the increase in residence time at all the ϕ values. However, the increase in concentration of CO at higher equivalence ratio, i.e., $\phi = 1.18$ is more than that at lower ϕ value, i.e., at $\phi = 0.95$. In this case, the nature of variation of CO is found to be the reverse of the variation trends of NO_2.

Figure 5 shows the variation of concentration of CO_2 in ppm with residence time at various equivalence ratios. It is observed that the concentrations of CO_2 remains the same at different residence time for all ϕ values, though lower concentration of CO_2 is found at $\phi = 1.18$, which gradually increases with decrease in ϕ values.
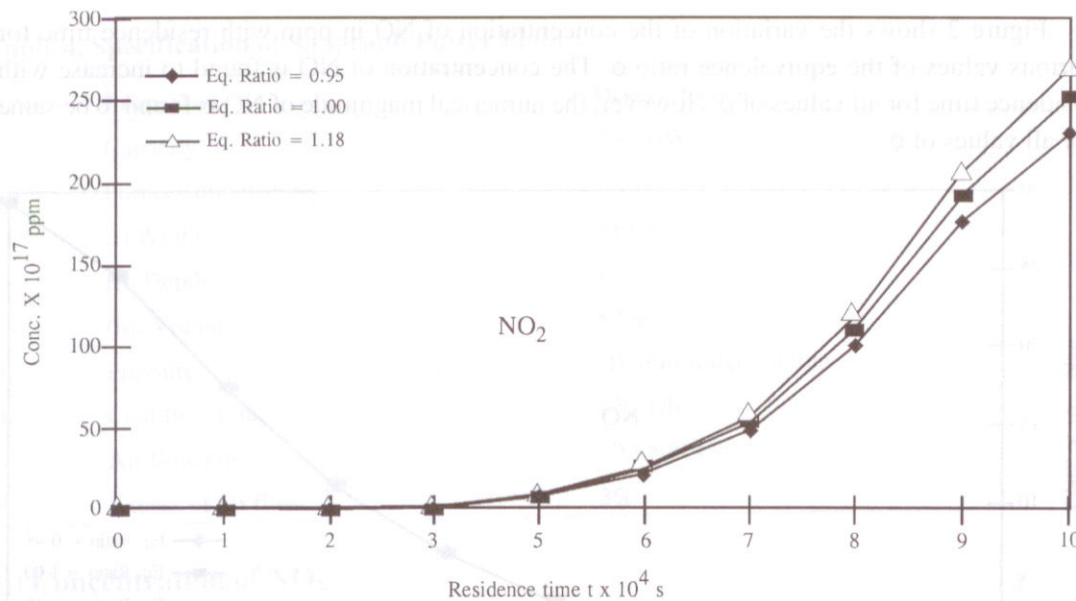
Figure 3. Variation of NO₂ in ppm with residence time t for different values of equivalence ratio φ
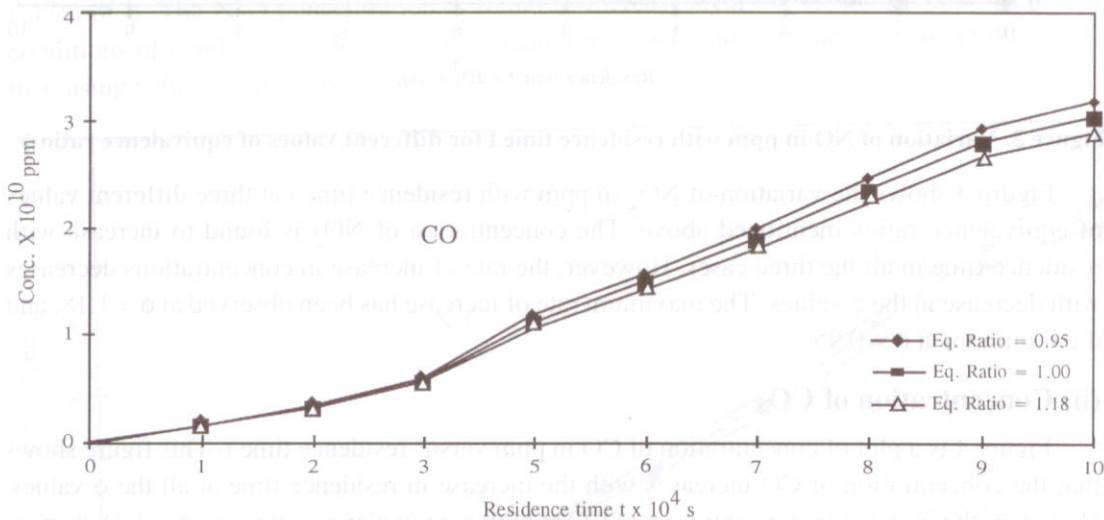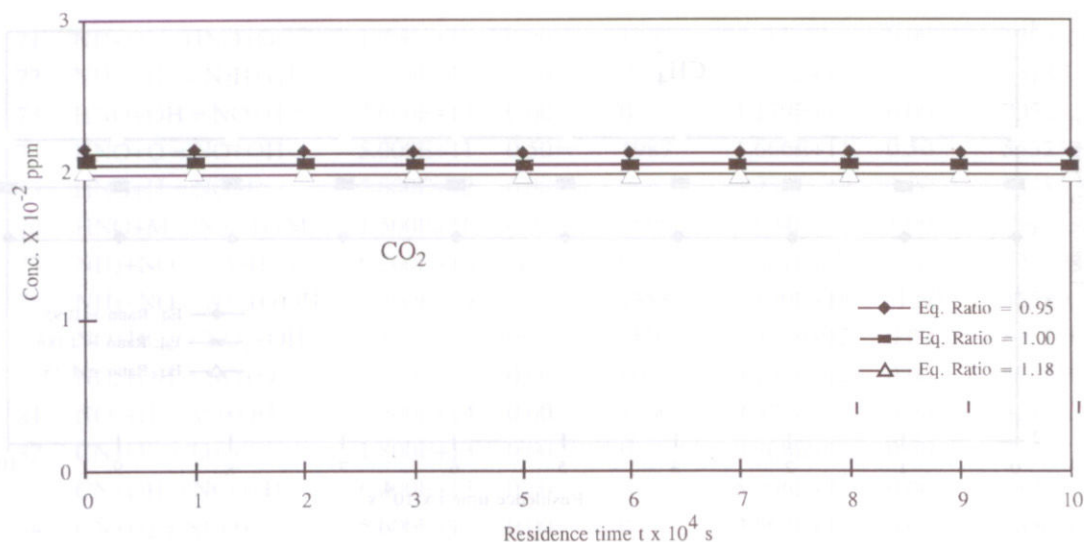

Figure 4. Variation of CO in ppm with residence time t for different values of equivalence ratio φ

(iii) Concentration of hydrocarbons

Figure 6 shows the plot of concentration of CH_3 in ppm with residence time t at various equivalence ratios. It is clear from this plot that the concentrations of CH_3 increases with increase in residence time for all the three equivalence ratios. However, the rate of increase in concentration increases with increase in φ values.

Figure 5. Variation of CO_2 in ppm with residence time t for different values of equivalence ratio ϕ
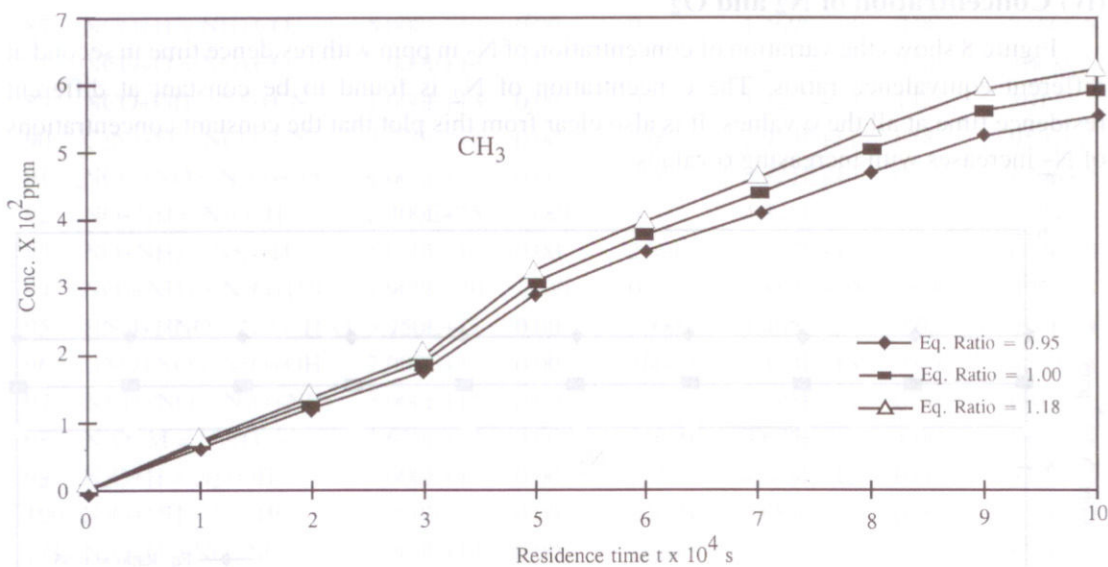

Figure 6. Variation of CH_3 in ppm with residence time t for different values of equivalence ratio ϕ

Figure 7 shows the dependence of CH_4 concentration in ppm with residence time in second. It is obvious from the figure that the CH_4 concentrations at all ϕ values remain the same as the lines are parallel to the residence time axis, though, concentrations of CH_4 is found to be higher for increasing ϕ values.
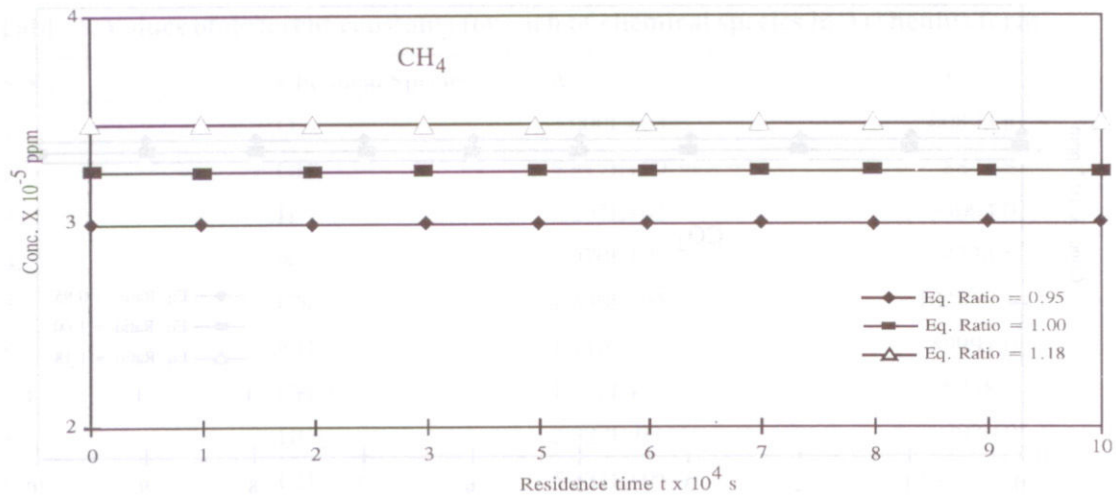
Figure 7. Variation of CH₄ in ppm with residence time t for different values of equivalence ratio φ

(iv) Concentration of N₂ and O₂

Figure 8 shows the variation of concentration of N_2 in ppm with residence time in second at different equivalence ratios. The concentration of N_2 is found to be constant at different residence time at all the φ values. It is also clear from this plot that the constant concentrations of N_2 increases with increasing φ values.
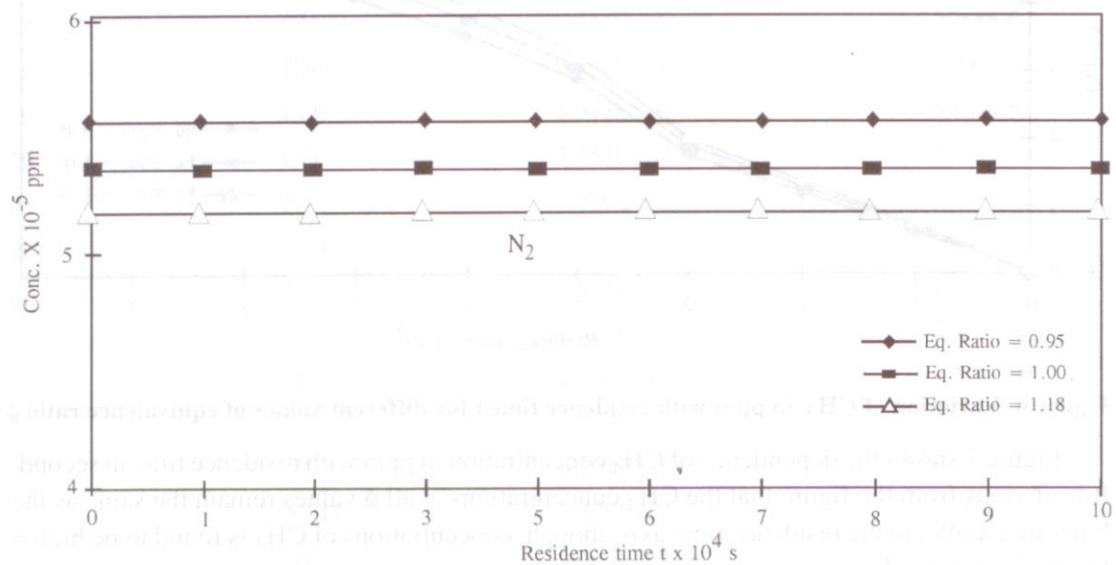

Figure 8. Variation of N₂ in ppm with residence time t for different values of equivalence ratio φ

Figure 9 is the plot of O_2 concentration in ppm and residence time in second at different equivalence ratios. It is clear from this figure that concentration of O_2 remains almost constant at different residence times but is found to increase with higher ϕ values.
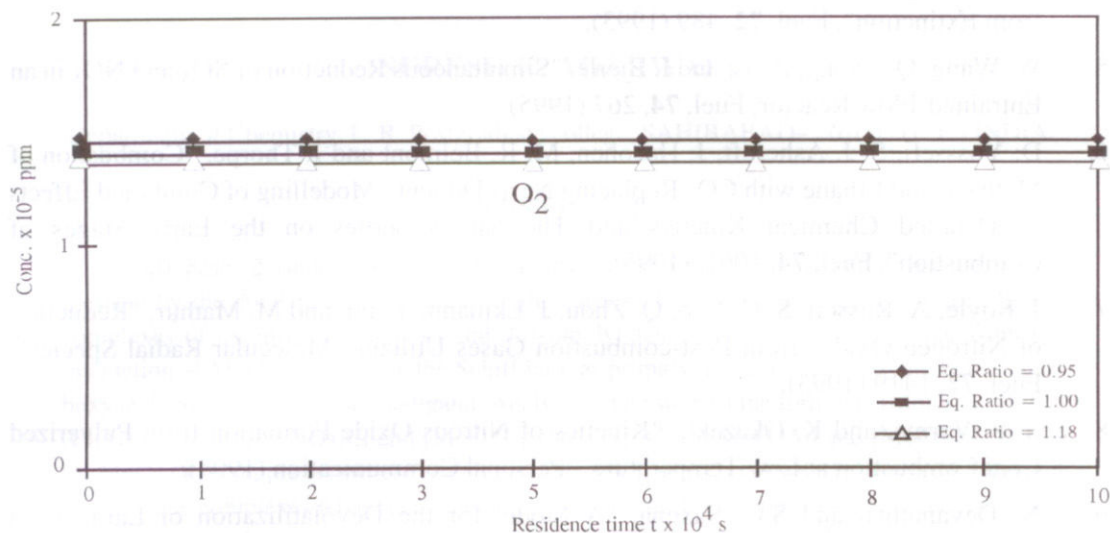

Figure 9. Variation of O₂ in ppm with residence time t for different values of equivalence ratio ϕ

CONCLUSION

The results, obtained so far (i.e., for a residence time one ms) indicate that the concentration of NO_x, CO_x and hydrocarbon pollutants in the emission of combustion of Singrauli coal are within the limit of tolerance as mentioned in the National Ambient Air Quality Standards (NAAQS, India). A final conclusion about the concentration of these pollutants in the emission of coal combustion can be drawn when the evaluations are carried out fully for a residence time 2-3 seconds.

ACKNOWLEDGEMENT

REFERENCES

1.   J. W. Mitchel and J. M. Tarbel, "A Kinetic Model of Nitric Oxide Formation during Pulverized Coal Combustion", AlChE J., **28**, 303 (1982).

2.   Jensen, J. E. Johnson, J. Andries and K. Laughlin, "Formation and Reduction of NO_x in Pressurized Fluidised Combustion of Coal", Fuel, **74**, 1555 (1995).

3.   Jensen and J. E. Johnson, "Modelling of NO_X Emissions from Pressurized Fluidised Bed Combustion - A Parametric Study", Chem. Eng. Sci., **52**, 1715 (1997).

4.   M. H. Yang, and I. K. Puri, "NO_X formation in Stretched Premixed Flame Established far from Extinction", Fuel, **72**, 489 (1993).

5.   W. Wang, Q. Zhong, Z. Ye and I. Bjerle, "Simultaneous Reduction of SO_X and NO_X in an Entrained-Flow Reactor, Fuel, **74**, 267 (1995).

6.   D. Yosssefi, S. J. Ashcroft, J. Hacohen, M. R. Belmont and I. Thorpe, "Combustion of Methane and Ethane with CO_2 Replacing N_2 as Diluent : Modelling of Combined Effects of Detailed Chemical Kinetics and Thermal Properties on the Early Stages of Combustion", Fuel, **74**, 1061, (1995).

7.   J. Boyle, A. Russell, S. C. Yao, Q. Zhou, J. Ekmann, Y. Fu. and M. Mathur, "Reduction of Nitrogen Oxides from Post-combustion Gases Utilizing Molecular Radial Species", Fuel, **72**, 1419 (1993).

8.   S. S. Verma, and K. Okazaki,. "Kinetics of Nitrous Oxide Formation from Pulverized Coal Combustion at Low Temperature", Personal Communication (1994).

9.   N. Devanathan and S.C. Saxena, "A Model for the Devolatilization of Large Coal Particles", Chem. Eng. Sci., **41**, 2442 (1986).

10.   H. Lomax and H. E. Bailey, "A Critical Analysis of Various Numerical Integration Methods for Computing the Flow of a Gas in Chemical Nonequilibrium", A Report, NASA TN D-4109, National Aeronautics and Space Administration, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 22151 (1967).

11.   M. W. Chase Jr., C. A. Davies, J. R. Downey Jr., D. J. Frurip, R. A. McDonald and A. N. Syverud, "Janaf Thermochemical Tables, Third Ed. Part I", J. Phys. Chem. Ref. Data, 14 (1985).