TURBULENT COMBUSTION MODELING OF COAL:BIOMASS BLENDS IN A SWIRL BURNER I - PRELIMINARY RESULTS

by

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ABSTRACT

A combustion model using three mixture fractions has been developed for accurate simulation of coal:manure combustion. This model treats coal and manure off gases separately. This model has been incorporated into the PCGC-2(Pulverized Coal Gasification and Combustion - 2 Dimensional, from Brigham Young University) code. Numerical results of this simulation are presented. The results are compared with those from the two mixture fraction model of the original code. While the overall simulation results from both models appear similar, there are significant differences in local temperature predictions in the near burner region.

NOMENCLATURE

f	Primary gas mixture fraction
h	Enthalpy
PDF,p	Probability density function
k	Kinetic energy of turbulence
m_p	Mass flow rate of primary gas
m_s	Mass flow rate of secondary gas
m_c	Mass flow rate of coal off-gas
m_m	Mass flow rate of manure off-gas
η_1	Coal off gas mixture fraction
η_2	Manure off gas mixture fraction

INTRODUCTION

As the nation moves towards the 21st century, coal still remains a major source of fuel for electrical power generation. Presently 75% of the electricity is generated from fossil fuels. Although the United States has massive reserves of coal, its use faces a major hurdle in environmental regulations.

In spite of the environmental concerns regarding the usage of coal, DOE has identified coal as the principal source of electricity well into the 21st century. This dependency on coal calls for better technologies to reduce the emissions from existing boiler burners as well as development of new technologies for the design of burners for the 21st century. The sulfur di-oxide emissions could be reduced either by using low sulfur coal or by exhaust clean up technology. For the power plants, the simplest solution is the preventive method where one uses low sulfur fuel (e.g. Wyoming coal) in order to avoid costly remediation technology. However, as demand for low sulfur coal increases, the fuel cost rises. Further, the deregulation in utilities is driving the utility cost downward. Thus power plants are compelled to look for cheaper fuel alternatives. One promising alternative is fuel blending.

For power plants located in the farm belt, the alternative fuels are generally agricultural waste ranging from corn husk to manure. Hence one can blend feedlot manure as a fuel along with coal. The huge beef industry in the farm belt is a source for a large amount of cattle manure (about 12,000 tons/day around Amarillo, Texas), the disposal of which remains a perennial problem for the feedlot operators. If manure could be successfully used as a fuel, the problems of unwanted accumulation of manure could be solved. At the same time, the power plants can be supplied with cheaper fuel alternatives which include coal-manure blends.

Frazzitta et al. (1994) conducted experimental studies on coal:manure blends. Figure 1 shows the combustor geometry used in the experimental and computational studies. The present paper attempts to numerically model the combustion of blends using PCGC-2 code which has been primarily developed for coal. These studies are important and necessary in the exploration of alternative technologies that will enable the use of non conventional fuels instead of low sulfur coal. The goal of this work is to improve the combustion model used in the PCGC-2.

LITERATURE SURVEY

There exists a large amount of literature on turbulent combustion modeling. They differ in the type of problem that

is modeled (premixed or non premixed combustion), the type of turbulence model used, the type of chemical reaction model used and on the particle phase model used. The general outline of a turbulent combustion model is given below:

1. modeling the flow field
2. modeling of the mixing of the fuel and oxidizer
3. modeling of the particle phase and source terms from particle phase
4. calculation of thermodynamic variables - species fractions, temperature, density etc.

Flow field modeling

Time averaged Navier-Stokes equations are used. The Reynolds stress terms are modeled using eddy viscosity, i.e. these terms are expressed as products of eddy viscosity and mean velocity gradients. The eddy viscosity is expressed as a function of kinetic energy of turbulence and its rate of dissipation. The turbulent kinetic energy and rate of dissipation are supplied by the k-e turbulent model. The presence of swirl in the flow calls for modifications to the k-e model and hence there are many 'swirl corrected' models. The k-e model is widely used in spite of its deficiencies and performs reasonably well in many cases.

Turbulent Combustion Models

Spalding (1971) discusses a model in which the turbulent reaction is assumed to be a function of concentration fluctuation and temperature. This model entails solving transport equations for mixture fraction and its variance. The mean volumetric rate of fuel consumption is expressed as a function of local velocity gradient, mixture fraction and the maximum fuel consumption rate(as a function of mixture fraction) and density. This is analogous to turbulent energy decay which could be expressed as a function of density and local velocity gradient.

Lockwood and Naguib (1975) present a turbulent combustion model for gaseous combustion. The mean and variance of concentration fluctuation are used to determine the probability density function of the concentration scalar. The mean values of thermodynamic variables are calculated using convolution of the variable with the pdf of the concentration scalar. Another widely used chemical reaction model is that of Magnussen and Hjertager (1977). This model is also based on the concept of eddy breakup. They present the following model for diffusion flames. The oxidizer and fuel occur in separate eddies and the chemical reaction can take place only when there is mixing between the oxidizer and the fuel at the molecular level. Turbulent eddies are destroyed at molecular scales due to viscosity and as such the rate of mixing is same as the rate of dissipation of the eddies. The rate of dissipation (breakup into molecular scales) can be expressed by the mean concentration of the reacting species. If the mixture is fuel lean the rate of dissipation of the fuel eddies is the controlling factor and for fuel rich mixtures, rate of dissipation of the oxidizer eddies is the controlling factor.

Kent and Bilger (1977) presents a different approach to turbulent combustion modeling by taking into account the density fluctuations. This is accomplished by the use of Favre averaged form of transport equations and Favre probability density functions. Flow field was predicted using a model very similar to k-e model and conserved scalar approach was used in the calculation of thermodynamic variables. Smith and Smoot [1980] describe a one dimensional model for pulverized coal combustion and gasification. This model is capable of handling detailed coal combustion mechanisms like devolatilisation and swelling, char reaction, particle-particle radiation, particle-wall radiation etc.,. It can also treat different particle sizes with different properties. But a major limitation of this model is that there is no turbulence model (turbulence models have been incorporated since) and instead the mixing of primary and secondary streams have to be specified as input. This code assumes that chemical equilibrium exists and hence the combustion is controlled by mixing of the fuel and oxidizer and not by kinetics. Thus it is not necessary to specify the composition of the volatiles, only the overall elemental compositions to the gas phase are needed. From elemental balances, calculated energy level and pressure, all other thermodynamic variables like species compositions, gas temperature etc., are obtained from equilibrium considerations. The model results are compared with experimental data from a laboratory combustor which essentially behaves as one dimensional combustor. Reasonably good predictions were obtained for species concentrations and particle burnout but no temperature comparisons were given.

Stickler et al. (1983) discusses a zero dimensional model for flame stability in pulverized coal burners. The flow field calculations are circumvented by specifying the mixing rates using time scales which were obtained from experiments. This model is based on time-history approach to combustion behavior. More importance is given to particle thermo-kinetic phenomena and gas phase chemical equilibrium is assumed. This model has inherent burner scaling capability and requires minimal computing time but needs more input from experiments to determine the mixing time scale.

Costa et al. (1990) describes the modeling of industry type pulverized coal flame. The essential features of this model are the use of time averaged conservation equations for the gas phase and a Lagrangian approach for particle phase calculations. They use a first order devolatilisation model and a diffusion controlled char reaction model which takes place entirely at the particle surface. The char reaction is taken to be first order with respect to oxygen. The standard k-e model is used without any modifications for swirl. Extensive experimental results are presented for three different types of flames and compared with predictions.

DESCRIPTION OF THE EXISTING MODEL

PCGC-2 is based on mixture fraction - equilibrium chemistry approach. Appendix B explains the application of this concept. This model has a single mixture fraction variable

) track the gases released by coal and one more mixture fraction to track the mixing of the primary and secondary gas streams. The version of PCGC-2 used in this work has the following capabilities:

i) modeling of axisymmetric swirling flows
ii) fuels: coal, gas and oil
iii) finite kinetic pyrolysis and heterogeneous oxidation
iv) k-e model for turbulence modeling
v) Equilibrium combustion calculations
and
vi) finite kinetic modeling of NO_x .

A more detailed description of the models and the governing equations is provided in PCGC-2(1988). Dhanapalan and Annamalai(1994) present simulation results for low sulfur Wyoming coal combustion using the PCGC-2 without any modifications.

IMPROVED COMBUSTION MODEL

The improved model uses three mixture fractions to calculate elemental balances, total enthalpy and pressure inside the combustor, instead of the two mixture fractions used in the original model. The chemical equilibrium calculations use these three variables to determine all other thermodynamic variables such as species compositions, gas temperature etc.

If the combustor is fed with two distinct gas streams 'A' and 'B' (no coal particles in either of the streams) the thermodynamic variables are functions only of mixture fraction of stream 'A' and total enthalpy, assuming constant pressure throughout the reactor. If coal particles were also injected, the gases from coal constitute yet another gas stream 'C'. The thermodynamic variables now are functions of mixture fraction of 'A', mixture fraction of 'C' and total enthalpy. This is the model used in PCGC-2. There is an implicit assumption here that gases from coal are of uniform composition at all times, during pyrolysis as well as char oxidation.

In particular for a fuel blend of two distinct fuel types the gases evolved by each fuel vary throughout the reactor and the relative proportion of the two types of gases will be different. Due to this reason, it will be inaccurate to use a single mixture fraction to represent the gases evolved by the blend. This problem can be overcome by using a separate mixture fraction variable for each fuel type in the fuel blend.

Flores and Fletcher (1995) also present a three mixture fraction approach to coal combustion, in which separate mixture fraction variables are used to track volatiles and char. In their model, the fluctuations of the third mixture fraction were ignored. Justifications for doing so were also provided. But a general three mixture fraction model which can be applied both for the simulation of coal combustion and fuel blend combustion can not ignore fluctuations of the third mixture fraction. A general model can be used explore the combustion of gases of different compositions. In addition, such a model can be applied to coal combustion in order to track volatile, char and moisture emissions separately.

INCORPORATION OF AN IMPROVED COMBUSTION MODEL IN PCGC-2

As stated in the previous section the assumption that the gases evolved by the solid fuel are uniform throughout the reactor is employed in the version of PCGC-2 used in this work. This assumption may be reasonable for a single fuel type (the new model will also be applied to coal combustion to track volatiles and char separately) but when a mixture of two fuels is used, this assumption becomes unrealistic. This is because the devolatilization and char oxidation behavior for each fuel type will be different. Due to this reason, the combined gas mixture evolved from the two fuel types will not always be of uniform composition. If one were to use an average composition, this will result in inaccuracies in the combustion calculations. The need for an additional mixture fraction variable is explained in more detail in the following section.

The above mentioned problem can be circumvented by tracking the gases evolved by the two fuel types separately. The inclusion of an additional mixture fraction in the model calls for quite a few modifications in the code. All the needed modifications will be discussed in the following sections. In brief, the modifications include addition of two turbulent scalar transport equations, an improved convolution routine to calculate equilibrium thermodynamic properties and proper accounting of source terms for mixture fraction transport equations.

Mixture fractions

The additional mixture fraction transport equations will be discussed in this section. For the sake of completeness, all three mixture fractions are defined below:

$$f = \frac{m_p}{m_p + m_s}$$

$$\eta_1 = \frac{m_c}{m_p + m_s + m_c}$$

$$\eta_2 = \frac{m_m}{m_p + m_s + m_c + m_m}$$

For steady state laminar combustion, only the transport equation for the mixture fraction is needed. In case of turbulent flow, the mean transport equation alone is not sufficient and the fluctuations of the mixture fraction must be taken into account during the simulation process. This is accomplished by solving a transport equation for the variance of the mixture fraction. Variance is simply the root mean square of the fluctuations. The numerical solution of the above two transport equations is very similar to any other scalar transport equation (PCGC-2, 1988) and follows a finite volume approach.

Particle source terms

The mixture fractions which track gases from particles must include the source terms in their transport equations. These source terms are the mass contributions from the particles to the gas phase at different numerical cells which lie along the particle trajectory. The PSI-cell (Crow et al., 1977) method is used to calculate particle trajectories. The particles are divided into various groups and each group is independently tracked. As each particle group moves in and out of the numerical cells, they contribute mass, momentum and energy to the gas phase along the particle paths.

In the original code which used a two mixture fraction approach, the mass contributions from both fuel types are lumped into a single mass source term. In the modified code these two mass sources need to be distinguished from each other. To perform this, the particle tracking routines were analyzed and the source term modifications were made at appropriate places.

Convolution model

The previous modifications provide information about the gas phase composition at the numerical cells in the combustor. Since transport equations for both mean and variance of the mixture fractions were solved, one can determine the probability density function for each of the mixture fraction variables. Due to the manner in which these mixture fractions were defined they are independent of each other (at least to the first order) and in effect they are independent random variables.

All the thermodynamic variables are functions of these random variables and these themselves are described by their probability density functions. The mean values of the thermodynamic variables are obtained by convolution of these variables with the probability density functions of the mixture fraction variables. This convolution process is shown below:

$$\overline{V} = \int_{-\infty}^{+\infty}\int\int V(f,\eta_1,\eta_2,h)\,p(f)\,p(\eta_1)\,p(\eta_2)\,df\,d\eta_1\,d\eta_2$$

where,

V = any thermodynamic variable

p = probability density function of the appropriate mixture fraction

If one focuses attention on the limits of the integrals it becomes obvious that they are physically unrealistic, because all the mixture fractions lie within the range $0 \leq f \leq 1$. Therefore all the PDFs are clipped at these limits and delta functions are added to account for the cut-off tails. These delta functions account for the intermittencies of the respective mixture fractions. Intermittency of a mixture fraction is a measure of the fraction of the time the pure gas stream identified by the intermittency is present. The triple integral is split into fifteen different terms to account for various events that can occur in each numerical cell. These events and the corresponding integral terms are shown in Figure 2. It should be noted that the fluctuations in enthalpy have been partially neglected. This is accomplished by decomposing the total enthalpy into two parts, adiabatic enthalpy and residual enthalpy. The fluctuations of the adiabatic enthalpy are automatically included during the convolution process, whereas the fluctuations of the residual enthalpy are ignored (PCGC-2, 1988).

Computing issues

The numerical integration process makes use of the Gauss quadrature and also requires thermodynamic property values for different values of mixture fractions. These property values are interpolated from the master thermodynamic table which stores property values using mixture fraction and enthalpy as independent variables. The resulting table is a 4 dimensional table and places huge toll on dynamic memory. The size of this data file varies from 35Mbytes to 150Mbytes.

The routine which generates the thermodynamic table and the interpolation routines have been rewritten. However, the equilibrium routines which perform the thermodynamic calculations are used in the existing form as they are independent of the number of mixture fractions used. In fact these 'fundamental routines' only require elemental atom fractions, total enthalpy and the pressure as input variables to perform the corresponding equilibrium calculations. The convolution routine for the three mixture fraction case is extremely CPU-intensive and requires many hours of CPU time. In order to reduce the execution time these routines have been provided with the capability to be executed in parallel. The Multiple Instruction Multiple Data paradigm is used to parallelize these routines for the Silicon Graphics Shared Memory - Symmetric Multiprocessor architecture.

RESULTS AND DISCUSSION

Combustion of fuel blend made of 90% coal 10% manure has been modeled using both the original code and the modified code. The properties of coal and manure are given in Table 1. The preliminary results indicate differences in species composition and temperature in the near region. The overall differences are not very dramatic because the source from coal dominates that from manure. But in small regions near the air:fuel inlet there are significant differences in the predictions. Figure 3 compares the centerline mole fraction distributions of O_2, CO and CO_2 as obtained from the two-mixture fraction and three-mixture fraction models. The three-mixture fraction model shows lower level of oxygen and higher levels of CO and CO_2. This indicates slightly higher burnout for the three-mixture fraction model. This fact is also supported by the variation of radial-averaged burnout along the burner axis. This can be explained as follows: In the three-mixture fraction approach the carbon atom fraction will be higher because the coal off gas composition is more accurately represented rather than being averaged with the manure off gas composition. It should be noted that the carbon atom content of manure off gas

is significantly lower than that of coal off gas. The three-mixture fraction model also predicts a higher temperature for the most part, as shown in figure 4, which is expected due to the higher carbon atom content in the gas phase predicted by the three mixture fraction model. Figures 5 and 6 show respectively the temperature and O_2 contours in the near burner region. It can be observed that there are localized regions where there is significant difference in the predictions from two and three mixture fraction models. The maximum temperature difference is about 350 K which can be significant in the prediction of NOx. If ignition location is defined as the distance at which there is rapid rise in temperature, then ignition distance is not altered significantly due to small amount of manure used in the blend.

CONCLUSION

Some initial results from a modified version of PCGC-2 as applied to coal:biomass manure were presented. The comparison of results from the two mixture fraction and three mixture fraction models shows differences in major species composition and temperature distribution in the near burner region.

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Table 1. Properties of coal and manure

Parameter	Coal	Manure
Moisture	10.8 %	36.61 %
Ash	5.68 %	25.25 %
Volatile Matter	52.8 %	31.57 %
Fixed Carbon	30.72 %	6.57 %
Heat Value(DAF) kJ/kg	26535	7865
Carbon	54.9 %	19.24 %
Hydrogen	4.33 %	2.22 %
Oxygen	23.2 %	14.68 %
Nitrogen	0.76 %	1.47 %
Sulfur	0.34 %	0.53 %

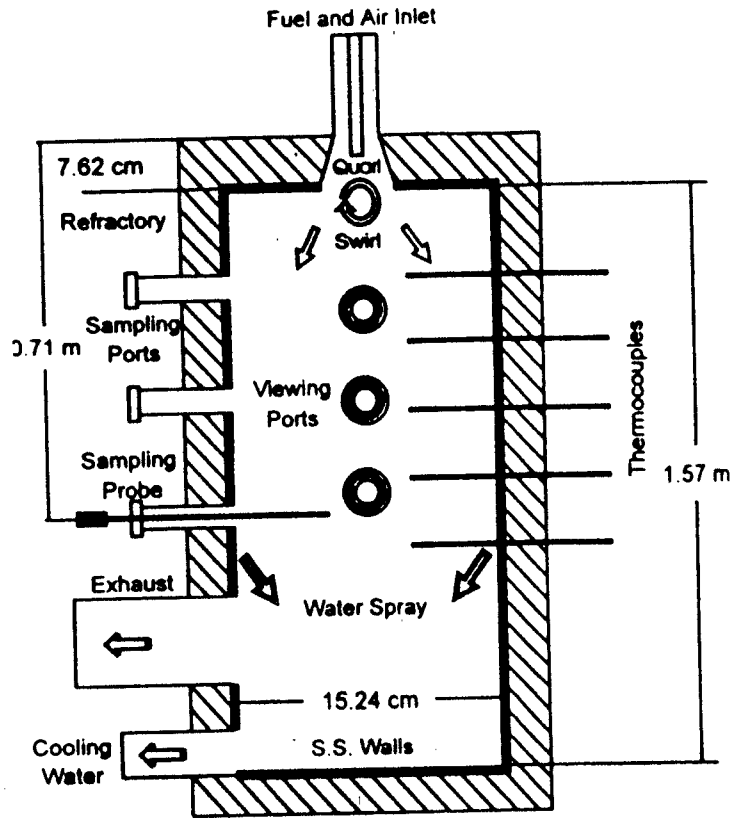

Figure 1. Boiler-Burner Schematic

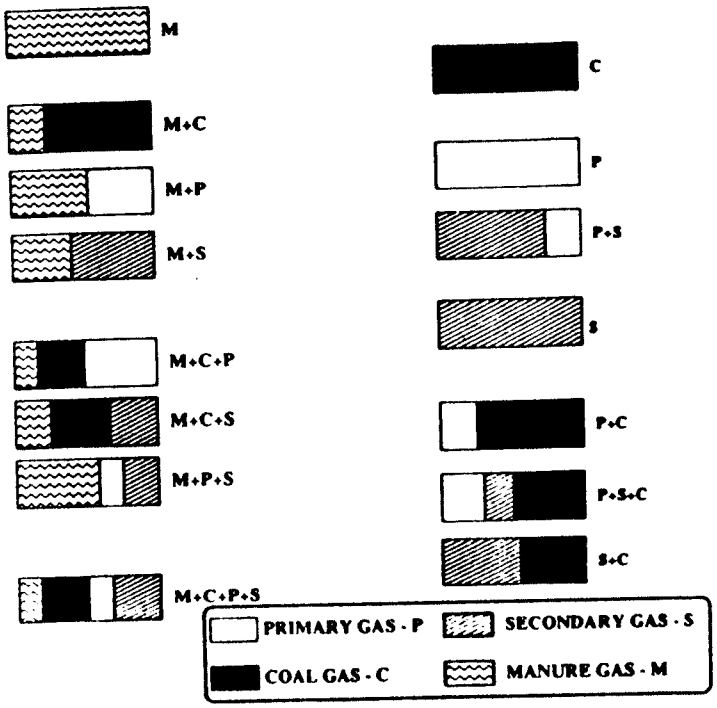

Figure 2. Coal:Manure Combustion - Possible events in a cell

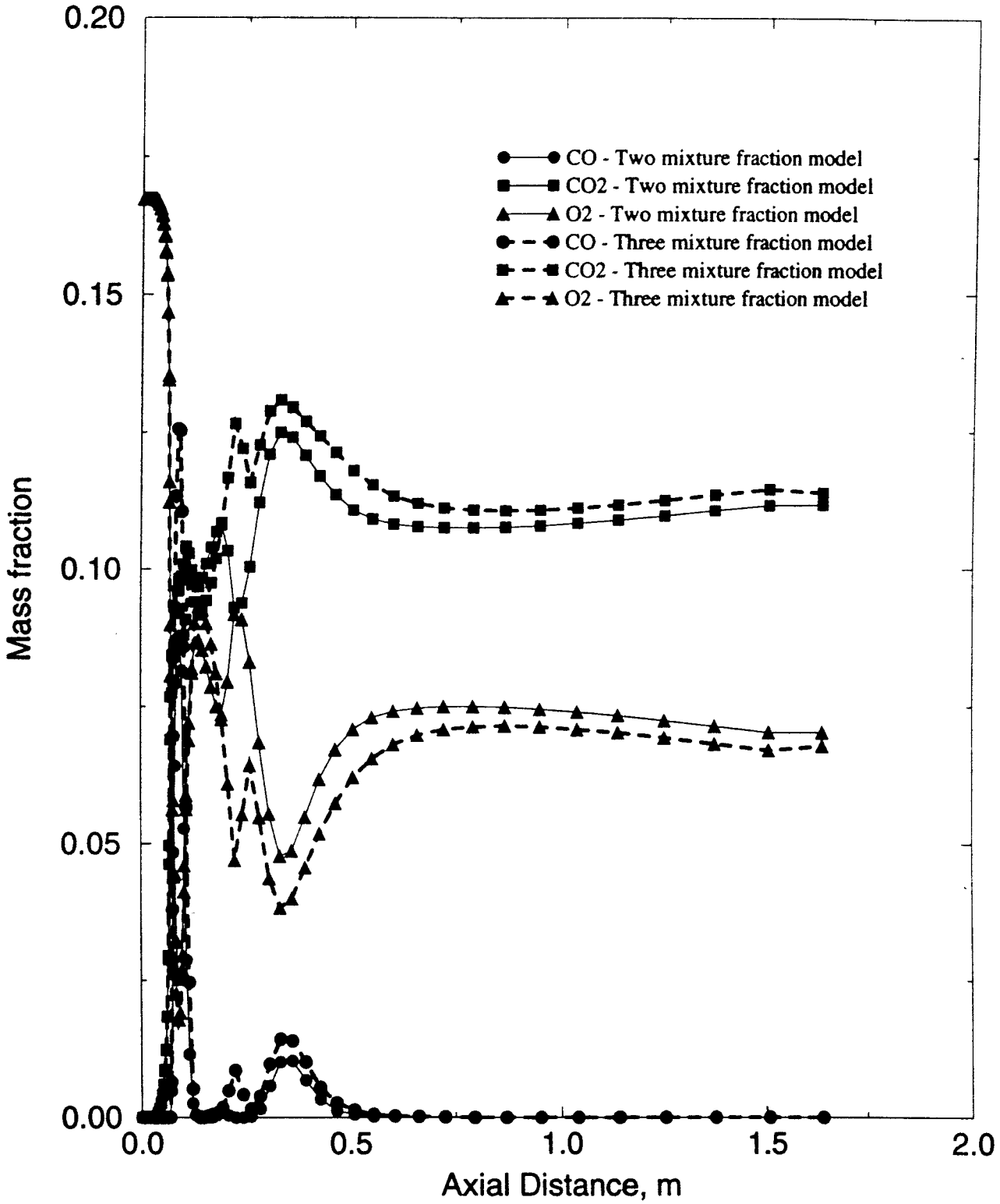

Figure 3. Centerline mass fraction distributions of mahor species

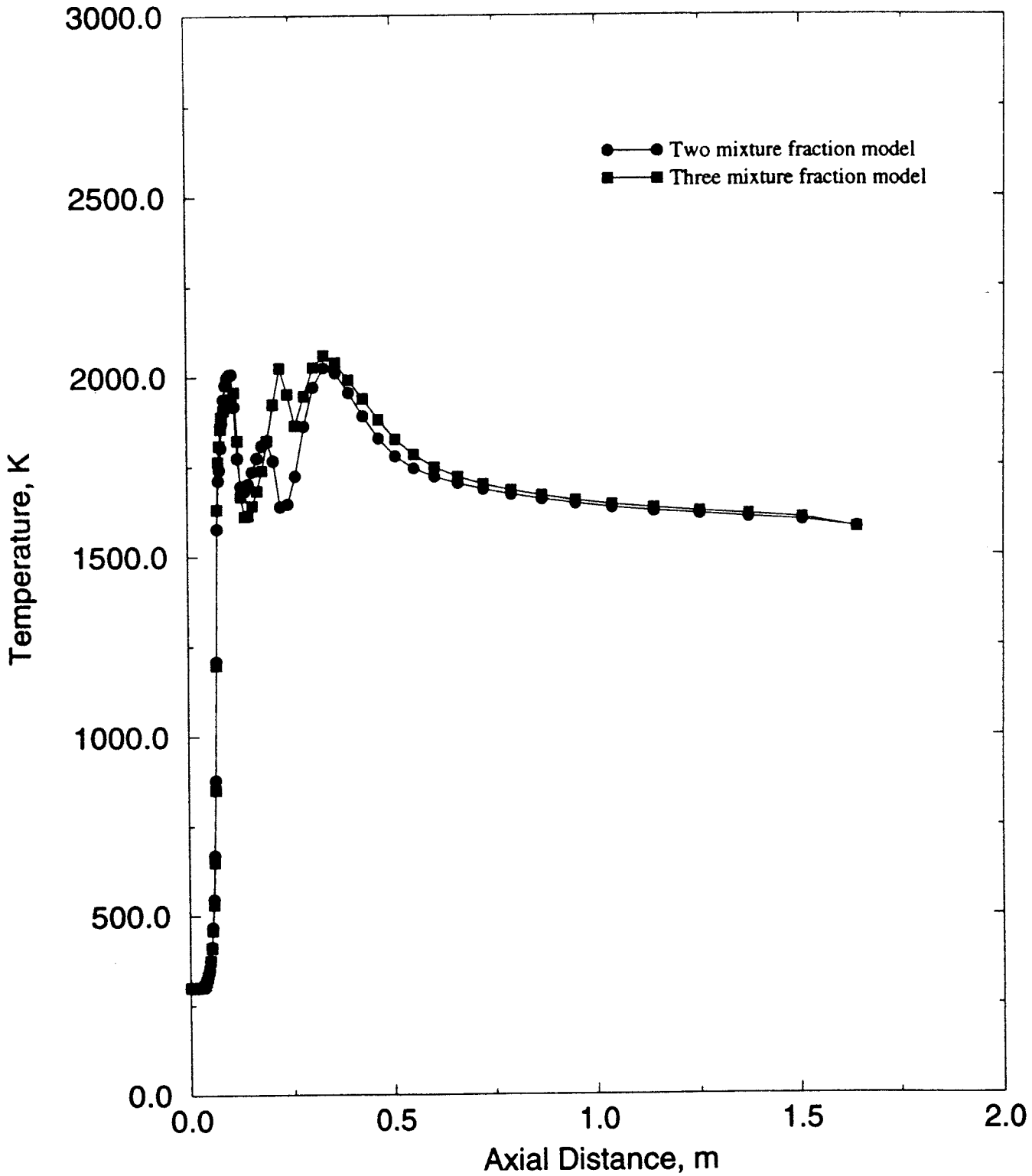

Figure 4. Centerline distribution of temperature.

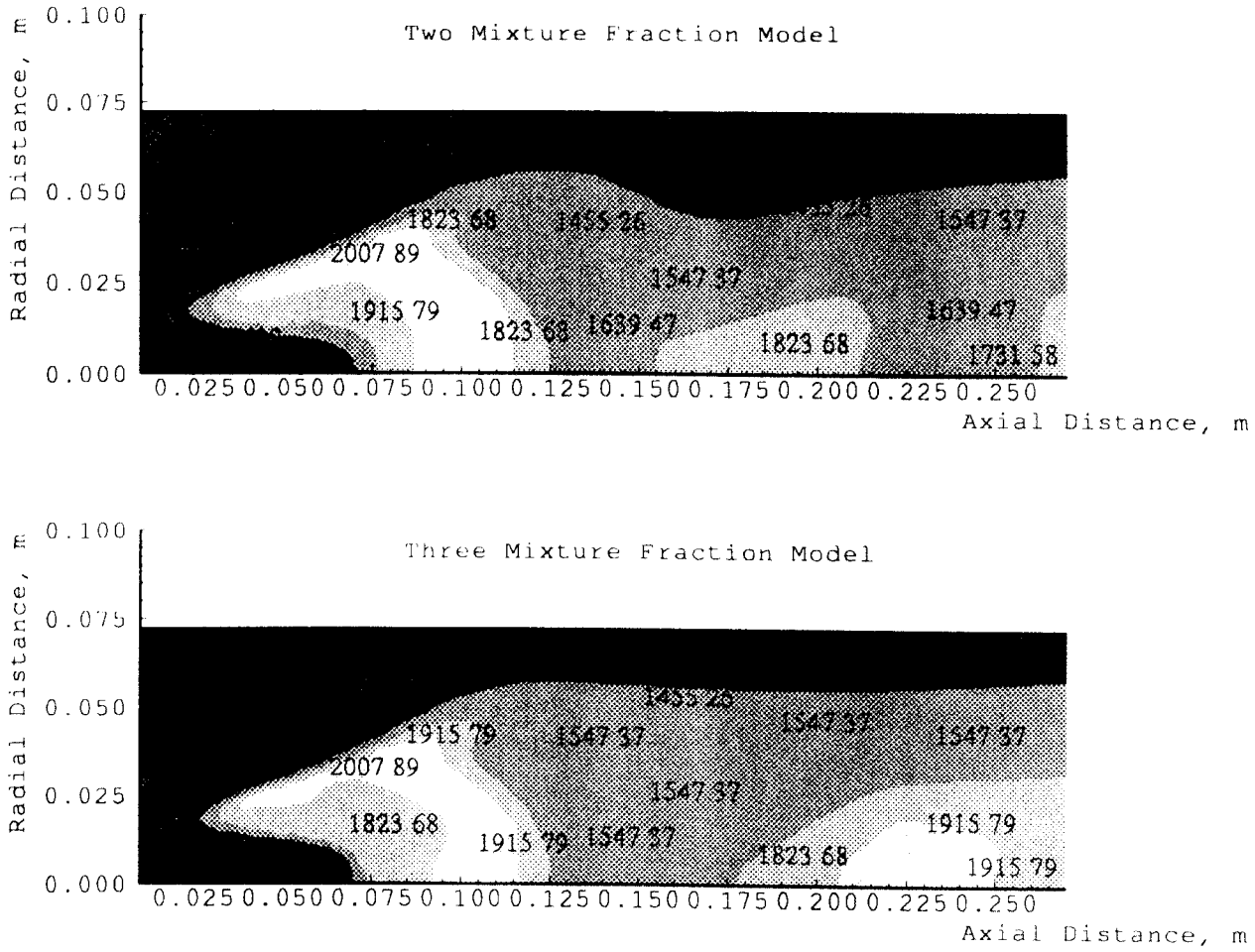

Figure 5. Near burner temperature (Kelvin) field predictions