

Extending the Mixture Fraction Concept to Address Under-Ventilated Fires

Floyd, J.E.¹ and McGrattan, K.B.²

¹ Hughes Associates, Inc.

3610 Commerce Dr., #817

Baltimore, Maryland, USA, 21227

P:410.737.8677, F:410.737.8688, jfloyd@haifire.com

²Building and Fire Research Laboratory, National Institute of Standards and Technology,

Gaithersburg, Maryland, USA

Abstract

A common technique in computational fluid dynamics (CFD) modeling of fire is to assume single step, infinitely fast combustion, in which case the transport equations of all gas species can be combined into one for a single conserved scalar called the mixture fraction. While this approach is adequate for many engineering applications, for fire scenarios that require predictions of CO formation or flame extinction this approach is inadequate. This paper describes a method of extending the mixture fraction concept to address two-step chemistry. The two-step chemistry allows for flame extinction and the prediction of CO formation and destruction. The mixture fraction is decomposed into components representing the states of the two-step chemistry. The new model is demonstrated with two test cases: a slot burner using direct numerical simulation (DNS) and a reduced scale enclosure using large eddy simulation (LES). Results of the new model are compared with experimental data and simulations using single-step chemistry.

Nomenclature

a, b, x, y, z	Mole proportions
$\frac{D}{Dt}$	Substantial derivative
D	Diffusion coefficient
K	Reaction rate constant
$\dot{m}_i'''$	Species i production rate (kg i /m ³ -s)
R	Universal gas constant
T	Time (s)
T	Temperature (K)
W_i	Molecular weight of species i (kg i /kmol i)
X_H	Hydrogen atom fraction
Y_i	Mass fraction of species i (kg i /kg)
Y_i^I	Fuel inlet mass fraction of species i (kg i /kg)
Y_i^∞	Ambient mass fraction of species i (kg i /kg)
y_i	Yield of species i (kg i /kg fuel)
s	Stoichiometric oxygen to fuel mass ratio
Z_i	Mixture fraction component
ϕ	Equivalence ratio
ρ	Density (kg/m ³)
ν_i	Stoichiometric coefficient of species i
ν_{CO}	Fixed yield stoichiometric coefficient of CO
ν'_{CO}	Stoichiometric coefficient of CO

The Mixture Fraction Concept

In the classic Burke-Schumann description of a diffusion flame [1], the combustion process can be described by way of a single conserved scalar, the mixture fraction, which represents the mass fraction of the gas originating in the fuel stream. It can be expressed in various ways, usually as linear combinations of fuel and product species. Here we adopt:

$$Z = \frac{sY_F - (Y_{O_2} - Y_{O_2}^\infty)}{sY_F^I - Y_{O_2}^\infty} = Y_F + \frac{Y_{H_2O}W_{H_2}}{W_{H_2O}} + \frac{Y_{CO_2}W_C}{W_{CO_2}} + \dots \quad (1)$$

where s is the stoichiometric oxygen to fuel mass ratio. For fire modeling with simple combustion chemistry, the mixture fraction is a useful concept, as it reduces the computational expense of having multiple gas species transport equations. However, the mixture fraction alone only provides one degree of freedom. In the absence of additional scalar parameters (i.e. some form of reaction progress variable), one is limited to the assumption that combustion is infinitely fast, or, in other words, fuel and oxygen burn instantly and completely on contact, regardless of temperature and other local conditions. This means that there is no way to model extinction, CO and soot production/destruction, pre-mixed combustion, ignition, and various other phenomena of interest in fire science.

Does this mean that we ought to abandon the mixture fraction approach? No. The principal reason for adopting a mixture fraction-based combustion model is to reduce the number of species transport equations that must be solved and thereby reduce the overall computer time required. To overcome its limitations, but keep its benefits, we have extended the mixture fraction approach to account for incomplete combustion. This method has been incorporated into the CFD model Fire Dynamics Simulator (FDS) [2][3] and a number of validation test cases have been run. Two examples are given in this paper: a methane-air slot burner and a small scale compartment fire experiment.

2. Generalizing the Mixture Fraction Concept

There exist in the combustion literature numerous reaction mechanisms for various hydrocarbon fuels. Many of these are intended for small scale simulations and involve dozens of reactions and species. For example one mechanism for methane combustion in air includes 58 reactions with 16 species [4]. This is a level of complexity that is undesirable for a practical fire model as tracking 16 species would greatly increase the computational resources required (both memory and time) and many of the reactions would occur at length scales never encountered in a typical large scale simulation. Simpler reaction mechanisms have been derived that collapse the very complex schemes down to four reactions [5] that include separate steps for the oxidation of H_2 to H_2O and CO to CO_2 . Even this, however, is more complex than desired as it involves five parameters (one each for fuel, CO_2 , CO , H_2 , and H_2O). It is additionally observed that for fire protection applications H_2 in under-ventilated fires is not as critical as CO , since H_2 is essentially non-toxic.

Since it is desired to minimize the complexity of a new combustion model and to ensure its applicability to simulations with large grid sizes, the simplest possible CO formation and extinction mechanism is used. The following two-step combustion is assumed [6]:



In the first step, fuel and oxygen react to form carbon monoxide and other combustion products. Other products (soot, water vapor) are considered to have fixed yields. In the second step, carbon monoxide reacts with oxygen to form carbon dioxide. No assumptions need be made at this point about reaction rates. This scheme is designed primarily for hydrocarbon fuels. Fuels containing oxygen, such as wood, can generate CO directly from pyrolysis reactions [7] and this method presumes that CO and other products are formed proportionately to oxygen consumption.

The description of the two-step reaction above, with extinction, requires three independent variables. One to keep track of the amount of fuel present, a second to track how much of that fuel has reacted to form CO, and a third to track how much of the CO has reacted to form CO₂. For practical reasons, the variables should be conserved, should provide a numerically stable method of computing the heat release rate, and should uniquely determine the gas species. To derive these variables, consider linear combinations of the transport equations for fuel, carbon monoxide, and carbon dioxide:

$$\frac{DY_F}{Dt} = \nabla \cdot D\rho \nabla Y_F + \dot{m}_{F,1}''', \quad (4)$$

$$\frac{DY_{CO}}{Dt} = \nabla \cdot D\rho \nabla Y_{CO} + \dot{m}_{CO,1}''' + \dot{m}_{CO,2}''', \quad (5)$$

and

$$\frac{DY_{\text{CO}_2}}{Dt} = \nabla \cdot D\rho \nabla Y_{\text{CO}_2} + \dot{m}_{\text{CO}_2,2}''' \quad (6)$$

where the numerical subscripts on the mass production terms refer to the two reaction steps.

Note that:

$$\frac{\dot{m}_{\text{F},1}'''}{W_{\text{F}}} = - \frac{\dot{m}_{\text{CO},1}'''}{\nu_{\text{CO}} W_{\text{CO}}} \quad (7)$$

and

$$\frac{\dot{m}_{\text{CO},2}'''}{\nu_{\text{CO}} W_{\text{CO}}} = - \frac{\dot{m}_{\text{CO}_2,2}'''}{\nu_{\text{CO}_2} W_{\text{CO}_2}}. \quad (8)$$

By substituting Eqs. (7) and (8) into Eqs. (5) and (6), respectively, and multiplying the equations by an appropriate scalar constant (scalar multiplication does not affect the conservation of mass), we derive the following transport equations for the three mixture fraction variables:

$$\frac{DZ_1}{Dt} = \nabla \cdot D\rho \nabla Z_1 + \dot{m}_{\text{F},1}''', \quad (9)$$

$$\frac{DZ_2}{Dt} = \nabla \cdot D\rho \nabla Z_2 - \dot{m}_{\text{F},1}''' + \frac{W_{\text{F}} \dot{m}_{\text{CO},2}'''}{\nu_{\text{CO}} W_{\text{CO}}}, \quad (10)$$

and

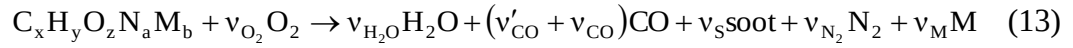
$$\frac{DZ_3}{Dt} = \nabla \cdot D\rho \nabla Z_3 - \frac{W_F \dot{m}_{CO,2}'''}{\nu_{CO} W_{CO}} \quad (11)$$

where $Z_1 = Y_F$, $Z_2 = \frac{W_F}{\nu_{CO} W_{CO}} Y_{CO}$, and $Z_3 = \frac{W_F}{\nu_{CO_2} W_{CO_2}} Y_{CO_2}$. Note that the source terms in the mixture fraction transport equations sum to zero. Physically, this is simply mass conservation. The decrease in Z_1 (fuel combining with oxygen to form CO and other products) is equal to the increase in Z_2 , and the decrease in Z_2 (CO combining with oxygen to form CO₂) is equal to the increase in Z_3 . When the three mixture fraction variables are summed, the resulting quantity represents all the mass that was originally fuel, and is equal to the mixture fraction itself:

$$Z_1 + Z_2 + Z_3 = Y_F + \frac{W_F}{\nu_{CO} W_{CO}} Y_{CO} + \frac{W_F}{\nu_{CO_2} W_{CO_2}} Y_{CO_2} = Z \quad (12)$$

In short, we can replace the transport equations for all the gas species with the three mixture fraction variables. The source terms in these equations depend on the specific form of the combustion model which will be described below.

Recovering the species mass fractions from the mixture fraction variables is relatively easy and computationally efficient. To derive the necessary formulae, first consider Eqs. 2 and 3 written completely in terms of all the species:



$$v'_{CO} \left(CO + \frac{1}{2} O_2 \rightarrow CO_2 \right) \quad (14)$$

The parentheses in Eq. (14) are there to indicate that the two reactions sum to the complete combustion reaction for the fuel. Note that CO has two stoichiometric coefficients where v'_{CO} applies to the CO that can be converted to CO_2 and v_{CO} applies to the CO that exists post-flame. The combustion model to be discussed later in this paper is not capable of predicting the small levels of CO that still exist in well ventilated fires; hence, the need to preserve this empirical value. M is a species that representing that portion of the fuel that is not C, H, O, or N.

Next, some additional quantities are defined. The fuel stream may be specified as diluted given by Y_F^I , the mass fraction of fuel in the fuel stream. The diluent is presumed to be nitrogen with a mass fraction of $Y_{N_2}^I = 1 - Y_F^I$. The ambient mass fractions of oxygen, $Y_{O_2}^\infty$, and nitrogen, $Y_{N_2}^\infty = 1 - Y_{O_2}^\infty$, are also specified. Accounting for fuel dilution and the atom fraction of hydrogen in the soot, X_H , the mixture fraction parameters are given as:

$$Z_1 = \frac{Y_F}{Y_F^I}, \quad (15)$$

$$Z_2 = \frac{W_F}{W_{CO}(x - (1 - X_H)v_S)} \frac{Y_{CO}}{Y_F^I}, \text{ and} \quad (16)$$

$$Z_3 = \frac{W_F}{W_{CO_2}(x - (1 - X_H)v_S)} \frac{Y_{CO_2}}{Y_F^I}. \quad (17)$$

The mass fractions of the species are then given by:

$$\begin{bmatrix} 0 & Y_F^I & 0 & 0 \\ Y_{N_2}^\infty & Y_{N_2}^I & \frac{\nu_{N_2} W_{N_2}}{W_F} Y_F^I & \frac{\nu_{N_2} W_{N_2}}{W_F} Y_F^I \\ Y_{O_2}^\infty & 0 & -\frac{\nu'_{O_2} W_{O_2}}{W_F} Y_F^I & -\frac{\nu_{O_2} W_{O_2}}{W_F} Y_F^I \\ 0 & 0 & \frac{(\nu'_{CO} + \nu_{CO}) W_{CO}}{W_F} Y_F^I & 0 \\ 0 & 0 & 0 & \frac{\nu_{CO_2} W_{CO_2}}{W_F} Y_F^I \\ 0 & 0 & \frac{\nu_{H_2O} W_{H_2O}}{W_F} Y_F^I & \frac{\nu_{H_2O} W_{H_2O}}{W_F} Y_F^I \\ 0 & 0 & \frac{\nu_S W_S}{W_F} Y_F^I & \frac{\nu_S W_S}{W_F} Y_F^I \\ 0 & 0 & \frac{\nu_M W_M}{W_F} Y_F^I & \frac{\nu_M W_M}{W_F} Y_F^I \end{bmatrix} \times \begin{bmatrix} 1 - Z_1 - Z_2 - Z_3 \\ Z_1 \\ Z_2 \\ Z_3 \end{bmatrix} = \begin{bmatrix} Y_F \\ Y_{N_2} \\ Y_{O_2} \\ Y_{CO} \\ Y_{CO_2} \\ Y_{H_2O} \\ Y_S \\ Y_M \end{bmatrix}. \quad (18)$$

The stoichiometric coefficients are given by:

$$\begin{aligned}
\nu_{N_2} &= \frac{a}{2} & \nu_{H_2O} &= \frac{y}{2} - X_H \nu_S \\
\nu'_{O_2} &= \frac{\nu'_{CO} + \nu_{H_2O} - z}{2} & \nu'_{CO} &= x - \nu_{CO} - (1 - X_H) \nu_S \\
\nu_{O_2} &= \nu_{CO_2} + \frac{\nu_{H_2O} - z}{2} & \nu_{CO} &= \frac{W_F}{W_{CO}} y_{CO} \\
\nu_{CO_2} &= x - (1 - X_H) \nu_S & \nu_S &= \frac{W_F}{W_S} y_S \\
\nu_M &= b & W_S &= X_H W_H + (1 - X_H) W_C
\end{aligned} \tag{19}$$

where y_{CO} and y_S are the user specified post-flame yields of CO and soot and a , b , x , and y are from the specification of the fuel molecule in Eq. (13). In short, the individual gas species mass fractions are just linear combinations of the three mixture fraction variables, and the solution of transport equations for the three mixture fraction variables rather than the eight species reduces the computational expense of the entire simulation by roughly 30 %.

3. Numerical Advantages of the Mixture Fraction Decomposition Method

The decomposition of the mixture fraction discussed in the previous section is not the only way to generalize the concept. There are combustion models that still retain the “total” mixture fraction, Z , for species tracking, but also solve a transport equation for a “progress variable” (often denoted by the letter c) that indicates, via a value between zero and one, the completeness of the combustion reaction [8]. Z and c alone can describe a single reaction with the possibility of local extinction. The formulation can be extended, via another

progress variable, to account for CO production/destruction. Indeed, the decomposition of the mixture fraction described in the previous section can also be reformulated in terms of only two mixture fraction variables, Z_1 and Z_3 , if we want to neglect the incomplete combustion step and only allow complete combustion with the possibility of local extinction.

Mathematically, these various formulations of the basic transport equations are equivalent. They are simply book-keeping strategies designed to reduce the computational expense of the simulation. However, there are numerical advantages to the mixture fraction decomposition ($Z = \sum_i Z_i$) when implemented in a large scale fire model. The first advantage has to do with the calculation of the heat release rate; the second has to do with boundary and initial conditions.

A very important consideration in a fire model is the computation of the local volumetric heat release rate. In the classic formulation, the heat release rate is proportional to the gradient of Z across the “flame sheet;” that is, the interface between fuel and oxygen. On a relatively coarse numerical grid, this computation can be awkward, as the value of Z can change dramatically at the interface when there are not a sufficient number of grid cells to resolve it. Consider a horizontal profile of Z across a coarsely defined fire, shown in Figure 1 (shaded region is burner location). A common problem with finite differencing schemes whose spatial accuracy is higher than first order is that regions with steep gradients typically exhibit “under-shoots,” where the variable drops below some obvious lower

bound. For example, in the figure, the mixture fraction, Z , drops below zero. Although a negative value of the mixture fraction is physically meaningless, the numerical scheme is mass conserving overall. In other words, a local dip below zero is offset somewhere else (the slight increase in Z above zero seen near the dips). There are numerous ways of correcting these local defects [9], but all of these methods will compromise the accuracy of any heat release rate calculation that is based on the gradient of the mixture fraction across the flame sheet, where these under-shoots typically occur. The reason for the inaccuracy is that the correction of the under-shoot is typically achieved by redistributing fuel mass across the flame sheet, which effectively alters the heat release rate.

The advantage of the mixture fraction decomposition approach is that Z_f represents the fuel mass fraction, and the heat release rate can be computed directly from the conversion rate of fuel to products. There is no need to compute gradients of a single mixture fraction variable, and thus the problem associated with under-shoots is eliminated. This was a crucial consideration in the adoption of the decomposition approach in FDS, starting with version 5, released in October, 2007 [2].

A second major advantage of the mixture fraction decomposition approach has to do with boundary conditions. Because the mixture fraction components, Z_i , represent linear combinations of species mass fractions, their initial and boundary conditions are easily formulated. However, the same cannot be said for the progress variable, c . The progress variable is well defined within the fuel and product streams because it indicates the relative

completeness of the combustion process. However, its value initially and in the far field is not well defined, as there are no reactants or products initially or in the far field. Over the course of a fire simulation, the value of the progress variable in the exhaust plume might go from 1 (complete combustion) to 0 (no combustion). What value should be assigned to c in the far field that is consistent with these two extremes? Whether it be 0 or 1, there will inevitably be problems associated with the “artificial” diffusion of c that are inherent in any finite difference formulation of the transport equations. Artificial diffusion is essentially the “smearing” of the variable’s value over the numerical mesh, another unavoidable consequence of the numerics. Because c represents the state of the combustion process, changes in its value imply a reaction has or has not occurred. As with the problem associated with the calculation of the heat release rate, we do not want to adopt any numerical scheme for which unavoidable numerical defects compromise the integrity of the underlying physical model.

This discussion of the advantages and disadvantages of these various mixture fraction formulations may seem completely divorced from the actual physics of fire. It is important to keep in mind, however, that these abstract concepts do have physical meaning, and the choice of one scheme over another often has more to do with numerical, rather than physical, considerations. Indeed, up to this point, the actual physics of the combustion process have not even been discussed, but rather the numerical framework that is to support the combustion model. The physical assumptions underlying the combustion model are discussed next.

4. Combustion Model

In this section we discuss the details of the combustion model that was implemented in FDS. The model is fairly simple and empirically based because of the fact that FDS is used for large scale fire simulations, and the numerical grid is typically on the order of 10 cm or higher. It is important to keep in mind that the mixture fraction decomposition idea put forward in the previous section will support any number of variants on the combustion model discussed below.

Consider the two-step reaction outlined in Eqs. (2) and (3). The first reaction step, the incomplete reaction of fuel and oxygen that forms CO and other products, could potentially occur in any grid cell that contains both fuel and oxygen, assuming conditions are appropriate. One possible means of determining flammability is via the critical adiabatic flame temperature [10]. On coarse numerical grids typical of large-scale fire simulations, there is only limited information with which to determine the viability of a flame in a particular region of the flow field. Using only the local temperature and oxygen concentration, an argument can be made that a flame is viable for values that lie in the upper right half of the diagram shown in Figure 2. For local temperatures and oxygen concentrations falling below the line, the critical flame temperature cannot be reached and Step 1 is not allowed. Details are given in Reference [2].

There are several limitations associated with this simple flammability argument. First, the rule is applicable to low strain rate flames typically found in fires and cannot predict phenomena such as blow off. Second, if flammability is permitted, there is often an abundance of fuel or oxygen in the particular grid cell due to the numerical error that inevitably results from using a coarse grid. Allowing either the fuel or oxygen to be consumed instantaneously leads to an unrealistic local heat release rate, but limiting the reaction rate is problematic as well because the local temperature is only an average over a fairly large grid cell and cannot be used to estimate the reaction rate. Empirical arguments must be used to control the rate of reaction. In FDS, an upper limit is placed on the volumetric heat release rate. Recent research has suggested that low strain rate diffusion flames cannot achieve heat release rates greater than about 200 kW/m^2 of flame area [11]. Dividing this value by the width of the grid cell provides a limit on the local volumetric heat release rate. In the specific FDS version used for this paper, no additional limitations were applied based on mixing constraints; however, such limitations are currently being investigated.

The second step of the reaction, the conversion of CO to CO₂, can occur in any grid cell where oxygen and CO exist. However, unlike Step 1, it can be argued that the computed local temperature away from the flame region *can* be relied upon for use in calculating the reaction rate, even on a relatively coarse grid, because the gradient of temperature is not nearly as steep. Of course, “away from the flame” is somewhat vague, especially in regard to a compartment undergoing flashover. In FDS, the strategy is as follows. If fuel, oxygen and CO exist in a grid cell for which flammability is viable, Step 1 of the reaction takes

preference in consuming the fuel and oxygen, followed by the instantaneous conversion of CO to CO₂ if there is enough oxygen left over and if the upper bound in the volumetric heat release rate has not been reached. It is presumed that a flame, and therefore a flame temperature, is present and CO will oxidize rapidly consuming the maximum possible amount of CO and O₂ in the grid cell. Away from the flame, that is, where fuel is not present or oxygen levels do not meet the criteria in Figure 2, it is presumed that a flame is also not present and therefore the computed cell temperature is appropriate in the following expression for the oxidation rate of CO [12].

$$k(T) = 2.53 \times 10^{12} e^{\frac{-199547}{RT}} \text{ cm}^3/\text{mol-s} \quad (20)$$

In summary, the two-step reaction mechanism described above consists of a fast (instantaneous) reaction of fuel and oxygen to form CO and other products, followed by a slow conversion of CO to CO₂ if the temperature is high enough and there is enough oxygen available. This process is illustrated in the flowchart shown in Figure 3.

4. Validation

The extended mixture fraction, two-step combustion model was implemented in FDS, version 5, and compared against two very different experiments. The first was a small methane-air, Wolfhard-Parker slot burner diffusion flame [13]-[15]. The second was a set of selected experiments performed at NIST in a reduced scale enclosure (RSE) [16]. The objective of the exercise was to (1) ensure that the new methodology is valid, (2) determine if the two-step approach is significantly better than the one-step, and (3) make sure that the methodology is sound not just for small laminar diffusion flames simulated using direct numerical simulation (DNS), but also for practical, large-scale fire scenarios performed with large eddy simulation (LES).

For both geometries, the current FDS submodels for radiation heat transfer and surface heat transfer were used. Surface heat transfer is computed using a one-dimensional, multi-layer, heat conduction solver. Radiation heat is computed using a finite volume method [17] using 104 control angles. Spectrally, the slot burner used a wide band approach that uses 9 spectral bands whereas the reduced scale enclosure used a gray gas approach. Absorption coefficients are precomputed using RADCAL [18] and tabulated as a function of the mixture fraction components, temperature, and spectral band.

4.1 Slot Burner

The Wolfhard-Parker slot burner consisted of an 8 mm wide central slot flowing fuel surrounded by two 16 mm wide slots flowing dry air with 1 mm separations between the

slots. The slots were 41 mm in length and 3 mm high. Velocity, temperature, and species profiles for a methane flame for various heights above the burner are archived on the NIST web page [13]. The experimental errors were reported as 5 % for temperature [14] and 10 % - 20 % [14] for the major species.

A three dimensional simulation was performed for one quarter of the slot burner with a uniform 0.5 mm numerical grid. The grid study used grids of 0.25 mm, 0.5 mm, and 1.0 mm. The 0.5 mm and 0.25 mm grid had no change in flame position and differences in the peak temperature, peak velocity, and CO and CO₂ gas concentrations were less than 10. Symmetry boundary conditions were assumed because the flow field was laminar. The computational domain was 32 mm by 32 mm by 48 mm with 393,000 grid cells. A two dimensional simulation was also performed, but the results were less accurate because radiative losses along the axis of symmetry are not possible in a 2D computation. The 3D simulation was run for 4 s of physical time, requiring 104 hours of CPU time on a 2.4 GHz Intel processor. While this might sound like a very costly calculation, it is typical of direct numerical simulation. While DNS is typically not practical for fire protection engineering applications, it is a useful approach for evaluating the new combustion methodology.

Figure 4 shows predicted temperature profiles using both a single and two-step reaction scheme, plotted as a function of the distance from the burner centerline at heights of 7 mm and 11 mm above the burner. Both the single and two-step models predicted a flame that is slightly narrower and slightly cooler than the data. The single and two-step models respectively predicted a 5.5 mm and 6 mm wide flame vs. the measured 6.5 mm (15 % and

8 % error). It is possible that the width error resulted from assumptions made in creating the FDS input. The fuel and air inlets were presumed to be uniform in both temperature and mass flux. Some or all of the width errors could be accounted for by non-uniformities in the inlet flow. Additionally, above the region displayed was a screen to stabilize the flame. That region was not included and its omission may also contribute to the error in width. Lastly, there is a noticeable shift in the width when going from 1-step to 2-step chemistry, and some portion of the width error could result from the lack of species such as H_2 . The peak flame temperature, however, should not be greatly affected by these assumptions. It is observed that the one-step reaction scheme under-predicted the peak measured temperatures by 11 % and 7 % at 7 mm and 11 mm, respectively, while the two-step scheme only under-predicted these measurements by 3 % and 4 %, respectively. The two-step version predicted higher centerline temperatures and the single-step version predicted slightly lower centerline temperatures. If the two-step profiles are expanded by the 0.5 mm width error (presuming the width error was due to input uncertainties), then the two-step predictions would match the measured data except along the centerline.

The overall results are not surprising as the first reaction step is infinitely fast. Thus, combustion occurs at the grid cell immediately above the lip of the burner. In reality, the cold fuel and air streams do not react infinitely fast and some oxygen penetrates the flame at the base. This lower amount of combustion in the experiment at the burner lip results in cooler gasses being entrained into the core of the flame with a resulting drop in the centerline temperature. The single-step version predicted lower temperatures throughout

the flame and this was likely a result of the single parameter model not capturing the appropriate heat release distribution vertically over the burner.

Figure 5 shows predicted and measured fuel and oxygen profiles for the single and two-step reaction schemes, plotted as a function of the distance from the burner centerline at a height of 7 mm and 11 mm above the burner. The two-step predictions of the fuel concentration lie within the uncertainty at all locations. The one-step predictions lie below the uncertainty bounds near the edge of the flame but are otherwise within the uncertainty bounds. Both schemes predicted oxygen concentrations above the uncertainty bounds, but the two-step predictions are significantly improved. The over-prediction of the oxygen concentration resulted primarily from the prediction of a narrower flame, as seen in the temperature predictions shown in Figure 4. If the predicted width were stretched to match the experimental width, the two-step predictions would match the measured data. Notice that both reaction schemes failed to predict the small amount of oxygen that was measured at the burner centerline because both schemes employ a fast primary reaction that does not allow any oxygen to penetrate the flame sheet.

Figure 6 shows predicted and measured carbon dioxide and carbon monoxide concentration profiles at two elevations above the burner. The two-step predictions for CO_2 generally lie within the uncertainty bounds of the measurements, except for regions outside the flame resulting from the narrower flame prediction. The one-step scheme over-predicted CO_2 inside the flame -- not surprising as the scheme only produced CO_2 in a one-step complete reaction. The two-step predictions of CO at the 7 mm height generally lie within the

uncertainty bounds except near the edge of the flame (due to the narrower flame prediction) and at the flame centerline. At the 11 mm height, the two-step predictions are lower than the measured data. The CO predictions show a decrease in the peak value as a function of height above the burner whereas the measurements show a slight increase (errors in the peak concentrations of CO are 5 % at 7 mm and 30 % at 11 mm). This result was likely due to a combination of the infinitely fast first reaction combined with allowing the second reaction to be infinitely fast in those cells where the first reaction has occurred.

The predictions of CO provide an excellent illustration of the two-step combustion model. In the grid cells in the vicinity of the burner lip, fuel and oxygen react and form CO, but there was not enough oxygen available to complete the reaction. Further up in the flame, additional air was entrained and CO oxidizes to form CO₂. The two-step combustion model is relatively simple, but it does at least have the necessary mechanism to describe this very basic process. Next, the model will be shown to work well for a more practical fire scenario.

4.2 NIST Reduced Scale Enclosure Experiments

The NIST Reduced Scale Enclosure (RSE) was a 40 % scaled version of the ISO 9705 compartment. It measured 0.98 m wide by 1.46 m deep by 0.98 m tall, with a door centered on the small face that measured 0.48 m wide by 0.81 m tall. A 15 cm diameter natural gas burner was positioned in the center of the compartment. The burner was on a stand so that its top was 15 cm above the floor. Species measurements were made inside

the upper layer of the compartment at the front near the door and near the rear [16]. Heat release rate uncertainties were reported as 8.6 %, and CO and CO₂ concentration measurements had reported uncertainties of 0.24 %.

FDS was used to simulate eight fires in the compartment: 50 kW, 75 kW, 150 kW, 200 kW, 300 kW, 400 kW, 500 kW, and 600 kW. The tests were modeled using properties of a typical natural gas supplied to the test facility [19],[20]. The simulation included the compartment interior along with a 0.6 m deep region outside the door that was modeled using a 2.4 cm grid resolution for a total of 240,000 grid cells. The grid study used the 500 kW fire with grid sizes of 1.9 cm, 2.4 cm, and 3.5 cm as well as a study using the 2.4 cm with a 50 % lower CFL limit (i.e. reduced the time steps by a factor of two). Between the 1.9 cm and the 2.4 cm grids as well as the reduced time step there was no significant change in the location and magnitude of the heat release rate contours and discernable differences in upper layer temperatures and CO and CO₂ concentrations were less than 10 %. The wall boundary condition used a reduced material density for the compartment lining. This was done so that the computation would reach steady state in less time. Each fire size was simulated for 300 s which for the new approach took approximately 45 hours on a 2.4 GHz processor.

Simulations were performed with both the single and two-step reaction schemes. While the one-step reaction scheme does not predict CO formation, it does allow the specification of a fixed post flame CO yield. Setting an increased CO yield to account for a higher equivalence ratio would be a typical practice for an engineer using the one-step model;

therefore the correlation in Eq. 21 [21] was used to set the CO yield for each simulation with the equivalence ratio, ϕ , determined using Eq. 22.

$$Y_{\text{CO}} = \frac{0.19}{180} \tan^{-1}(10(\phi - 0.8)) + 0.095. \quad (21)$$

$$\phi = \frac{\dot{m}_{\text{burner}} \frac{\nu_{\text{O}_2} W_{\text{O}_2}}{W_{\text{F}}}}{\frac{Y_{\text{O}_2}^{\infty}}{2} A_{\text{door}} \sqrt{H_{\text{door}}}}. \quad (22)$$

The predicted and measured CO and CO₂ concentrations at the front and rear locations are shown in Figure 7. The equivalence ratios in the figure are based upon the computed mass flow rates derived from temperature measurements made during the tests; they differ from the presumed equivalence ratios used to set the CO yield for the one-step model. Both reaction schemes capture the general trends seen in the CO₂ data. The one-step scheme over-predicted the concentrations while the two-step scheme under-predicted them. Moreover, the two-step scheme over-predicted the CO concentrations, but the amount of over-prediction was consistent with the amount of under-prediction in CO₂. The one-step scheme, using an equivalence ratio correlation for CO yield, could not replicate the measured values at the two specific locations inside the compartment. Not surprisingly, the under-prediction of CO by the one-step scheme was consistent with its over-prediction of CO₂.

At 600 kW, the two-step predictions of CO₂ at the front and rear locations were 4.9 % and 6.3 % respectively vs. the 6.1 % and 7.1 % in the data. For CO the corresponding results were 3.6 % and 2.9 % vs. 2.9 % and 2.1 %. Note, however, that the absolute front and rear under-prediction in CO₂ of 1.2 % and 0.8 % was similar to the 0.7 % and 0.8 % over-prediction of CO. This implies that a significant contributor to the model error was likely the infinitely fast chemistry assumption of the first reaction combined with the sequential vs. simultaneous reaction steps.

The predicted and measured lower and upper temperatures are shown in Figure 8. The two-step predictions show a similar trend to the data (reaching plateau at higher equivalence ratios) that is not seen in the single-step predictions. Both approaches over predict the upper layer temperatures; however, the degree of over prediction is much less for the two-step scheme.

5. Conclusion

A generalization of the mixture fraction concept has been proposed as a means of maintaining the practicality and efficiency of a CFD fire model while extending its ability to handle fire phenomena such as CO production and extinction. By decomposing the mixture fraction into three parts -- fuel, products of incomplete combustion, and products of complete combustion -- we can introduce a two-step combustion model that allows for extinction and CO production. The ability of the new approach to predict CO

concentrations was tested using two sets of experiments: a methane-air slot burner diffusion flame and small compartment experiments performed.

For the small-scale slot burner simulations performed at high spatial resolution, the new model predicted species concentrations generally within the 10 % to 20 % experimental uncertainty range with prediction errors of 6 % to 25 %. Temperature predictions were within the 5 % experimental uncertainty range. Improvements in all predicted quantities were achieved with the new approach and were demonstrably better than results using only a one-step reaction scheme.

For the larger scale geometry, the new model matched experiments for both well-ventilated and under-ventilated fires, whereas the one-step approach only performed well for well-ventilated fires. The two-step scheme under-predicted the oxidation of CO; however, the predictions were still within 20 % to 30 % of the measured data, a level of performance which was not possible with the one-step scheme. Upper temperature predictions were also greatly improved with the two-step scheme.

There is clearly room for improvement in the current approach. Developing improved criteria for allowing the oxidation of fuel and oxygen in the first step and perhaps the inclusion of a rate equation or mixing limitation should reduce over-predictions of CO formation. However, given the conditions discussed in the introduction, developing criteria that are broadly applicable over many length scales would not be trivial. Such criteria would have the added benefit of potentially extending the applicability of the model to re-

ignition problems such as backdrafts. The mixture fraction decomposition idea could also be extended to include additional parameters. For example the mixture fraction could be decomposed further to add a term for tracking soot formation and destruction. However, it is noted that at some point the expense of working with a large number of mixture fraction variables becomes comparable to the cost of working with the primitive variable approach of tracking individual species, in which case its advantages disappear.

Acknowledgements

This work was funded by the United States Department of Commerce, National Institute of Standards and Technology, Building and Fire Research Laboratory through the Fire Grants Program.

References

- [1] Kuo, K. Principles of Combustion. John Wiley & Sons. New York, NY. 1986.
- [2] McGrattan, K., Hostikka, S., Floyd, J., Baum, H., Rehm, R. Fire Dynamics Simulator (Version 5): Technical Reference Guide. NIST SP 1018-5. National Institute of Standards and Technology. Gaithersburg, MD. 2007.
- [3] Floyd, J, McGrattan, K, Hostikka, S, and Baum, H. CFD Fire Simulation Using Mixture Fraction Combustion and Finite Volume Radiative Heat Transfer. Journal of Fire Protection Engineering. 2003. 13 (1):11-36.
- [4] Bilger, R.W. and Stårner, S.H. On Reduced Mechanisms for Methane-Air Combustion in Non-Premixed Flames. Combustion and Flame. 80:135-149. 1990.
- [5] Jones, W.P. and Lindstedt, R.P. "Global Reaction Schemes for Hydrocarbon Combustion." Combustion and Flame. 73:233-249. 1988.
- [6] Westbrook, C and Dryer, F. Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames. Combustion Science and Technology. 1981, 27:31-43.

- [7] Zhou, X. and Mahalingam, S. A Suitable Mixture Fraction for Diffusion Flames of Wood Pyrolysis Gas. *Combustion and Flame*. 133: 197-199. 2003.
- [8] Ferraris, S., Wen, J., and Dembele, S. Large Eddy Simulation of Backdraft Phenomenon. *Fire Safety Journal*. 2008. (in press)
- [9] Boris, J., Landsberg, A., Oran, E., and Gardner, J. LCPFCT – A Flux Corrected Transport Algorithm for Solving Generalized Continuity Equations. NRL/MR/6410-93-7192. Naval Research Laboratory. Washington, DC. 1993.
- [10] Beyler, C. Flammability Limits of Premixed Diffusion Flames. In DiNenno, P., ed. *Handbook of Fire Protection Engineering*, 3rd ed. Quincy, MA: National Fire Protection Association. 2002.
- [11] Linteris, G. and Rafferty, I. 2003. Scale Model Flames for Determining the Heat Release Rate from Burning Polymers. *Fourth International Symposium on Scale Modeling (ISSM-IV)*. 2003.
- [12] Tsang, W. and Hampson, R.F. Chemical Kinetic Database for Combustion Chemistry. Part I. Methane and Related Compounds. *J. Phys Chem. Ref. Data*. 15. 1986.
- [13] Smyth, K. <http://fire.nist.gov/fire/flamedata>. 1999.
- [14] Norton, S., Smyth, K., Miller, J., and Smooke, M. Comparison of Experimental and Computed Species Concentration and Temperature Profiles in a Laminar Two-Dimensional, Methane/Air Diffusion Flame. *Combustion Science and Technology*. 1993, 90:1-34.
- [15] Smyth, K. NO Production and Destruction in a Methane/Air Diffusion Flame. *Combustion Science and Technology*. (1996). 155: 151-176.

- [16] Bryner, N, Johnsson, E, and Pitts, W. Carbon Monoxide Production in Compartment Fires – Reduced-Scale Test Facility. NISTIR 5568. National Institute of Standards and Technology. Gaithersburg, MD. 1994.
- [17] Hostikka, S., McGrattan, K.m and Hamins, A. Numerical Modeling of Pool Fires Using LES and Finite Volume Method for Radiation. 7th International Symposium on Fire Safety Science. International Association for Fire Safety Science. Worcester, MA. 2003.
- [18] Grosshandler, W. RADCAL: A Narrow-Band Model for Radiation Calculations in a Combustion Environment. NIST Technical Note TN-1402. Gaithersburg, MD: National Institute of Standards and Technology. 1993.
- [19] Bundy, M., Hamins, A., Johnsson, E., Kim, S., Ko, G., and Lenhert, D. Measurements of Heat and Combustion Products in Reduced-Scale Ventilation-Limited Compartment Fires. NIST Technical Note TN-1483. Gaithersburg, MD: National Institute of Standards and Technology. 2007.
- [20] Johnsson, E., Bundy, M. and Hamins, A. Reduced-Scale Enclosure Fires – Heat and Combustion Product Measurements. Interflam 2007. London, England. Interscience Communications. 2007.
- [21] Gottuk, D. and Lattimer, B. Effect of Combustion Conditions on Species Production. SFPE Handbook of Fire Protection Engineering, 3rd Edition. Chapter 2 Section 5. Society of Fire Protection Engineers. Bethesda, MD. 2002.

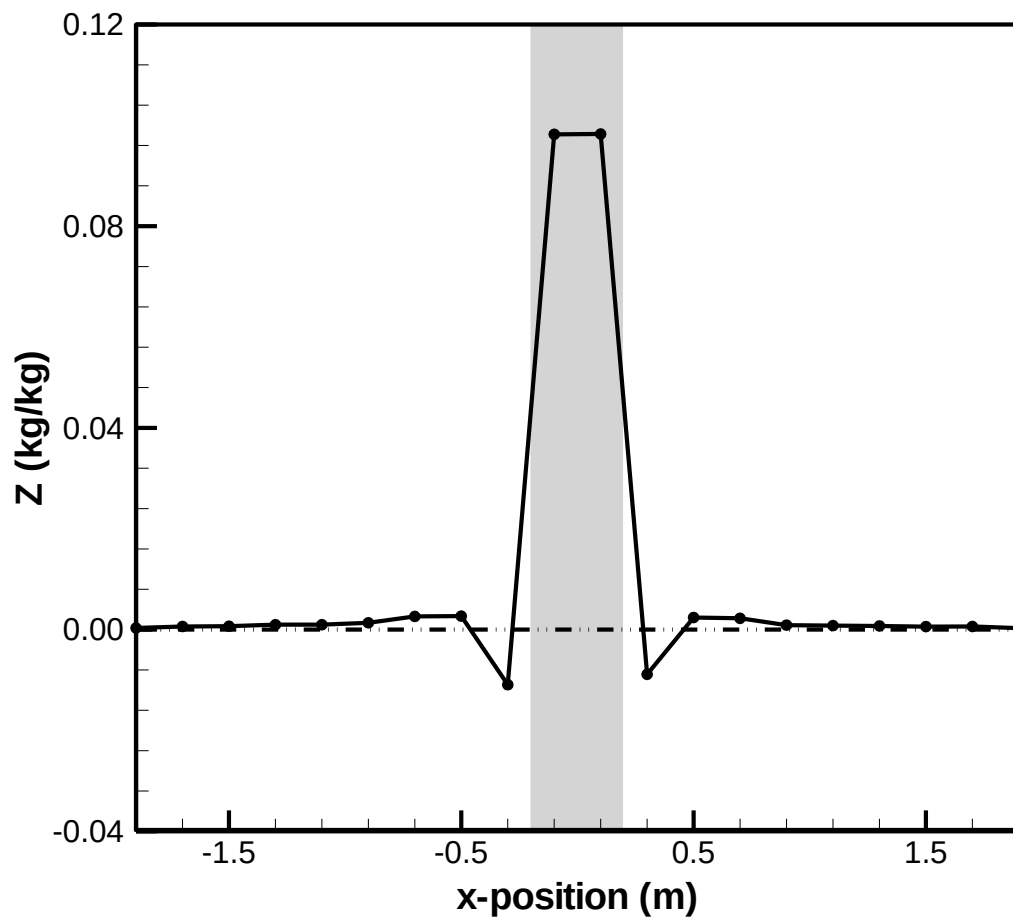


Figure 1: An example of a numerical “under-shoot.”

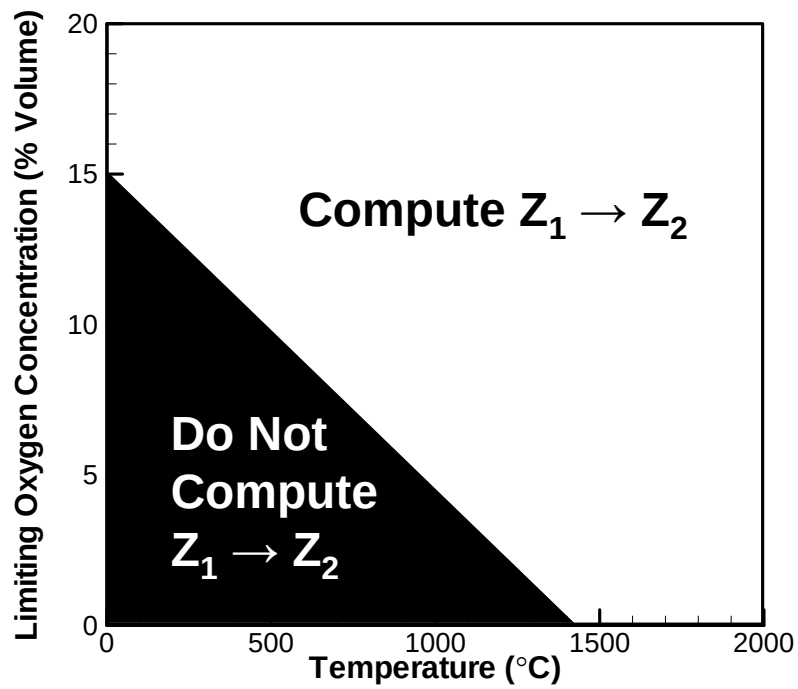


Figure 2: Flammability criteria for reaction step 1

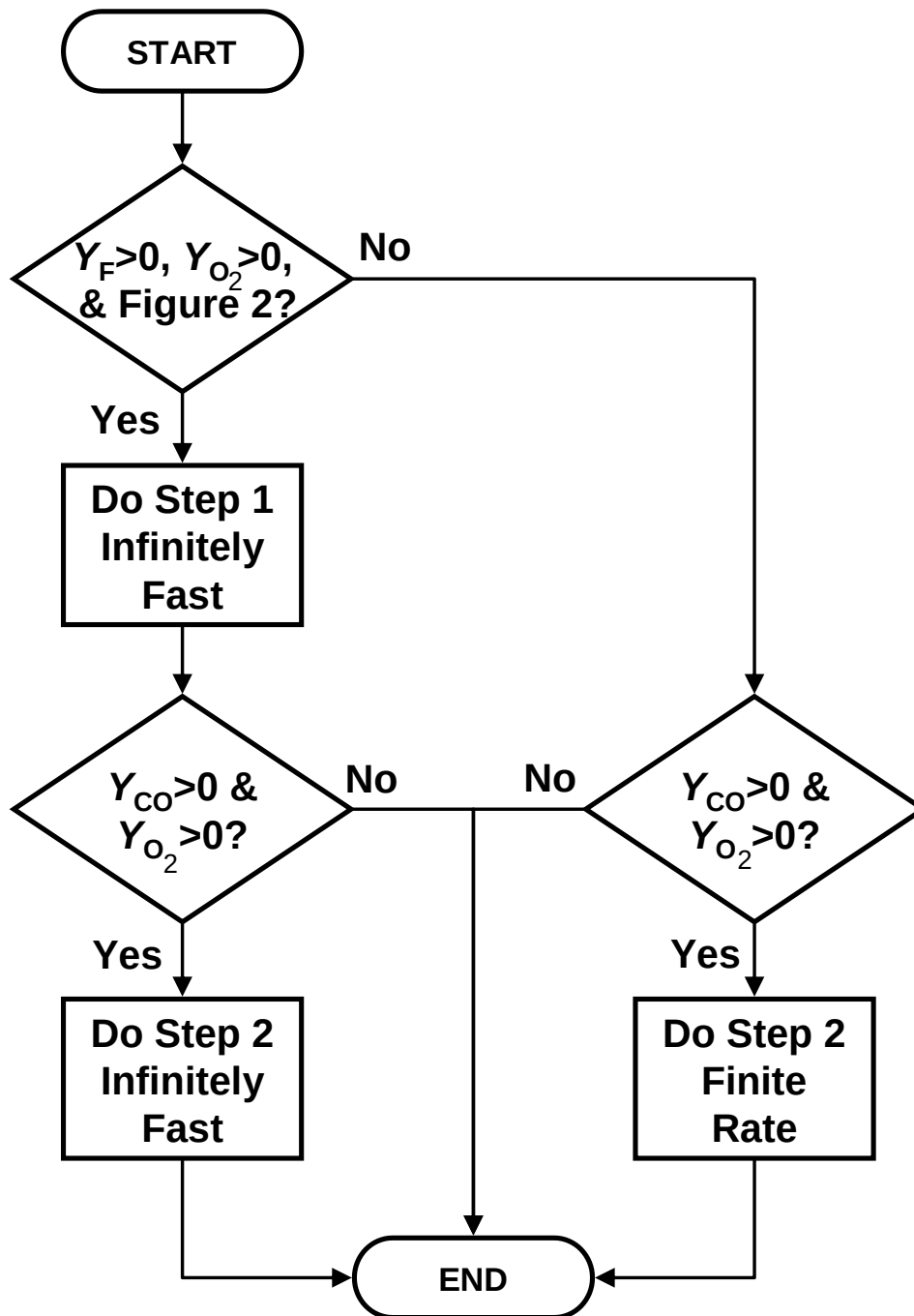


Figure 3: Flowchart of two-step combustion model

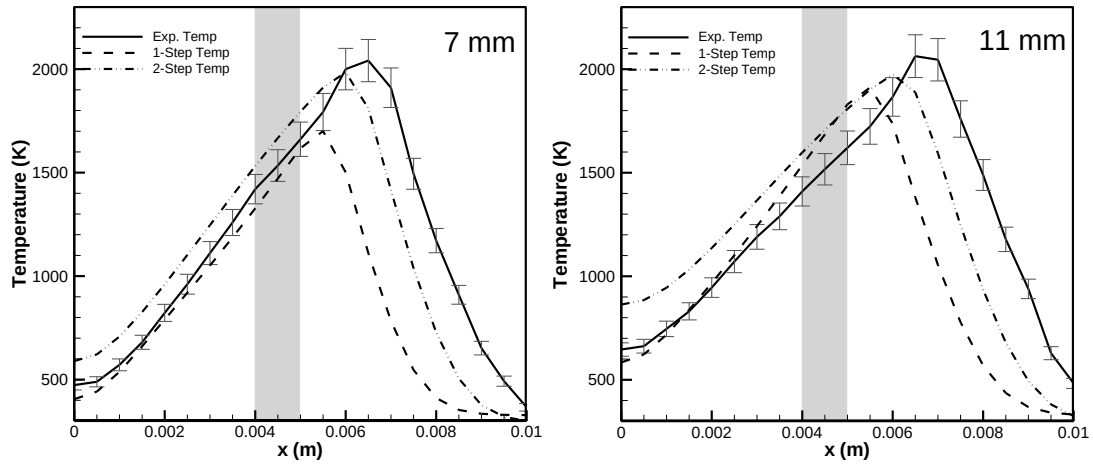


Figure 4: Predicted and measured temperature profiles over the half-width of a methane-air slot burner ($x=0$ is burner centerline, shaded region is burner lip) at two elevations above the burner.

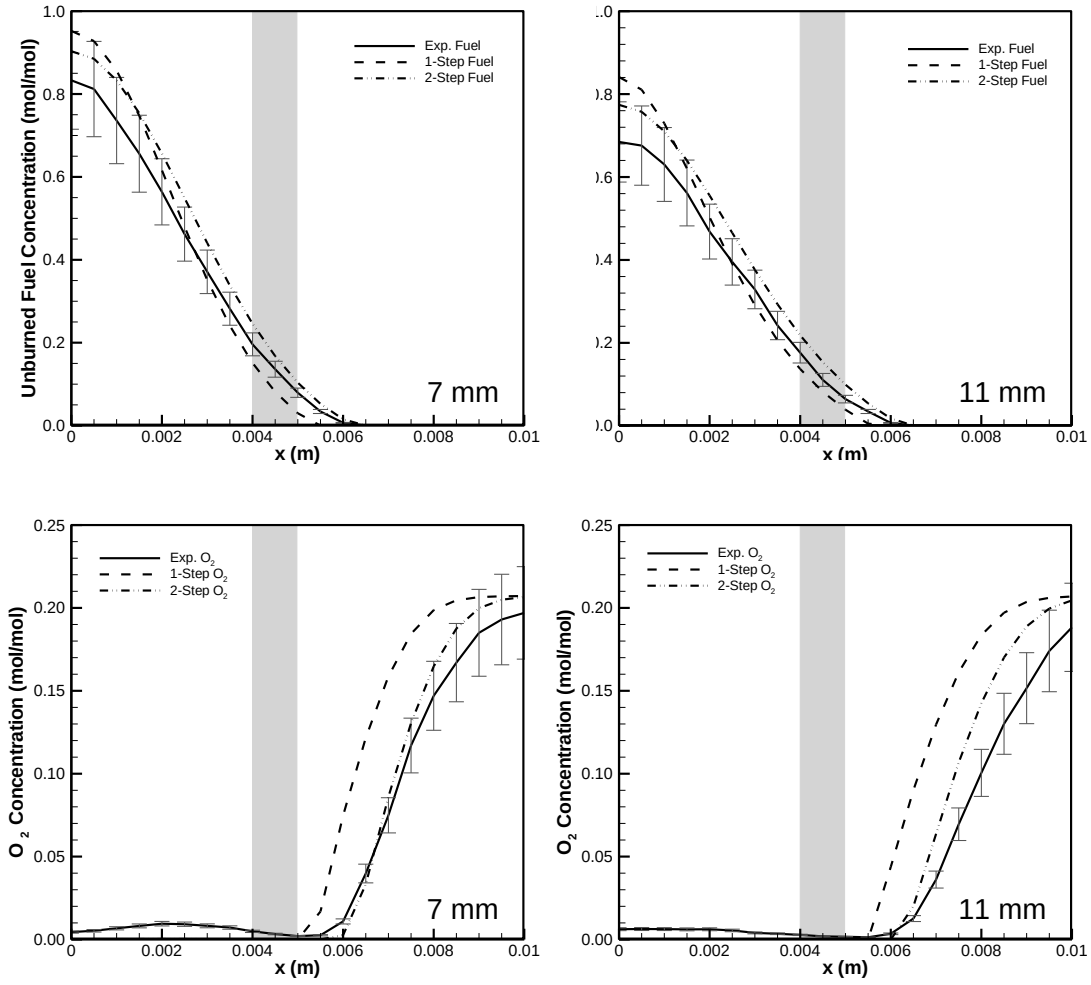


Figure 5: Predicted and measured fuel (top) and oxygen (bottom) concentrations for a methane-air slot burner ($x=0$ is burner centerline, shaded region is burner lip) at two elevations above the burner.

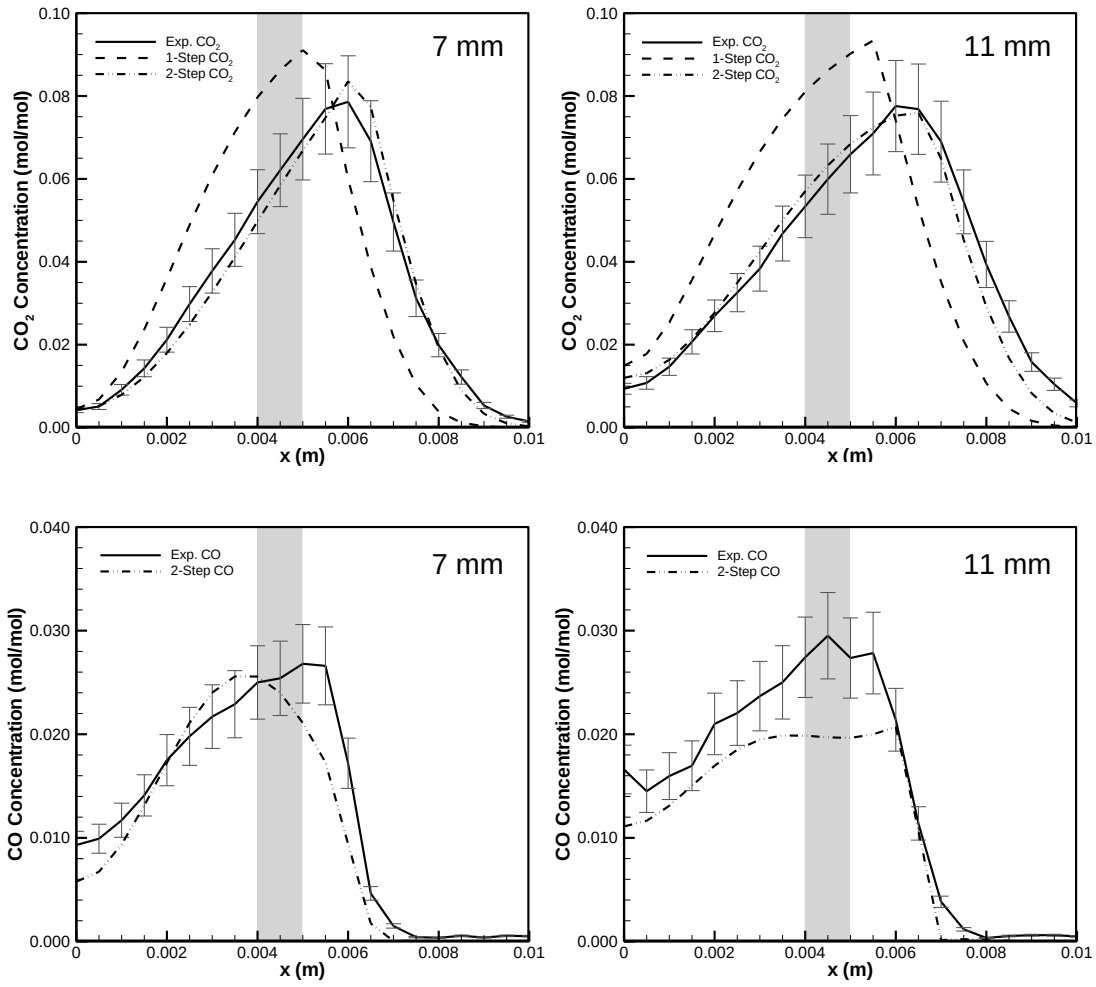


Figure 6: Predicted and measured carbon dioxide and carbon monoxide concentrations for a methane-air slot burner ($x=0$ is burner centerline, shaded region is burner lip) at two elevations above the burner..

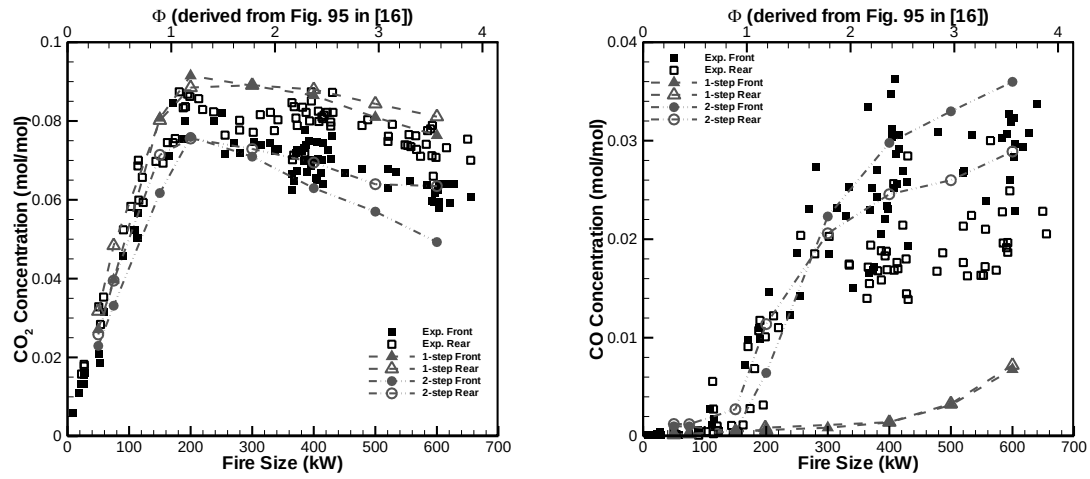


Figure 7: CO₂ and CO predictions compared against measurements in a reduced scale enclosure (lines for predictions added as a visual aid)

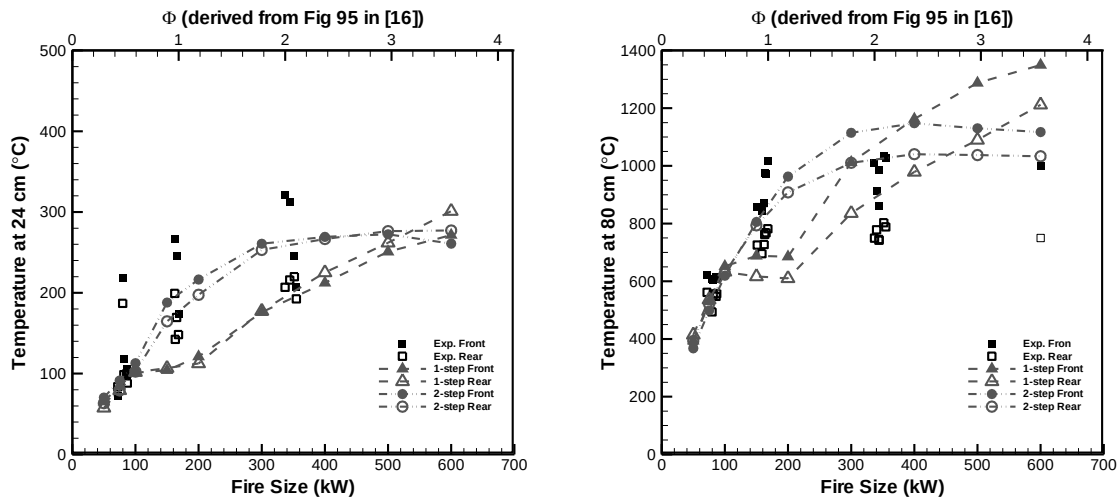


Figure 8: Lower (left) and Upper (right) predictions compared against measurements in a reduced scale enclosure (lines for predictions added as a visual aid)