Current and Future Parameters Used by FDS

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ABSTRACT

This paper discusses important input parameters used by the Fire Dynamics Simulator (FDS), a computational fluid dynamics (CFD) model of fire. Suggestions are made for new or enhanced sub-models and measurements specifically for CFD models of fire.

Keywords

Fire modeling, compartment fires, input parameters

Introduction

The Fire Dynamics Simulator (FDS) was publicly released in 2000, and over the past 20 years it has undergone six major revisions. With each new revision comes new capabilities and new algorithms and, of course, new input parameters. There are currently more than 1000 input parameters for FDS. Roughly half of these parameters are numerical in nature, controlling the grid size, time steps, convergence tolerances, and so on. The other half are physical parameters, some of which are well-defined quantities one can find in handbooks, and some of which are effective properties that are either unique to fire or unique to FDS. A goal of the FDS developers has been to reduce the need for end users to specify numerical parameters, and to reduce the number of fire-specific or "effective" physical parameters, which are often vaguely-defined or difficult to measure, in favor of ones backed by standard test methods and applicable to other fields of the thermal sciences. All this being said, there still remains certain physical phenomena that are difficult to model at large-scale for which special parameters or sub-models are still needed.

This paper describes some of the key input parameters and proposes suggestions for future improvements. Note that much of the discussion is focused on the solid phase. This is ironic

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because most of the computational expense of FDS lies in the gas phase flow solver. However, most of the input parameters are dedicated to the solid phase. The reason is that the governing Navier-Stokes equations, the properties of the gas species, the relatively simple combustion chemistry, and the simple assumptions underlying the gray-gas radiation assumption are all fairly well described in basic textbooks and handbooks of chemistry and physics.

Thermal Boundary Conditions

CONVECTION

There are a variety of empirical models governing convective heat transfer; for example, in Refs. [1, 2]. The selection depends largely on the spatial grid resolution and/or the nature of the turbulence and boundary layer model. For relatively smooth walls, these models are fairly easy to implement, verify and validate. However, walls, ceilings, and floors in actual buildings are rarely "smooth." In some instances, this might not matter, but in some configurations, like tunnels, the surface roughness might be important and should be specified as an input parameter.

Suggestion: For simulations of fires in tunnels, hallways, stairwells, etc., it would be good to have some measure of the *surface roughness*, a length scale that indicates the extent to which the walls are not smooth. This is particularly important if one is considering a significant pressure loss along the length of the tunnel or shaft. Given that the surface roughness is dictated largely by random pieces of equipment, cabling, baffles, etc., the roughness parameter will probably be deduced from a flow test in the actual facility, rather than some empirical value.

For typical large-scale fire simulations where the numerical grid is on the 10 cm or more, empirical heat transfer coefficients are fairly accurate and easy to implement. This is largely due to the fact that the temperature and velocity of the gases in the near-surface grid cell can simply be taken as the "free-stream" values in the expression for the coefficient. However, as simulations become more finely-resolved—say down to centimeters or less in resolution—it is no longer appropriate to take the nearest gas phase cell as the "free stream." What is needed is a model for convective heat transfer that naturally transitions from one grid resolution to the next.

This is particularly important if one is doing a grid resolution study, where the numerical grid is systematically made finer and finer until the result of the simulation no longer changes significantly. Transitioning naturally from a large eddy simulation (LES) to a direct numerical simulation (DNS) without having to change sub-models is a long term goal of FDS.

THERMAL INERTIA OF SOLID BOUNDARIES

A common parameter for describing the thermal inertia of a solid boundary is the product of the conductivity, density, and specific heat, $k\rho c$. For example, it appears in the empirical formula for the flame spread velocity

$$V_{\rm p} = \frac{\phi}{k\rho c(T_{\rm ig} - T_{\rm s})^2} \tag{1}$$

where ϕ is an empirical parameter, $T_{\rm ig}$ is the ignition temperature, and $T_{\rm s}$ is the surface temperature ahead of the flame front. Both the expression and the lumped parameter $k\rho c$ are inappropriate for a CFD model, where usually the 1-D heat conduction equation with a reaction source term is solved in depth along an axis normal to the surface. In such cases, one needs individual values of k, ρ, and c, not the lumped parameter, $k\rho c$, which does not appear in the governing equations.

Difficulties arise when the solid boundary is not really "solid," but includes air gaps, cracks, and so on. Even a simple cardboard box is not really so simple if one desires to include its thermal impact on the flow field or its burning behavior. In such cases, having a robust method to measure the effective thermal conductivity is most important, even if this method produces something like the apparent "R-value" that characterizes insulation materials, δ/k (thickness / conductivity).

PYROLYSIS

In FDS, the user can model a fire in several different ways, depending on the data available and objective of the simulation.

1. The fire's heat release rate as a function of time is specified by the user, either in terms of the

heat release rate per unit area or a mass loss rate of fuel per unit area in combination with an effective heat of combustion. This is still by far the preferred method used in practice due to either a lack of data or the need to satisfy a design requirement. If this model is applied, one needs to know the heat release rate of the fire and the yields of the relevant products of combustion, all of which are typically assumed to be constant.

2. Thermal properties (density, specific heat, conductivity) of combustible materials, an effective ignition temperature, and the burning rate following ignition are all specified by the user. This is the preferred method for modeling a spreading fire, where intermediate combustibles are allowed to heat up, ignite, and burn. A key input for this model is the ignition temperature and burning rate per unit area, both of which can be obtained using a cone calorimeter or similar apparatus.

3. Thermal and kinetic properties of a solid or liquid are specified.

Option 3 is still difficult to apply in practice due to a lack of data and the added cost of finer numerical grids. The difficulty of tabulating these properties is substantial. Consider that a solid material may be composed of N_m components. Each component, α, undergoes $N_{\mathrm{r},\alpha}$ reactions at a rate of $r_{\alpha,\beta}$, where β is the index of the reaction. The local *component density* of α, $\rho_{\mathrm{s},\alpha}(\mathbf{x},t)$, evolves in time according to

$$\frac{\partial}{\partial t}\left(\frac{\rho_{\mathrm{s},\alpha}}{\rho_\mathrm{s}(0)}\right) = -\sum_{\beta=1}^{N_{\mathrm{r},\alpha}} r_{\alpha\beta} + \sum_{\alpha'=1}^{N_\mathrm{m}}\sum_{\beta=1}^{N_{\mathrm{r},\alpha'}} \nu_{\alpha,\alpha'\beta}\, r_{\alpha'\beta} \quad ; \quad \rho_\mathrm{s} = \sum_{\alpha=1}^{N_\mathrm{m}} \rho_{\mathrm{s},\alpha}$$

$$r_{\alpha\beta} = \left(\frac{\rho_{\mathrm{s},\alpha}}{\rho_\mathrm{s}(0)}\right)^{n_{\mathrm{s},\alpha\beta}} A_{\alpha\beta}\, \exp\left(-\frac{E_{\alpha\beta}}{RT_\mathrm{s}}\right) T_\mathrm{s}^{n_{\mathrm{t},\alpha\beta}} \tag{2}$$

$\rho_\mathrm{s}(0)$ is the initial density of the material layer and $\nu_{\alpha,\alpha'\beta}$ is the yield of component α due to reaction β of component α'.

This is the pyrolysis model used in FDS, and it is similar, but with subtle differences, to others used in fire science. The decomposition rates of almost any solid can be modeled to a fair degree of accuracy using this type of scheme, albeit with a complex array of kinetic parameters.

To date, there is no agreement in the field as to how to develop a database of thermal and kinetic properties of the vast number of materials that might be consumed in a fire. A key issue is the fact that measured kinetic parameters are typically designed to be used as a set, with a particular form of the governing equations. One cannot simply take a pre-exponential constant, A, from one paper and activation energy, E, from another. If the reaction order, n_s, is not one or if the rate equation is written differently than those above, it is very likely that unit inconsistencies will result.

Suggestion: The MaCFP[3] Condensed Phase Subgroup should create a series of verification cases in which Eq. 2 is solved numerically for a set of kinetic parameters, and the solutions should be posted on the web site. Those interested in using the property data measured by the participating laboratories would then check their own solution against the benchmark to ensure that the tabulated properties are interpreted correctly. This is a critical *verification* exercise that is often overlooked, leading to unnecessary confusion when parameters are taken from one model and implemented in another.

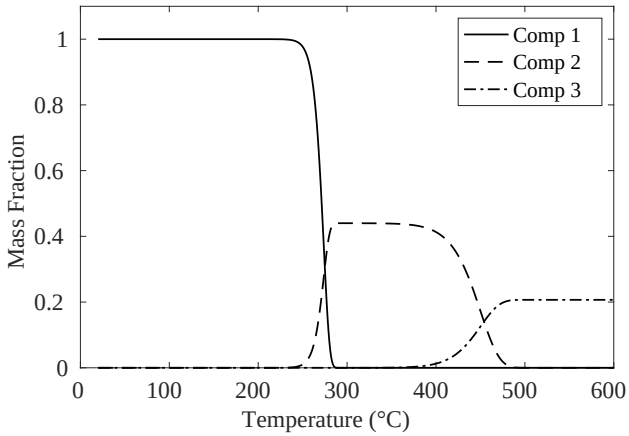
As an example, consider a solid material that initially consists of a single component, Comp 1, that decomposes upon linear heating of 5 °C/min to form another solid, Comp 2, and a gaseous product, Gas A. Comp 2 then decomposes upon further heating to form a third solid, Comp 3, and another product gas, Gas B. Figure 1 displays the component mass fractions and lists the kinetic parameters for this two-step process:

$$\text{Comp 1} \quad \rightarrow \quad \nu_{2,1,1}\,\text{Comp 2} + (1-\nu_{2,1,1})\,\text{Gas A} \tag{3}$$

$$\text{Comp 2} \quad \rightarrow \quad \nu_{3,2,1}\,\text{Comp 3} + (1-\nu_{3,2,1})\,\text{Gas B} \tag{4}$$

Assuming that one is using thermal degradation equations similar to those given in Eq. (2), one should be able to reproduce the plots in Fig. 1 exactly. If this exercise is successful, further verification cases can be developed to test the reaction energies and other aspects of pyrolysis. Over time, a "database" of material properties will evolve as interested parties adopt

[3]Measurement and Computational of Fire Phenomena



Symbol	Units	Value
ρ_1	kg/m^3	1430
ρ_2	kg/m^3	629
ρ_3	kg/m^3	296
$A_{1,1}$	s^{-1}	1.4×10^{33}
$E_{1,1}$	J/mol	3.67×10^5
$n_{s,1,1}$	–	1
$n_{t,1,1}$	–	0
$A_{2,1}$	s^{-1}	3.5×10^{12}
$E_{2,1}$	J/mol	2.07×10^5
$n_{s,2,1}$	–	1
$n_{t,2,1}$	–	0
$\nu_{2,1,1}$	kg/kg	0.44
$\nu_{3,2,1}$	kg/kg	0.47

Figure 1: (Left) Mass fraction of the material components of the sample solid. (Right) Kinetic parameters.

similar parameter naming conventions, units, and interpretation.

CHAR OXIDATION

With the growing interest in modeling wildland fire, there is a need to establish robust char oxidation models. The very simplest pyrolysis scheme for burning vegetation is as follows:

$$\text{Wet Vegetation} \rightarrow \nu_{H_2O}\,H_2O + (1-\nu_{H_2O})\,\text{Dry Vegetation} \tag{5}$$

$$\text{Dry Vegetation} \rightarrow \nu_{char}\,\text{Char} + (1-\nu_{char})\,\text{Fuel Gas} \tag{6}$$

$$\text{Char} + \nu_{O_2,char}\,O_2 \rightarrow (1+\nu_{O_2,char}-\nu_{ash})\,CO_2 + \nu_{ash}\,\text{Ash} \tag{7}$$

Numerous researchers [3, 4, 5, 6] have proposed kinetic parameters for the first two reactions, but the third reaction is more complicated because it is endothermic and it depends on oxygen penetration into the solid; that is, the reaction rate expression in Eq. (2) includes extra parameters related to the surrounding environment, including the mass or volume fraction of oxygen either at the surface or in depth and the flow conditions in the vicinity of the surface that affect the oxygen level. The endothermic nature of the reaction can lead to thermal run-away within the numerical model due to unrealistically high computed temperatures. In reality, the reaction rate limiter is the

oxygen transport in depth, but that is difficult to model. Often, semi-empirical charring models are developed that are tied directly to the geometry of the underlying solid, be it a tree branch or a block of wood.

Suggestion: It would be useful to have a robust char oxidation model that does not explicitly involve the oxygen concentration in depth, but rather the oxygen concentration in the gas phase beyond the surface boundary layer. This semi-empirical model may be as simple as a constant reaction rate limiter, or something more complex that involves gas phase flow characteristics in addition to oxygen concentration. Such a model would be appropriate for a large-scale CFD model.

Combustion

FDS by default applies a simple one step reaction to model the combustion of fuel gases.

$$\mathrm{C_xH_yO_zN_v} + \nu_{\mathrm{O_2}}\ \mathrm{O_2} \rightarrow \nu_{\mathrm{CO_2}}\ \mathrm{CO_2} + \nu_{\mathrm{H_2O}}\ \mathrm{H_2O} + \nu_{\mathrm{CO}}\ \mathrm{CO} + \nu_{\mathrm{S}}\ \mathrm{Soot} + \nu_{\mathrm{HCN}}\ \mathrm{HCN} + \nu_{\mathrm{N_2}}\ \mathrm{N_2} \qquad (8)$$

The products of incomplete combustion, i.e. CO, soot and HCN, are specified by the user in the form of yields; that is, the mass of the product species generated per mass of fuel consumed. These yields are of vital importance in fire hazard analyses because they often determine when a space becomes untenable for lack of visibility or an excess of toxic gases. However, these values are not readily available. Tewarson [7] measured some of these yields, and the data now can be found in the SFPE Handbook, but this data is limited to pure fuels and relatively small fires. By-product yields are dependent on fire size and fuel geometry. If the yields of major product gases are known, along with either measured or postulated fuel stoichiometry, the one-step reaction above can be implemented in the model such that carbon, hydrogen, oxygen, and nitrogen, can be accounted for. The CO and soot yields can be used to estimate the combustion efficiency and effective heat of combustion, which will decrease from its ideal value as more products of incomplete combustion are formed.

Of course, more detailed chemical reactions are limited by the coarse spatial and tempo-

ral resolution of a large-scale CFD simulation, but at least there is a consistent accounting for the major gas species and soot.

Suggestion: Fire testing labs should, when possible, create on-line repositories of measured heat release rates for common combustibles. Recently, Matt Bundy created an on-line database of calorimetry measurements performed in the National Fire Research Laboratory at NIST [8]. The database contains the heat release rate, along with soot and CO yields, for a variety of commodities burned in the lab. It would be of great benefit for other fire labs to do something similar because there are an infinite number of things that can burn and a very small database of basic combustion yields for these items. In particular, the soot yield of common commodities is vitally important in fire protection engineering because visibility if often the most important factor in an ASET/RSET (Available/Required Safe Egress Time) analysis.

Thermal Radiation

In simple models, the fire is typically assumed to be cylindrical or conical in shape with a surface emissive power (SEP) given by:

$$\dot{E} = A\,\sigma\,T_{\mathrm{f}}^4\,\left(1-\mathrm{e}^{-\overline{\kappa}L}\right) \tag{9}$$

where A is the surface area, σ is the Stefan-Boltmann constant, T_{f} is the effective flame surface temperature, and $\overline{\kappa}$ is an effective absorption/emission coefficient over a path length, L, which is typically taken as the diameter of the cylinder that represents the fire. None of these parameters are appropriate for a CFD model, and even for simpler empirical models they have proven to be difficult to define and measure precisely. FDS uses the narrow band model called RadCal to compute spatially-resolved absorption/emission coefficients for gas mixtures over a range of composition and temperature. The radiative heat flux from a fire to a target is obtained by solving the radiative transport equation in three-dimensions where each cell either absorbs or emits energy depending on its composition and temperature.

The spatially resolved absorption/emission coefficient, $\kappa(\mathbf{x})$, along with a computed gas temperature, should be sufficient to compute the emission source term in the radiative transport equation under the gray-gas approximation:

$$B(\mathbf{x}) = \frac{\kappa(\mathbf{x})\,\sigma\,T(\mathbf{x})^4}{\pi} \quad ; \quad \mathbf{x} = (x,y,z) \tag{10}$$

Unfortunately, the computed gas temperature, T, in a given grid cell is typically less than the actual flame temperature that governs radiation emission because FDS can only compute a bulk-average temperature in a cell as opposed to the actual flame temperature. Because of this, the radiation emission from the fire can be under-predicted. To remedy this problem, FDS takes a user-specified *radiative fraction*, χ_r, which is loosely defined as the fraction of the fire's chemical energy release in the form of thermal radiation. It is by default 35 %, but can range between approximately 20 % for "clean" fuels like natural gas and 40 % for "dirty" fuels like heavy hydrocarbons and plastics. This parameter is not easily found in the fire literature because there is no rigorously defined test method for it. It is typically estimated by making a far-field radiation measurement which is then divided by $4\pi R^2$, where R is the distance from the fire.

Suggestion: There is sparse data in the literature listing the radiative fraction of common combustibles at full-scale. Fire testing labs should, when possible, report the radiative fraction of experimental fires using at a minimum a single radiometer measurement that is several fire diameters or flame lengths set back from the fire. Also, the radiometer should be approximately at the mid-height of the luminous flame to offset any errors in view factor. The radiative fraction is a more useful and robust quantity for any model than the expression for the SEP in Eq. (9).

Conclusion

The input parameters discussed in this paper are just a small fraction of those used by FDS or any CFD model of fire, combustion, or other thermal processes. These CFD models require far more parameters than their predecessors. One way to make progress is to deprecate parameters that were originally developed solely for simple fire models in favor of parameters that are used

outside of the relatively small field of fire. Lumped parameters like $k\rho c$ and methods developed by the fire community to measure them should be replaced by similar parameters (k and ρ and c, for example) that have importance beyond just fire. Fire-specific test methods should be replaced by broader-based methods because CFD models cannot use many of these fire-specific parameters and methods. In essence, the fire community invented empirical compartment and zone models, along with parameters and measurement methods appropriate for these models. The fire community did not invent CFD, and parameters appropriate for CFD models come from other branches of the thermal sciences. FDS has more in common with a meteorological model than a zone model; thus, its parameters are not necessarily found in a reference book on fire.

For many topics in fire modeling, it is not appropriate to talk about parameters outside of the context of the sub-model for which it is intended. This is especially true of pyrolysis. In order to make progress, there needs to be some standardization of the sub-model, i.e. solid decomposition reactions. For example, a pre-exponential factor, A, for a reaction cannot be listed in a table without reference to the particular reaction rate expression. For this reason, standards documents like ASTM E 1591 are not particularly useful for CFD models. The input parameters needed by a CFD cannot be obtained by a handful of measurement methods. Rather, the parameters come from reference texts, handbooks, and industry consortia like the MaCFP. The simpler models that still in use by the fire protection engineering community are best discussed in reference texts like the SFPE Handbook [9].

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