Modeling Smoke Movement through Compartmented Structures

WALTER W. JONES
Building and Fire Research Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899

INTRODUCTION

PREDICTING THE ENVIRONMENT in a building subject to a fire is a complex undertaking. Time scales vary from picosecond times for molecular interactions to hours for collapse of building barriers. Space scales vary from millimeters to tens of meters. To account for these broad ranges in a practical way, we use a simplification known as a zone model. A zone model is a particular implementation of the class of mathematical models known as finite element models. The concept of a zone or control volume model was pioneered by Kawagoe [1]. This model embodied several approximations which reduce the computational complexity without unduly sacrificing accuracy. However, the first true multicompartment model of this type was formulated by Tanaka [2]. The important approximation which Tanaka stated is that flow generally occurs between like atmospheres. In other words, vent gases are assumed to flow between adjacent lower layers or upper layers. Although a drastic simplification, this rule works surprisingly well.

We have developed a deterministic model, CFAST [3,4,5], which has built on this prior work, adding greater versatility while retaining the

This paper was presented at the Thirty-Ninth Sagamore Army Materials Research Conference, Plymouth, MA, September 16–17, 1992.

Reprinted from JOURNAL OF FIRE SCIENCES, *VOL. 11 – MARCH/APRIL 1993*

Journal of Fire Sciences, Vol. 11, No. 2, 172-183, March/April 1993.

basic tenets of the zone model. For example, the lower layer is treated just like the upper layer in that it can gain and absorb energy and thus change temperature. However, the most important advance incorporated into the CFAST model is that the conservation equations are solved in their original differential form. The pressure is not assumed to be in steady state, nor the lower layer temperature to be at ambient conditions. As will be seen later, this form provides several benefits, one of which is the luxury of adding physical processes simply by adding to the source terms for the various predicted quantities. It also provides a model which will work over a much wider range of initial conditions.

The emphasis in this article is on the improvements which have been made to include phenomena which have been observed experimentally [6,7], but which have not been incorporated in prior models of smoke spread. Further motivation to improve the model is supplied by experience in its use in reconstructing the original path of fire growth and smoke movement in fire incidents. From these real world experiences there exists a great deal of anecdotal evidence that the model works well. Much of this latter comes from liability adjudication, fire reconstruction and product testing. As might be expected, many of these comparisons are unavailable for citation, although a recent case [8] is illustrative. Nevertheless, we use these cases as confirmation of the fundamental correctness of the zone model concept, and this implementation in particular. However, these comparisons also reveal phenomena which are lacking. One improvement which will not be discussed in this article, but is significant in the development of such models is an improved numerical scheme [9]. The speed improvement is typically two to ten times faster than FAST [3], its predecessor. It also solves the pressure equation completely, with no damping as was done in FAST.

We begin with a *brief* description of the predictive equations contained in the original model. This is done to provide a basis for discussion. In the interest of clarity and completeness, some of the earlier derivations are included. The conservation equations are turned into predictive equations for the sensible variables. The right-hand side of these equations, the source terms discussed below, are the forcing functions for the ordinary differential equations. The term forcing function is used in the mathematical sense of the right-hand side of an ordinary differential equation [10]. The refinements are discussed in terms of the original formulation of the source terms for these predictive equations. Finally we show some sample calculations to demonstrate how the refinements and improvements have affected the model from a theoretical standpoint.

THE PREDICTIVE EQUATIONS

All current zone fire models take the mathematical form of an initial value problem for a system of differential equations. These equations are derived from the conservation of mass, energy and momentum. Subsidiary equations are the ideal gas law, and definitions of density and internal energy (for example, see Reference [11]). These conservation laws are invoked for each zone or control volume. It is necessary to use a complete, but orthogonal set of equations so that the system is completely defined but not over constrained. Any complete set can be used. The implications for various choices of the basis set are discussed by Forney and Moss [12].

The basic element of one of these models is a zone. The basic assumption of a zone model is that properties such as temperature can be approximated throughout the zone by some uniform function. The usual approximation is that temperature, density and so on are uniform within a zone. This is not a necessary approximation. For example, a temperature which increases monotonically from the bottom of the zone to the top uniformly would, perhaps, improve the precision somewhat. However, the assumption of uniform properties is reasonable and yields good agreement with experiment. In general, these zones are grouped within compartments. The usual grouping is two gas layers per compartment. Once again, more could be utilized with a concomitant increase in computing time, but little improvement in accuracy.

Until the development of FAST [3], all models of this type assumed that the pressure equilibrated instantaneously, and thus the dP/dt term could be set to zero. This was an attempt to solve the numerical problem known as stiffness. The time for significant change in each of the variables is significantly different for each equation. This is particularly acute for the pressure equation. It is not a matter of equilibration of the density or pressure within the compartment. Rather it is how strong the coupling is between the time rate of change of the variable (dP/dt for example), and the forcing function, or right-hand side of the predictive equation. Writing each of the predictive equations in the form

$$\frac{dx}{x} = A d\tau, \tag{1}$$

the coefficient A varies by orders of magnitude amongst the equations. Typically, the ratio of these coefficients for the pressure to any other

variable is $\approx c_p$, or about 1000. By setting the dP/dt term to zero, this difference vanishes. However, as has been shown [13], it is much easier to solve these equations in the differential than the algebraic form if the proper solver is used.

Each formulation can be expressed in terms of mass and enthalpy flow. These rates represent the exchange of mass and energy between zones due to physical phenomena such as plumes, natural and forced ventilation, convective and radiative heat transfer, and so on. For example, a vent exchanges mass and energy between zones in connected rooms, a fire plume typically adds heat to the upper layer and transfers entrained mass and energy from the lower to the upper layer, and convection transfer energy from the gas layers to the surrounding walls.

We use the formalism that the mass flow to the upper and lower layers is denoted $\dot{m}_U$ and $\dot{m}_L$ and the enthalpy flow to the upper and lower layers is denoted $\dot{s}_U$ and $\dot{s}_L$. It is tacitly assumed that these rates may be computed in terms of zone properties such as temperatures and densities. These rates represent the net sum of all possible sources of mass and energy due to phenomena such as those listed above. The numerical characteristics of the various formulations are easier to identify if the underlying physical phenomena are decoupled in this way.

Many approximations are necessary when developing physical submodels for the mass and enthalpy terms. For example, most fire models assume that (1) the specific heat terms c_p and c_v are constant even though they depend upon temperature, (2) hydrostatic terms can be ignored in the equation of state (the ideal gas law) relating density of a layer with its temperature. However, the derivations which follow are all based on the basic conservation laws.

DERIVATION OF EQUATIONS FOR A TWO-LAYER MODEL

We divide a compartment into two control volumes, a relatively hot upper layer and a relatively cooler lower layer. The gas in each layer has attributes of mass, internal energy, density, temperature, and volume denoted respectively by m_i, E_i, ϱ_i, T_i, and V_i where $i = L$ for the lower layer and $i = U$ for the upper layer. The compartment as a whole has the attribute of pressure P. These eleven variables are related by means of the following seven contraints

$$\varrho_i = \frac{m_i}{V_i} \text{ (density)} \tag{2}$$

$$E_i = c_v m_i T_i \text{ (initial energy)} \tag{3}$$

$$P = R\varrho_i T_i \text{ (ideal gas law)} \tag{4}$$

$$V = V_L + V_U \text{ (total volume)} \tag{5}$$

The specific heat at constant volume and at constant pressure c_v and c_p, the universal gas constant, R, and the ratio of specific heats, γ, are related by $\gamma = c_p/c_v$ and $R = c_p - c_v$. For air, $c_p \approx 1000$ kJ/kg K and $\gamma = 1.4$. This leaves four unconstrained, or independent, variables. So we require four equations for a unique solution. The four are the conservation of mass and energy for each layer.

The differential equations for the mass in each layer are

$$\frac{dm_L}{dt} = \dot{m}_L, \quad \frac{dm_U}{dt} = \dot{m}_U \tag{6}$$

The first law of thermodynamics states that the rate of increase of internal energy plus the rate at which the layer does work by expansion is equal to the rate at which enthalpy is added to the gas. In differential form this is

$$\begin{array}{ccccc} \text{internal} & & & & \\ \text{energy} & + & \text{work} & = & \text{enthalpy} \\ \uparrow & & \uparrow & & \nearrow \\ \dfrac{dE_i}{dt} & + & P\dfrac{dV_i}{dt} & = & \dot{s}_i \end{array} \tag{7}$$

A differential equation for pressure can be derived by adding the upper and lower layer versions of Equation (7), noting that $dV_U/dt = -dV_L/dt$, and substituting the differential form of Equation (3) to yield

$$\frac{dP}{dt} = \frac{\gamma - 1}{V}(\dot{s}_L + \dot{s}_U) \tag{8}$$

Similar derivations can be done for volume, density, energy and temperature. These equations for each of the eleven variables are summarized in Table 1. The time evolution of these solution variables can be computed by solving the corresponding differential equations together

Table 1. Conservative zone modeling differential equations.

Equation Type	Differential Equation
ith layer mass	$\frac{dm_i}{dt} = \dot{m}_i$
pressure	$\frac{dP}{dt} = \frac{\gamma - 1}{V}(\dot{s}_L + \dot{s}_U)$
ith layer energy	$\frac{dE_i}{dt} = \frac{1}{\gamma}\left(\dot{s}_i + V\frac{dP}{dt}\right)$
ith layer volume	$\frac{dV_i}{dt} = \frac{1}{\gamma P}\left((\gamma - 1)\dot{s}_i - V\frac{dP}{dt}\right)$
ith layer density	$\frac{d\varrho_i}{dt} = -\frac{1}{c_p T_i V_i}\left((\dot{s}_i - c_p \dot{m}_i T_i) - \frac{V_i}{\gamma - 1}\frac{dP}{dt}\right)$
ith layer temperature	$\frac{dT_i}{dt} = \frac{1}{C_p \varrho_i V_i}\left((\dot{s}_i - c_p \dot{m}_i T_i) + V_i\frac{dP}{dt}\right)$

with appropriate initial conditions. The remaining seven variables can be determined from the four independent solution variables.

The current version of CFAST is set up to use the equation set for layer temperature, layer volume, and pressure as shown in Equations (9), (10), (11) and (12). However, the internal structure of the model is such that it will allow any of the formulations above to be substituted with minimal effort.

$$\frac{dP}{dt} = \frac{\gamma - 1}{V}(\dot{s}_L + \dot{s}_U) \tag{9}$$

$$\frac{dV_U}{dt} = \frac{1}{\gamma P}\left((\gamma - 1)\dot{s}_U - V_U\frac{d\Delta P}{dt}\right) \tag{10}$$

$$\frac{dT_U}{dt} = \frac{1}{C_p \varrho_U V_U}\left((\dot{s}_U - c_p \dot{m}_U T_U) + V_U\frac{dP}{dt}\right) \tag{11}$$

$$\frac{dT_L}{dt} = \frac{1}{C_p \varrho_L V_L}\left((\dot{s}_L - c_p \dot{m}_L T_L) + V_L\frac{dP}{dt}\right) \tag{12}$$

The sensible variables in each compartment are described by the set

of predictive equations. The form of the equations is that the physical phenomena are source terms on the right-hand side of these equations [3]. Such a formulation makes the addition (and deletion) of physical phenomena and changing the form of algorithms a *relatively* simple matter.

The source terms important to smoke transport in buildings are radiation transfer between the zones and walls, and burning object(s), convective heating by boundaries, plume flow and vent flow, species generation and loss, and finally the fire or fires. There are subsidiary equations which must be solved also, but will not be discussed here. An example of the latter is heat conduction through partitions such as ceilings and walls. Most of the phenomena have been discussed adequately in the papers by Jones [3,14] and Jones and Peacock [4,15].

With this structure, adding and deleting physical models is *relatively* straightforward. CFAST now includes:

- normal horizontal flow (through doors, windows and so on)
- vertical flow (through holes in ceiling and floors)
- forced flow (mechanical ventilation)
- a ten wall two layer radiation model
- multiple fires in one or more compartments
- HCl deposition
- multiple compartments (15 in version 1.6)
- two zones per compartment plus plume and ceiling jet
- correct chemistry (using species production rates)
- free burn and oxygen limited fires
- multilayered walls, ceilings and floors in each compartment
- four wall conductive heat transfer
- 3D specification of the fire and asymmetric ceiling jet cooling
- fire plumes
- convective heat transfer (inside and out)
- wind and different internal and external ambient

COMPARISON OF THE PREDICTIVE MODEL WITH FULL SCALE EXPERIMENTS

We performed a comparison with five different full scale experiments. The first was a single compartment with a burning sofa. In a similar configuration, a single wall was burned. The next was a three room configuration using a gas burner. The third consisted of three compartments connected by a long corridor. This too used a gas burner, but a

great deal of effort was put into sealing the spaces so that they were airtight. The fourth was a seven story office building. Four of these are shown in Figure 1, beginning with the single compartment in the upper left and moving around the figure clockwise. The wall burning experiment is similar to the furniture configuration and is not shown separately. Figure 2 shows a comparison of the predicted and measured upper layer temperatures. Similar comparisons can be made for interface height, lower layer temperature, pressure and any other pair of variables which has been measured. All show comparable agreement between measured and predicted values. In the figure, the compartments are numbered 1, 2,. . . These are arbitrary designations, but pairs should be compared between the model predictions and the experimentally measured values, e.g., 1 with 1.

CONCLUSIONS

As has been shown here, as well as by Nelson et al. [7] and Peacock et al. [6], the predictions of sensible quantities from this model compare favorably with experimental measures of these quantities. As with any theoretical model there are pieces which have been omitted and others which could be implemented more completely. Given the limitations, the model seems to do a credible job. The next steps will be to include a self consistent flame spread model and to reformulate the equations for long corridors where zone models run into difficulty. This latter will involve a term for horizontal momentum. To data we have assumed this is not important. In long corridors the details of the flow are important if we are to model the real world of buildings.

NOMENCLATURE

m mass in kilograms
$\dot{m}$ rate of mass change in kilograms per second
$\dot{E}$ defined quantity–total enthalpy ($\dot{Q}$ + $\dot{h}$)
V volume in cubic meters
P pressure in newtons per square meter
R gas constant (239 joules per kilogram per kelvins for air)
T temperature in kelvins
c specific heat (joules per kilogram per kelvins)
t time in seconds
$\dot{s}$ defined quantity–sum of $\dot{E}$s

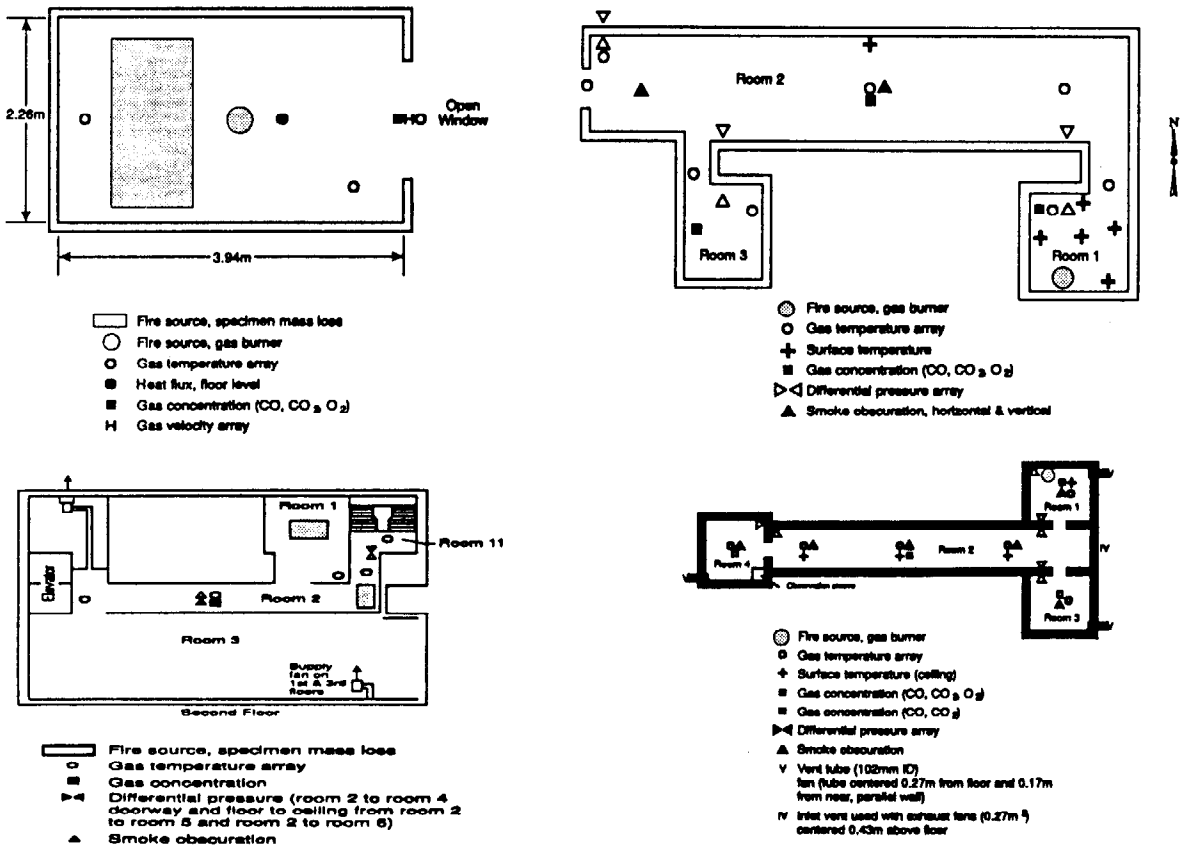

Figure 1. Schematic of the four experiments.

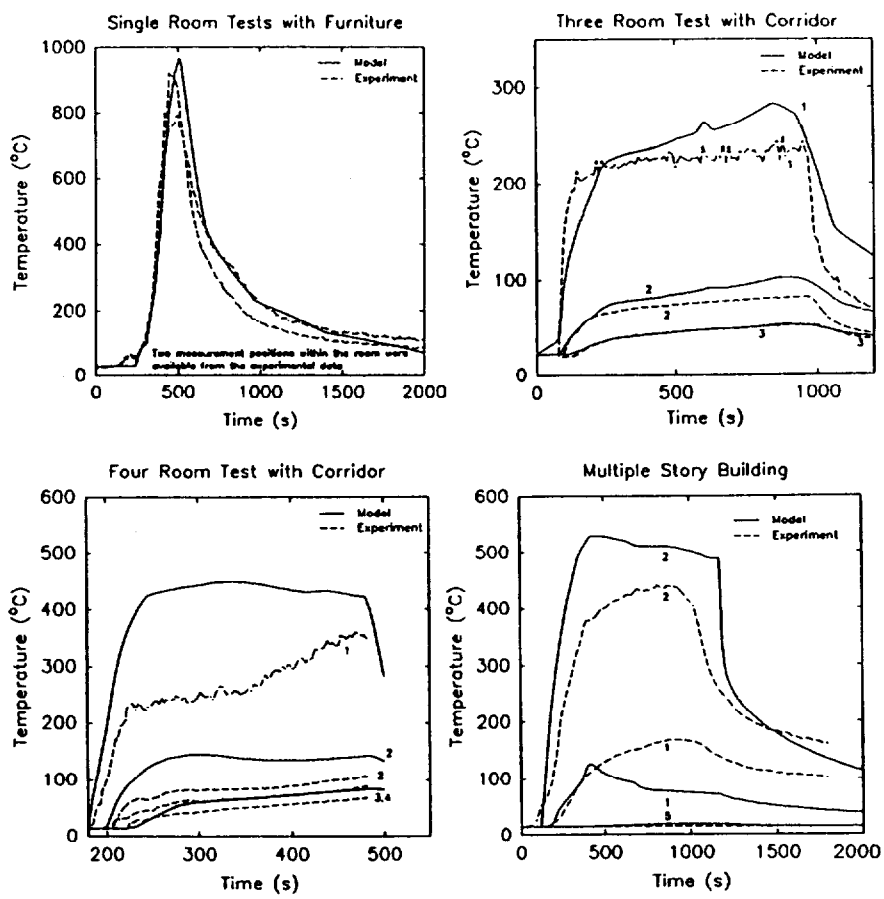

Figure 2. Upper layer temperature predictions and measurements.

γ ratio of specific heat c_p/c_v
β $\gamma/(\gamma - 1)$
ϱ mass density in kilograms per cubic meter
g gravitational constant, 9.8 meters per second
v velocity in meters per second
z height in meters

Subscripts

R reference
c convective

i,j compartment indices
f fire
p pressure (c_p for specific heat at constant pressure) and pyrolysis
u,l upper or lower layer, respectively (k is used as an index over $\{u,l\}$)
v volume (c_v which is the specific heat at constant volume)
a ambient
i,o compartment on the inside to compartment on the outside
v heat capacity (constant volume)
p heat capacity (constant pressure)

ACKNOWLEDGEMENT

The work described herein was sponsored in part by the Office of Naval Technology for the Surface Ship Technical Block Program (ONT 211).

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