ANALYZING AND EXPLOITING NUMERICAL CHARACTERISTICS OF ZONE FIRE MODELS

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ABSTRACT

In order to design robust and stable zone fire modeling algorithms, the numerical properties of the fire modeling differential equations must be understood. This paper examines some of these properties. Many sets of differential equations for zone fire modeling can be derived using the conservation of mass and energy. A comparison between various possible formulations is made in terms of numerical properties. One property that many formulations possess is the presence of multiple time scales. Pressures equilibrate much faster than other quantities such as density and temperature. Numerically, this property is known as stiffness. Stiffness, in the context of fire modeling, and numerical methods for handling it are discussed.

INTRODUCTION

The basic premise used to formulate a zone fire model is that an enclosure can be divided into a number of regions or zones each with approximately uniform conditions. These zones interact by exchanging mass and energy[1]. Mass and energy conservation along with expressions relating mass, density, volume, internal energy, temperature and pressure can be used to show that many formulations exist for tracking conditions in zones. These formulations are equivalent in the sense that one formulation may be converted to another using physical laws such as the ideal gas law or definitions such as that for density or internal energy. Computationally, zone fire modeling is challenging due to the numerical characteristics of the basic conservation equations used to simulate mass and energy exchange between various zones. The purpose of this paper then is to provide a numerical foundation for the design of fire modeling algorithms. It is important to understand when differences in these algorithms are numerically significant so that the best possible fire modeling algorithms can be designed and implemented.

ZONE FIRE MODELING FORMULATIONS

The zone fire models presented here take the mathematical form of an initial value problem for a system of differential equations. These equations are derived using the conservation of mass or continuity equation, the conservation of energy or the first law of thermodynamics,

the ideal gas law, and definitions of density and internal energy (for example, see [2]). The conservation of momentum is ignored. These conservation laws are invoked for each zone or control volume. A zone may consist of a number of interior regions (usually an upper and a lower gas layer), and a number of wall segments. The basic assumption of a zone fire model is that properties such as temperatures can be uniformly approximated throughout the zone. It is remarkable that this assumption seems to hold for as few as two gas layers.

Many differential equation formulations based upon these assumptions can be derived. One formulation can be converted into another using definitions of density, internal energy and the ideal gas law. Though equivalent analytically, these formulations differ in their numerical properties. One property that many share is the presence of multiple time scales. Physically, the pressure in a compartment equilibrates much quicker than densities and temperatures. Numerically, this property is known as stiffness and requires the use of special differential equation solvers.

Each differential formulation can be expressed in terms of mass and energy flow rates. These flow rates represent the exchange of mass and/or energy between zones due to physical phenomena or sub-models such as fire plumes, natural and forced vents, convective and radiative heat transfer *etc.* 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 transfers energy from the gas layers to the surrounding walls.

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

Many approximations are obviously necessary when developing physical sub-models for the mass and energy flow rate 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. We wish to distinguish between various formulations according to whether they are mathematically equivalent to the conservation laws of mass and energy. A formulation which is equivalent to the conservation laws will be denoted *conservative* otherwise it will be identified as *approximate*. Conservative formulations in this sense are not necessarily better than approximate ones. The next two sections discuss formulations which are conservative and approximate. Again, two conservative formulations that are equivalent mathematically need not be equivalent numerically.

Conservative Formulations

A compartment can be divided into two control volumes, an upper layer of hot gases and smoke and a lower layer of air as illustrated in Figure 1. 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 constraints. We get seven by counting density, internal energy and the ideal gas law twice (once for each layer).

$$\rho_i = \frac{m_i}{V_i} \quad \text{(density)} \tag{1}$$

$$E_i = c_v m_i T_i \quad \text{(internal energy)} \tag{2}$$

$$P = R\rho_i T_i \quad \text{(ideal gas law)} \tag{3}$$

$$V = V_L + V_U \quad \text{(total volume)} . \tag{4}$$

The specific heats 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

$$\gamma = \frac{c_p}{c_v} ,$$

$$R = c_p - c_v .$$

For air, $c_p \approx 1000$ kJ/kg K and $\gamma = 1.4$.

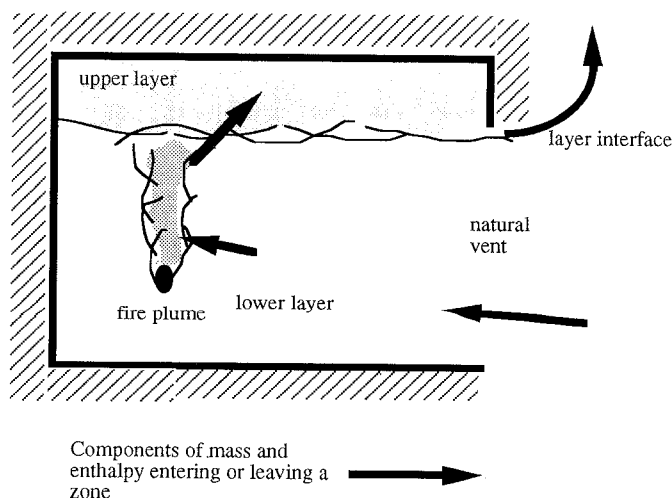The differential equations for mass in each layer are trivially

FIGURE 1: Schematic illustrating various physical sub-models contributing to the mass and energy flow in a zone fire model

$$\frac{dm_L}{dt} = \dot{m}_L$$

$$\frac{dm_U}{dt} = \dot{m}_U .$$

The first law of thermodynamics in differential equation form is

$$\overbrace{\frac{dE_i}{dt}}^{\text{internal energy}} + \overbrace{P\frac{dV_i}{dt}}^{\text{work}} = \overbrace{\dot{q}_i}^{\text{enthalpy}} \qquad (5)$$

A differential equation for pressure can be derived by adding the upper and lower layer versions of equation (5), noting that $\frac{dV_U}{dt} = -\frac{dV_L}{dt}$ and

$$\frac{dE_i}{dt} = \frac{d(c_v m_i T_i)}{dt} = \frac{c_v}{R}\frac{d}{dt}(PV_i) \qquad (6)$$

to obtain

$$\frac{dP}{dt} = \frac{\gamma - 1}{V}(\dot{q}_L + \dot{q}_U) . \qquad (7)$$

Differential equations for the layer volumes can be obtained by substituting equation (6) into equation (5) to obtain

$$\frac{dV_i}{dt} = \frac{1}{P\gamma}\left((\gamma - 1)\dot{q}_i - V_i\frac{dP}{dt}\right) . \qquad (8)$$

Equation (5) can be rewritten to eliminate the $\frac{dV_i}{dt}$ term to obtain

$$\frac{dE_i}{dt} = \frac{1}{\gamma}(\dot{q}_i + V_i\frac{dP}{dt}) .$$

Differential equations for the densities can be derived by applying the quotient rule to $\frac{d\rho_i}{dt} = \frac{d}{dt}\left(\frac{m_i}{V_i}\right)$ and using equation (8) to eliminate $\frac{dV_i}{dt}$ to obtain

$$\frac{d\rho_i}{dt} = \frac{-1}{c_p T_i V_i}\left((\dot{q}_i - c_p \dot{m}_i T_i) - \frac{V_i}{\gamma - 1}\frac{dP}{dt}\right) . \qquad (9)$$

Differential equations for temperatures can be derived by applying the quotient rule to $\frac{dT_i}{dt} = \frac{d}{dt}\left(\frac{P}{R\rho_i}\right)$ and using equation (9) to eliminate $\frac{d\rho_i}{dt}$ to obtain

$$\frac{dT_i}{dt} = \frac{1}{c_p \rho_i V_i}\left((\dot{q}_i - c_p \dot{m}_i T_i) + V_i\frac{dP}{dt}\right) . \qquad (10)$$

Differential equations for each of the eleven variables are summarized in Table 1. Notice that a $\frac{dP}{dt}$ term occurs in all but the mass equations. As is shown later this term can be set to zero except when modeling sealed structures. As is pointed out in [3], even supposedly sealed structures consisting of reinforced concrete walls will collapse due to the pressure induced by small fires. Therefore it is valid to neglect the dP/dt or work term in the temperature, density and volume differential equations. For the example presented later, the time period over which these two variants (ODE's with and without dP/dt term) are different is o(10^{-4}) seconds.

Using the constraint equations (1) to (4), it can be shown that four of the eleven variables can be chosen as solution variables. The time evolution of these solution variables can be computed by solving the corresponding differential equations together with appropriate initial conditions. The remaining seven variables can be determined from the solution variables. There are, however, many possible differential equation formulations. The numerical characteristics of some of these formulations will be discussed in the next section.

Table 1: Conservative Zone Modeling Differential Equations

Equation Type	Differential Equation
i'th layer mass	$\frac{dm_i}{dt} = \dot{m}_i$
pressure	$\frac{dP}{dt} = \frac{\gamma - 1}{V}(\dot{q}_L + \dot{q}_U)$
i'th layer energy	$\frac{dE_i}{dt} = \frac{1}{\gamma}(\dot{q}_i + V_i\frac{dP}{dt})$
i'th layer volume	$\frac{dV_i}{dt} = \frac{1}{\gamma P}((\gamma - 1)\dot{q}_i - V_i\frac{dP}{dt})$
i'th layer density	$\frac{d\rho_i}{dt} = \frac{-1}{c_p T_i V_i}((\dot{q}_i - c_p \dot{m}_i T_i) - \frac{V_i}{\gamma - 1}\frac{dP}{dt})$
i'th layer temperature	$\frac{dT_i}{dt} = \frac{1}{c_p \rho_i V_i}((\dot{q}_i - c_p \dot{m}_i T_i) + V_i\frac{dP}{dt})$

Table 2: Conservative Zone Model Equation Selections

Zone Fire Model	Equations	Substitutions
CFAST, FAST [11]	$\frac{d\Delta P}{dt}, \frac{dV_U}{dt}, \frac{dT_U}{dt}, \frac{dT_L}{dt}$	$\Delta P = P - P_{\text{ref}}$
CCFM.HOLE [12]	$\frac{d\Delta P}{dt}, \frac{dy}{dt}, \frac{d\rho_U}{dt}, \frac{d\rho_L}{dt}$	$\Delta P = P - P_{\text{ref}}, y = V_L/A_{room}$
CCFM.VENTS [2]	$\frac{d\Delta P}{dt}, \frac{dy}{dt}, \frac{dm_U}{dt}, \frac{dm_L}{dt}$	$\Delta P = P - P_{\text{ref}}, y = V_L/A_{room}$
FIRST, HARVARD V [13]	$\frac{dE_U}{dt}, \frac{dE_L}{dt}, \frac{dm_U}{dt}, \frac{dm_L}{dt}$	

Numerical Characteristics of Several Zone Fire Modeling Differential Equations

There are 330 different ways to select four variables from eleven to form a system of differential equations. Many of these systems are incomplete due to the relationships that exist between the variables given in equations (1) to (4). For example the variables, ρ_U, V_U, m_U and P form a dependent set since $\rho_U = m_U/V_U$. Table 2 shows the solution variable selection made by a few zone fire models. The variable y that appears in this table is the height of the upper layer above the compartment floor.

The number of differential equation formulations can be considerably reduced by not mixing variable types between layers; that is, if upper layer mass is chosen as a solution variable, then lower layer mass must also be chosen. For example, for two of the solution variables choose m_L and m_U, or ρ_L and ρ_U, or T_L and T_U. For the other two solution variables pick E_L and E_U or P and V_L or P and V_U. This reduces the number of distinct formulations to nine. Since the numerical properties of the upper layer volume equation are the same as a lower layer one, the number of distinct formulations can be reduced to six.

The next several subsections discuss the numerical implications of using these formulations. Some of the problems discussed can be solved by ignoring the pressure equation.

Pressure

Some of the numerical problems that arise in zone fire modeling are due to the difficulty of computing accurate pressure differences across vent openings. When adjacent room pressures are close, a catastrophic cancellation will lead to a loss of significant digits. If the pressures are too close, the result of the subtraction is roundoff noise. This can cause problems if the noise is amplified in the next stage of the computation; that is, the noise is propagated and may dominate some later stage

of the calculation. This problem is compounded by the fact that the base pressure in a room at 1 atmosphere is about 10^5 pascals (Pa). Pressure drops across a vent as low as .1 Pa can cause significant mass flow through a vent. Therefore, if pressure is used as a solution variable, seven accurate digits must be carried in order to have one significant digit in the vent flow calculation. One way around this problem is to solve for an offset pressure, ΔP, where for some reference pressure, P_{ref}, the room pressure is given by

$$P = P_{ref} + \Delta P .$$

The differential equation for relative pressure, ΔP is given by

$$\frac{d\Delta P}{dt} = \frac{dP}{dt} - \frac{dP_{ref}}{dt}$$
$$= \frac{dP}{dt} \text{ if } P_{ref} \text{ is constant .}$$

Internal Energy The problem with using internal energy in a formulation is the difficulty in accurately determining the offset pressure, ΔP, needed for accurate vent flow calculations. In large part this is due to the fact that energy is not an intensive variable, it is proportional to layer volume as well as temperature. To illustrate, consider that the total room pressure can be expressed in terms of lower and upper layer internal energy and room volume by using equations (1) to (4) to obtain

$$P = \frac{\gamma - 1}{V}(E_L + E_U) .$$

Substituting $E_L = E_{ref} + \Delta E_L$, $E_U = E_{ref} + \Delta E_U$ and $P = P_{ref} + \Delta P$ into the above equation and solving for E_{ref} and ΔP we obtain

$$\Delta P = \frac{\gamma - 1}{V}(\Delta E_L + \Delta E_U)$$

$$E_{\text{ref}} = \frac{P_{\text{ref}} V}{2(\gamma - 1)}.$$

The term, ΔP can be small while the term $|\Delta E_L| + |\Delta E_U|$ is large. This will result in cancellation errors. The term, ΔP, will not be zero in general, therefore we can not assume that $\Delta E_L = -\Delta E_U$.

Temperature and Density The temperature and density differential equations have several advantages and disadvantages in common. As seen in Table 1, both the density and temperature equations have the term $\dot{q}_i - c_p \dot{m}_i T_i$. The vent flow component of this term is identically zero for flows leaving a zone since the enthalpy flow rate for a vent flow is $\dot{q}_{\text{vent}} = c_p \dot{m}_{\text{vent}} T_{\text{vent}}$. An unnecessary subtraction can be avoided by setting this vent flow component to zero analytically, thereby avoiding a loss of significant digits. This property of the density and temperature equation is due to the fact that, ignoring pressure transients, the temperature and density of a room is not affected by flows leaving it. Similar cancellations must also be eliminated in the pressure equation for this strategy to be useful. Unfortunately, this is not possible unless the pressure equation is dropped from the equation set.

The density and temperature equations also have a problem in common. Both have layer volume terms in the denominator which may vanish. Although these singularities are removable (if they were not the derivatives $\frac{d\rho}{dt}$ and $\frac{dT}{dt}$ would be infinite), they cause numerical problems since it is difficult to determine proper values for $\frac{d\rho}{dt}$ and $\frac{dT}{dt}$ in this case. One method used to solve this problem is to prevent layers from vanishing.

Mass The mass equation does not have the vanishing denominator problem of the density or temperature equation. Using the mass equation allows sensible initial conditions. The mass for a layer with zero height is just zero. However, quantities derived from mass such as density are only valid when a layer volume has a

significant number of accurate digits.

Approximate Formulations

The formulations discussed in this section are approximate in the sense that certain terms deemed negligible are removed from the modeling differential equations. Two types of approximations and their error behavior are discussed. One involves the elimination of the pressure transient, ($\frac{dP}{dt}$), terms. A second way approximates the differential equations by assuming that the conditions in the lower layer remain at ambient. Some fire models along with their variable choices that use some of the approximation techniques discussed in this section are listed in Table 3. ASET assumes the pressure remains at ambient and uses a non-dimensional form of the layer height and upper layer density equations. BRI assumes that the pressure relaxes to quasi-steady values instantly. BRI solves a non-linear algebraic equation equivalent to equation (7) with $\frac{dP}{dt}$ set to zero. First, we examine the behavior of pressure as motivation for making these approximations.

Behavior of the Pressure Equation for a Heated Enclosure with a Small Leak
The pressure in a compartment approaches steady state rapidly if other compartment properties such as layer temperatures, fire size, and vent sizes are constant. The equilibrium pressure value depends on the fire size and vent areas or more generally on the sources and sinks of energy in the room. To characterize the equilibrium pressure value and the time required to reach equilibrium, consider a room with a fire that is vented to the outside as illustrated in Figure 2.

To simplify the analysis assume that the vent is a slit located at the floor so that Bernoulli's law,

$$\dot{m}_{\text{vent}} = c_{\text{vent}} A_{\text{vent}} \sqrt{2\rho_{\text{vent}} \Delta P},$$

can be used to model the mass flow through the vent. The conclusions found here hold for more general vent algorithms since they all use or compute pressure differences. Here A_{vent} denotes the area of the vent, c_{vent},

Table 3: Approximate Zone Model Equation Selections

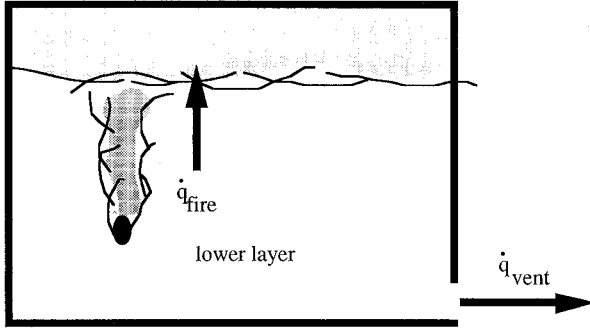| Zone Fire Model	Equations	Substitutions
ASET [14, 15]	$P = P_{\text{amb}}, \frac{dy^*}{dt}, \frac{d\rho_U^*}{dt}, T_L = T_{\text{amb}}$	$y = V_L/A_{room}$
BRI [16, 17]	$\frac{dP}{dt} = 0, \frac{dV_U}{dt}, \frac{dT_U}{dt}, \frac{dT_L}{dt}$	
LAVENT [18, 19]	$P = P_{\text{amb}}, \frac{dy}{dt}, \frac{dm_U}{dt}, T_L = T_{amb}$	$y = V_L/A_{room}$

FIGURE 2: One Room Test Case

the vent coefficient, while ρ_{vent} denotes the density of the vent flow gas. Further, assume that the density and temperature of the gas flowing through the vent is constant over the time period required to reach pressure equilibrium. This is reasonable since this time period is typically rather short.

The source of energy in the room is the fire and is denoted by $\dot{q}_{fire}$. Most entrainment models used by fire plume models do not affect the calculation of the pressure rise or transient time since the energy entrained from the lower layer cancels with the energy added back into the upper layer. The energy flow rate out of the room is due to the vent and is denoted by $\dot{q}_{vent}$. The initial value problem for the pressure drop across the vent is

$$\frac{d\Delta P}{dt} = \frac{\gamma - 1}{V}(\dot{q}_{fire} - \dot{q}_{vent}) \qquad (11)$$
$$\Delta P(0) = 0$$

where ΔP is the pressure drop across the vent, V is the volume of the room, and the other terms have been defined previously. Setting

$$a = \frac{\gamma - 1}{V}\dot{q}_{fire}$$
$$b = \frac{\gamma - 1}{V}c_p c_{vent} A_{vent} T_{vent} \sqrt{2\rho_{vent}} ,$$

problem (11) simplifies to

$$\frac{d\Delta P}{dt} = a - b\sqrt{\Delta P}$$
$$\Delta P(0) = 0 .$$

This differential equation is separable and can be integrated to obtain the implicit solution

$$t = \frac{2\Delta P_\infty}{a}\left(ln\left(\frac{1}{1 - \sqrt{\Delta P/\Delta P_\infty}}\right) - \sqrt{\Delta P/\Delta P_\infty}\right), \qquad (12)$$

or equivalently

$$\Delta P = \Delta P_\infty\left(1 - e^{\frac{-at}{\Delta P_\infty}}e^{-\sqrt{\Delta P/\Delta P_\infty}}\right)^2 \qquad (13)$$

with the equilibrium pressure ΔP_∞ given by

$$\Delta P_\infty = \left(\frac{a}{b}\right)^2 \approx 1.00 \times 10^{-11}\left(\frac{\dot{q}_{fire}}{A_{vent}}\right)^2 . \qquad (14)$$

where $T_{vent} = 300K$, $\rho_{vent} = 1.2kg/m^3$, $c_{vent} = .68$ and $c_p = 1000kJ/kgK$. Taking the limit as $t \to \infty$, equation (13) verifies that ΔP_∞ is the equilibrium pressure and equation (12) shows how long it takes to achieve it. Substituting $\Delta P/\Delta P_\infty = .99$ into equation (12) gives the time required for the pressure to reach 99 per cent of ΔP_∞ or

$$t_{.99} \approx 21.5\frac{\Delta P_\infty}{\dot{q}_{fire}/V} .$$

For a room with volume $18m^3$, a 100 kW fire, and an equilibrium pressure of 0.1 Pa, the time required to reach 99 per cent of the equilibrium value is approximately 0.00038 seconds.

Figure 3 shows the dependence of equilibrium pressure on fire size and vent area. Figure 4 shows how the time required to reach equilibrium is affected by these same two quantities.

This analysis shows that pressures tend towards equilibrium values very quickly. The equilibrium pressure value is a function of quantities that affect the sources or sinks of energy in a room. The flow of enthalpy through a vent into and out of a room is affected by vent area, layer heights and temperatures *etc*. The fire also contributes to the energy gain in a room. As these quantities (vent area, layer heights, fire size, *etc*) change, the room pressure adjusts almost instantly to a new quasi-steady state value. Numerically, this property is known as stiffness. A numerical challenge of zone fire modeling is to determine pressures accurately and efficiently.

For a one room model the algebraic equation (14) can be used to determine the equilibrium pressure instead of the pressure differential equation (11). Furthermore, the $\frac{dP}{dt}$ term in the other zone modeling differential equations (as expressed in Table 1) can be dropped in cases when $\frac{dP}{dt}$ goes to zero almost instantly.

Algebraic Pressure Approximation The pressure differential equation (7) can be approximated by determining the pressure that satisfies the non-linear equation

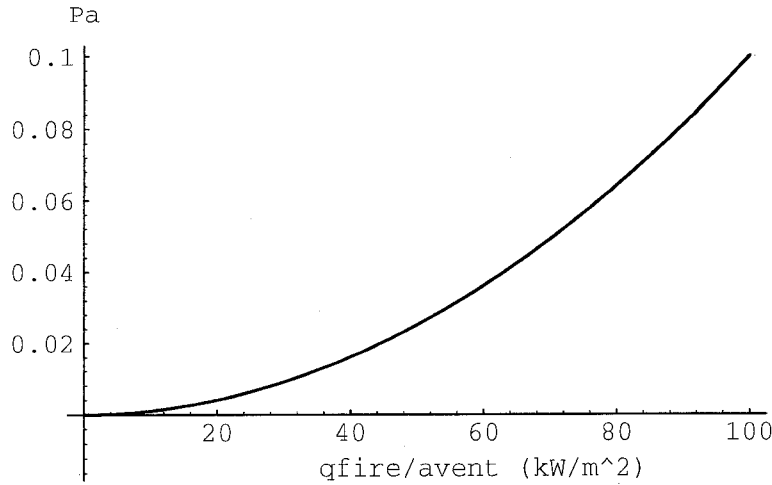$$\dot{q}_L(P) + \dot{q}_U(P) = 0 . \qquad (15)$$

Pa

FIGURE 3: Plot of equilibrium pressures versus fire size where the energy release rate of the fire is normalized by vent area
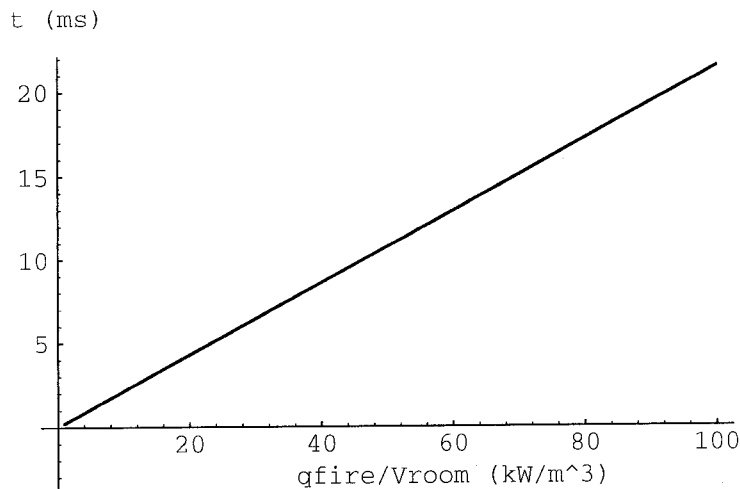
t (ms)

FIGURE 4: Plot of the time it takes the pressure to reach 99 per cent of its final equilibrium value versus fire size where the energy release rate of the fire is normalized by the room volume.

This pressure in general varies with time. For simple cases, such as a one room model with one fire and layer height above a thin slit vent, this equation can be solved analytically for P. For example, using equation (14) for the equilibrium pressure offset ΔP_∞, this equation has the solution

$$P = P_{\text{ref}} + \left(\frac{\dot{q}_{\text{fire}}}{c_p c_{\text{vent}} A_{\text{vent}} T_{\text{vent}} \sqrt{2\rho_{\text{vent}}}} \right)^2 . \quad (16)$$

Rehm and Baum in [4] similarly calculate the equilibrium pressure rise in the context of a field model. Table 4 gives the approximate zone modeling differential equations corresponding to the conservative ones given previously in Table 1. The equations in this table were obtained by neglecting the dP/dt terms in Table 1.

For multiple room simulations the approximation is more complicated. An equilibrium pressure offset must be calculated for each room using an equation similar to (15). This results in a system of equations since the equi-

Table 4: Approximate Zone Modeling Differential Equations

Equation Type	Differential Equation
i'th layer energy	$\frac{dE_i}{dt} = \frac{\dot{q}_i}{\gamma}$
i'th layer volume	$\frac{dV_i}{dt} = \frac{(\gamma-1)\dot{q}_i}{\gamma P}$
i'th layer density	$\frac{d\rho_i}{dt} = -\frac{\dot{q}_i - c_p \dot{m}_i T_i}{c_p T_i V_i}$
i'th layer temperature	$\frac{dT_i}{dt} = \frac{\dot{q}_i - c_p \dot{m}_i T_i}{c_p \rho_i V_i}$

librium pressure in one room depends on the equilibrium pressure in another *via* vent connections. Solvers such as Petzold's DASSL [5, 6] can solve algebraic and differential equations simultaneously. This was tried with CCFM.VENTS. It was found that there was no advantage to doing this. The algebraic pressure equation version could not track rapidly changing pressures and run times were not significantly shorter.

A One Zone Approximation Conditions in the lower layer are essentially ambient for many fire scenarios of interest. This observation may be exploited by replacing the differential equation for lower layer density (equation (9)) with $\rho_L = \rho_{amb}$ or the differential equation for lower layer temperature (equation (10)) with $T_L = T_{amb}$. This is equivalent to assuming that the rate of mass and energy additions to the lower layer satisfy $\dot{q}_L/(c_p \dot{m}_L) = T_{amb}$ which will be true as long as the temperature of flows added to the lower layer are at ambient.

ZONE FIRE MODELING NUMERICAL CHARACTERISTICS

Vent Flow

Physical models of natural and forced vent flow, fire plumes, radiation, conduction, convection *etc* are used to exchange or transfer mass and/or energy between zones. As with the differential equation formulations discussed in the previous section, two physical models for computing these phenomena may be identical physically but be different numerically. This section addresses some of the numerical issues important in the design of physical algorithms, some miscellaneous numerical considerations appropriate for any fire model and finally discusses the numerical properties of systems of differential equations.

Numerical difficulties can arise when calculating vent flow because of its dependence on the square root of pressure differences. This is especially a problem when the pressure drop across the vent is small relative

to the pressure computed in each room adjacent to the vent. To illustrate this phenomena consider two rooms. Suppose the first room has a fire and is connected to the outside and to a second room which does not have a fire. This second room is assumed to be connected only to the first room and not to the outside. To simplify the analysis assume that the vents are narrow slits located at the floor. This configuration is depicted in Figure 5.
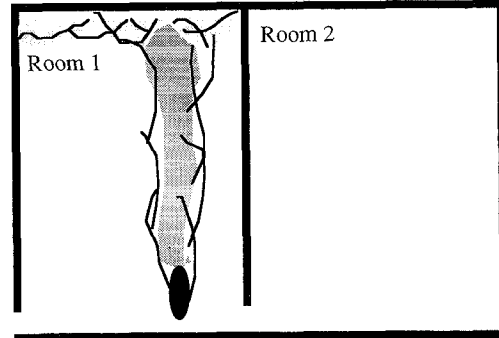

FIGURE 5: Test case illustrating a scenario than can cause numerical difficulties due to the fact that the pressure in both rooms are identical. Catastrophic cancellation occurs when the pressure drop accross the vent is computed. The resulting numerical noise is amplified (by $c_p T_{vent} \approx 300000$) when computing enthalpy flows.

Suppose that the pressure above ambient in rooms 1 and 2 are denoted ΔP_1 and ΔP_2. Theoretically, these pressure offsets will be the same after the initial pressure transient dies. Numerically, however, these two offsets will be different. Though this difference may be insignificant physically, the magnification of the cancellation error occurring in the vent flow computation may be significant numerically. Unfortunately, simply setting the pressure drop to zero for physically insignificant flows is not an adequate solution to this problem of unwanted error propagation as will be explained next.

In this test problem, the pressure in room 1 will rise to its equilibrium value as given by equation (14) in a time period given by equation (12). If a cut off pressure drop ΔP_{cut} is chosen so that $\frac{d\Delta P_2}{dt} = 0$ for $|\Delta P_2 - \Delta P_1| < \Delta P_{cut}$, then ΔP_1 will continue to rise (since $\frac{d\Delta P_1}{dt}$ is not zero) while ΔP_2 remains fixed. Eventually $|\Delta P_2 - \Delta P_1|$ will exceed ΔP_{cut} so that $\frac{d\Delta P_2}{dt}$ will not be zero. Again, ΔP_2 will rapidly approach ΔP_1 until $|\Delta P_2 - \Delta P_1| < \Delta P_{cut}$. This type of algorithm will result in a drastic reduction in time step size as the differential equation solver tries to track the solution due to the "stair stepping" behavior of ΔP_2 illustrated in Figure 6.
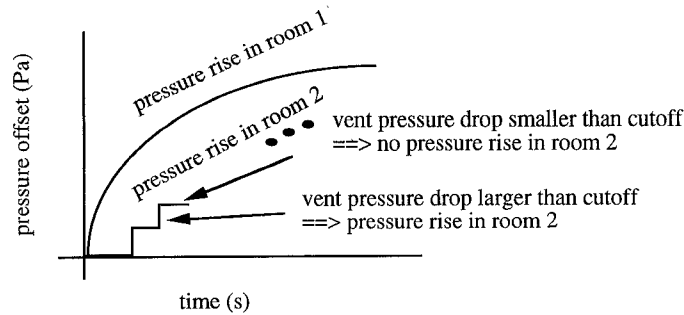
FIGURE 6: Behavior in room pressure exhibited when the numerical error resulting from computing the pressure drop accross vent is not adequately damped.

Although the Bernoulli law for computing vent flow is known to break down for small pressure differences, the problems discussed here are solely numerical and are a consequence of the fact that only a finite number of digits are used to compute and represent the pressure offsets ΔP_1 and ΔP_2. For example, if ΔP_1 and ΔP_2 each have a relative error of $\epsilon_P = 0.0001$ and the first four digits match then the subtraction $\Delta P = \Delta P_1 - \Delta P_2$ will result in total cancellation. In other words, ΔP will consist entirely of numerical error or noise. This noise will be amplified when computing mass and enthalpy vent flow since both depend on ΔP. In situations where the pressures ΔP_1 and ΔP_2 are supposed to be the same (for example in Figure 5), the computation of ΔP will not be exactly zero due to numerical error. Though generally it is a good idea to use double precision because of the pressure calculation, its use here will not solve this problem since the above cancellation error eliminates all information from the computed pressures. The ODE solver is essentially integrating noise which it accomplishes by cutting the time step to zero.

The above problem can be solved by smoothly damping the roundoff noise present in the computation $\Delta P = \Delta P_1 - \Delta P_2$, by using

$$\Delta \hat{P} = \Delta P \left(1 - e^{-\frac{\Delta P}{\epsilon_{\text{cut}}}}\right)$$

where ϵ_{cut} is defined by

$$\epsilon_{\text{cut}} = 10\epsilon_p \max(1, \Delta P_1, \Delta P_2) .$$

and ϵ_p is an error tolerance used in the solution of the variables ΔP_1 and ΔP_2. When ΔP is large relative to ϵ_{cut}, ΔP and $\Delta \hat{P}$ are essentially the same. On the other hand, when ΔP is small relative to ϵ_{cut}, $\Delta \hat{P}$ is essentially zero.

Stiffness

The key property that zone modeling differential equations possess is called stiffness. Differential equation solvers not taking this property into account will at best be grossly inefficient and at worst give wrong answers. Stiff systems of ordinary differential equations (ODE's) are an important class of problems that can occur when the modeled phenomenon possesses characteristic time scales that vary by several orders of magnitude. Physically, the system of ODE's used in zone fire modeling are stiff because the pressure adjusts to changing conditions much faster than other quantities such as upper and lower layer temperatures or layer heights.

The numerical difficulties encountered because of stiffness can not be avoided by exchanging the pressure equation for some other equation such as temperature, density, or internal energy. As shown in Table 1, each zone modeling differential equation contains a $\frac{dP}{dt}$ term. If the pressure is computed using an approximation such as equation (16) and $\frac{dP}{dt}$ is removed from the modeling differential equations, the resulting approximate ODE's are not stiff and a standard nonstiff solver may be used. However, the class of problems that can be solved is reduced since large pressure fluctuations can not be modeled properly.

The curious aspect of stiff ODE's is that the solution appears to be changing slowly and yet the computational costs of computing the solution are enormous when using standard nonstiff algorithms such as Runge-Kutta methods or predictor-corrector methods such as Adams-Bashforth. The question then is why does it cost so much to solve a problem whose solution changes slowly? To maintain stability, a nonstiff solver must use a stepsize that is small enough to track the part of the solution corresponding to the shortest time scale even when this solution component decays rapidly to some quasi-steady value. This stepsize is much smaller than required to

accurately track the desired part of the solution which corresponds to one of the longer time scales. So for stiff problems the choice of stepsize is dominated by considerations of stability, not accuracy.

Stiff differential equation solvers are expensive to use. This is because a nonlinear set of simultaneous equations involving the solution variables must be solved at each time step. Variants of Newton's method are typically used for this and require the solution of a system of linear equations at each iteration. (See for example, Gear, who gives a discussion in Chapter 11 of [7]). Consequently, it is inefficient to use stiff methods for nonstiff problems. Stiff methods work because their choice of stepsize is dominated by considerations of accuracy, not stability. As a result, they allow larger time steps to be taken than nonstiff methods. Even though the work per step is greater, the number of steps is sufficiently smaller that the total work is smaller.

There is no one definition of stiffness that is universally applied to initial value problems. One that is commonly applied is the following (see [8]). The initial value problem, $dy/dt = f(y, t), y(t_0) = y_0$ is called *stiff* if each eigenvalue of the Jacobian of f, has a negative real part and the range between the smallest and biggest real part is large (several orders of magnitude).

A physical interpretation of stiffness, which is imprecise mathematically, is to say that an initial value problem is stiff if the process being modeled possesses multiple time scales which vary widely. As has been discussed earlier, this is the case with zone fire models because pressures equilibrate much quicker than do layer volumes, masses, densities, or temperatures.

Good non-stiff ODE solvers such as DERKF and DEABM[9, 10] attempt to diagnose a problem as stiff so that the user will not use it inappropriately. ODE solvers are either explicit or implicit. Implicit solvers are generally stable for a much wider range of stepsizes than are explicit solvers.

The simulation time interval (t_0, t) for a zone fire model can be broken into two types of subintervals, stiff transient and stiff. In the stiff transient subintervals, the pressure is rapidly moving toward a quasi-steady state value. The simulation generally begins with a stiff transient. Each time layer height passes a vent boundary or the fire output takes a jump, a new stiff transient begins. During a stiff transient, stepsize will generally be small because it will be restricted by accuracy; that is, a small stepsize will be required to accurately track the rapidly changing pressure. Nonstiff solvers can generally integrate over the stiff transient time subinterval. Outside of these very short time intervals, a stiff solver is required. Since there is a large overhead associate with switching solvers, it is more efficient to use the stiff solver throughout the computation.

CONCLUSIONS

Natural vent flow is particularly susceptible to numerical problems due to the loss of significant digits that can occur when computing pressure differences. One approach for reducing this problem is to modify the subtraction $|\Delta P_1 - \Delta P_2|$ in order to damp out unwanted error that occurs when ΔP_1 and ΔP_2 are nearly equal.

Many model formulations can be derived from the basic mass and energy conservation equations some of which are analytically equivalent; that is, the equations in one formulation can be converted into those of another using the ideal gas law and definitions of density and internal energy. These formulations, however, are not equivalent numerically. When pressure changes are significant, the pressure equation should be included in a multi-room model. The significance of pressure changes can be evaluated in terms of flow through a vent since vent flow is quite sensitive to small pressure changes. When it is valid to assume that pressures are constant, the modeling differential equations can be simplified by setting $\frac{dP}{dt}$ to zero. The resulting ODE's have the added advantage that they are easier to solve since they are no longer stiff.

NOMENCLATURE

a, b	miscellaneous constants used in the equilibrium pressure relation, equation (14)
A_{vent}	area of vent m^2
$c_p(c_v)$	specific heat at constant pressure (volume) kJ/kg K
c_{vent}	vent coefficient, usually has a value of around 0.68
E	internal energy kJ
E_{ref}	reference internal energy kJ
f	a vector valued function which is the right hand side of the differential equation to be solved
f_y	Jacobian of the right hand side vector function f
m	mass kg lost due to cancellation in a subtraction

$\dot{m}_L, (\dot{m}_U)$	total mass flow rate into the lower (upper) layer kg
P	absolute pressure Pa
P_{cut}	pressure below which flows (through vents) are deemed to be negligible Pa
P_{ref}	reference pressure Pa
P_{amb}	ambient pressure usually about 101325 Pa
$\dot{q}_L, (\dot{q}_U)$	total enthalpy flow rate into the lower (upper) layer W
$\dot{q}_{fire}$	energy release rate of a fire W
$\dot{q}_{vent}$	energy flow rate through a vent W
R	universal ideal gas constant $\frac{m^2}{s^2 K}$
T	temperature K
t_0	initial time s
$t_{.99}$	time for pressure in a room to reach 99 percent of its final value
T_{vent}	temperature of gas flowing through vent K
t	independent variable, time, in the differential equations
T_{amb}	ambient temperature
V	volume m^3
y	layer height m
y	solution of the differential equation
y_0	solution of a differential equation at time t_0
ΔP	pressure drop across a vent Pa
$\Delta \hat{P}$	pressure drop across a vent modified to account for catastrophic cancellation errors Pa
ΔP	Pressure offset satisfying $P = P_{ref} + \Delta P$ Pa
$\Delta P_1, (\Delta P_2)$	pressure rise above floor pressure in room 1 (2) Pa
ΔP_{cut}	pressure below which flow is insignificant numerically Pa
ΔP_∞	Equilibrium pressure Pa
ϵ_p	error tolerance of pressure variables used in the calculation of vent flow
γ	ratio of specific heats c_p, c_v
ρ	density kg/m^3
ρ_{amb}	ambient density kg/m^3
ρ_{vent}	density of gas flowing through vent

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