REVIEW ON KEY EQUATIONS IN THE TWO-LAYER ZONE MODEL CFAST

S.S. Han
Department of Building Services Engineering, The Hong Kong Polytechnic University, Hong Kong, China

ABSTRACT

Two-layer zone model is now a practical engineering tool for fire safety design. In this paper, the key equations used in a typical zone model, CFAST, are reviewed. There might be errors in using zone model under some conditions. Uncertainties and limitations of those equations should be clearly identified. It is important to understand the physical and numerical algorithms included. Reporting those becomes the objectives of the paper.

1. INTRODUCTION

Computer modeling [1] of fire behavior plays a key role in fire safety engineering. Fire modeling itself is changing rapidly and many computer models [2,3] are now available in the market. Zone model [4-11] is a relatively simple approach which can be modified easily for practical applications. Almost all zone models can be run on personal computers with short CPU time. Although relatively simple, zone model cannot work well if the detailed flow field is unknown. It can provide adequate fire parameters fairly accurately. Because of so many advantages, zone model has been widely investigated and successfully used in fire safety engineering in the last few decades. Now, zone model is the commonest type of fire model and verified to be a practical tool for simulating building fires.

While using the fire models correctly without making any mistakes, the results are still uncertain or might even be wrong. Actually, there is no universal zone model which fits all applications. There must be some shortcomings. If the user cannot deal with the limitations well, the results will not be accurate. Practical fire behaviour and the physical basis of the model including its capabilities and limitations should be understood.

Most of the zone models are based on similar basic principles and only different in treating the fire phenomena. CFAST [12-18] is a well-developed zone model based on solving a set of equations which can predict state variables. It takes the form of an initial value problem for a mixed system of differential and algebraic equations. These equations are derived from the conservation of mass and energy. Subsidiary equations are the ideal gas law, definitions of variables such as density and internal energy and other fire physical phenomena.

2. KEY EQUATIONS IN A TWO-LAYER ZONE MODEL

In a two-layer zone model, two control volumes are taken as a comparatively hot upper layer and a cooler lower layer. There are eleven variables which 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, which i is L for the lower layer and i is U for the upper layer. The compartment is taken to have the same pressure P. These eleven variables are related by definitions of physical parameters:

Density: $$\rho_i = \frac{m_i}{V_i} \quad (1)$$

Internal energy: $$E_i = c_v m_i T_i \quad (2)$$

Ideal gas law: $$P = R\rho_i T_i \quad (3)$$

Total volume: $$V = V_L + V_U \quad (4)$$

There are seven constraints on density, internal energy and the ideal gas law. Four additional equations can be obtained from conservation of energy and mass:

$$\frac{dE_i}{dt} + P\frac{dV_i}{dt} = \dot{q}_i \quad (5)$$

$$\frac{dm_i}{dt} = \dot{m}_i \quad (6)$$

Solving the above equations, nine differential equations for P, V, E_i, ρ_i, T_i can be derived respectively and be included in the following five equations:

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

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

$$\frac{dE_i}{dt} = \frac{1}{\gamma}\left(\dot{q}_i + V_i \frac{dP}{dt}\right) \quad (9)$$

$$\frac{d\rho_i}{dt} = \frac{1}{c_P T_i V_i}\left(\left(\dot{q}_i - c_P \dot{m}_i T_i\right) - \frac{V_i}{\gamma - 1}\frac{dP}{dt}\right) \quad (10)$$

$$\frac{dT_i}{dt} = \frac{1}{c_P \rho_i V_i}\left(\left(\dot{q}_i - c_P \dot{m}_i T_i\right) + V_i \frac{dP}{dt}\right) \quad (11)$$

The time evolution of these solution variables can be computed by solving the corresponding differential equations together with appropriate initial conditions. Seven variables can be determined by using equations (1) to (4), four additional equations can be selected from these eleven differential equations (6) to (11).

3. EQUATIONS IN CAST

CFAST is set up to solve pressure, upper layer volume and the temperature of the two layers. The substitution pressure equation and selected differential equations are shown below.

$$\Delta P = P - P_{ref} \quad (12)$$

$$\frac{dP}{dt} = \frac{\gamma - 1}{V}\left(\dot{q}_L + \dot{q}_U\right) \quad (13)$$

$$\frac{dV_U}{dt} = \frac{1}{\gamma P}\left((\gamma - 1)\dot{q}_U - V_U \frac{dP}{dt}\right) \quad (14)$$

$$\frac{dT_U}{dt} = \frac{1}{c_P \rho_U V_U}\left(\left(\dot{q}_U - c_P \dot{m}_U T_U\right) + V_U \frac{dP}{dt}\right) \quad (15)$$

$$\frac{dT_L}{dt} = \frac{1}{c_P \rho_L V_L}\left(\left(\dot{q}_L - c_P \dot{m}_L T_L\right) + V_L \frac{dP}{dt}\right) \quad (16)$$

The conserved quantities in each compartment are described by the set of predictive equations above. The form of the equations is such that the physical phenomena are source terms (the $\dot{m}_i$ and $\dot{q}_i$ in equations (13) to (16)) on the right-hand side of these equations. This formulation can change the physical phenomena and alter the form of algorithms in a relatively simple manner. Source terms of these equations are:

- The fire itself
- The plumes
- Vent flow
- Heat transfer

All those will be reviewed in the following sections.

4. THE FIRE

The fuel source used in CFAST is a specified fire, for which the time-dependent characteristics are specified as a function of time. The specified fire can be unconstrained or constrained. Combustion chemistry is not calculated for unconstrained fires. The heat release rate for a constrained fire may be reduced below its specified value based on the concentration of fuel or oxygen available for combustion. The pyrolysis rate for both fire types is specified as $\dot{m}_f$, the burning rate as $\dot{m}_b$ and the heat of combustion as H_c, therefore the heat release rate $\dot{Q}_f$ is:

$$\dot{Q}_f = H_c \dot{m}_b - c_p\left(T_U - T_L\right)\dot{m}_b \quad (17)$$

For the unconstrained fire, $\dot{m}_b = \dot{m}_f$, whereas for the constrained fire, $\dot{m}_b < \dot{m}_f$, the burning rate may be less than the pyrolysis rate. An effective heat of combustion generally used is obtained from experimental data. The enthalpy released would be transferred away by radiation and convection:

$$\begin{cases} \dot{Q}_r(\text{fire}) = \chi_r \dot{Q}_f \\ \dot{Q}_c(\text{fire}) = (1 - \chi_r)\dot{Q}_f \end{cases} \quad (18)$$

where χ_r is the fraction of the heat release rate lost as radiation. The convective heat release rate $\dot{Q}_c(\text{fire})$ becomes the driving term in the plume flow. For a specified fire, there is radiation to both the upper and lower layers, whereas the convective part contributes only to the upper layer.

5. THE PLUMES

A fire generates energy at a rate $\dot{Q}$. Some fraction, χ_r, will exit the fire as radiation. Within CFAST, the radiative fraction defaults to 0.3. The plume correlation by McCaffrey [19] is adopted to estimate the mass entrained by the plume from the lower into the upper layer. This correlation divides the flame/plume into three regions as given below.

$$\frac{\dot{m}_e}{\dot{Q}} = \begin{cases} 0.011\left(Z/\dot{Q}^{0.4}\right)^{0.566} \textit{ for } 0.00 \le \left(Z/\dot{Q}^{0.4}\right) < 0.08 \\ \textit{in the continuous flame region} \\ 0.026\left(Z/\dot{Q}^{0.4}\right)^{0.909} \textit{ for } 0.08 \le \left(Z/\dot{Q}^{0.4}\right) < 0.20 \\ \textit{in the intermittent flame region} \\ 0.124\left(Z/\dot{Q}^{0.4}\right)^{1.895} \textit{ for } 0.20 \le \left(Z/\dot{Q}^{0.4}\right) \\ \textit{in the plume region} \end{cases} \quad (19)$$

McCaffrey's correlation is an extension of the common point source plume model, with a different set of coefficients for each region. These coefficients are experimental correlations, and are not based on theory. From conservation of mass and enthalpy:

$$\dot{m}_p = \dot{m}_f + \dot{m}_e \quad (20)$$

$$\dot{m}_p c_p T_p = \dot{m}_f c_p T_f + \dot{m}_e c_p T_L \quad (21)$$

where the subscripts p, f, e and l refer to the plume, fire, entrained air, and lower layer, respectively. The entrainment limit used in the CFAST model can be obtained:

$$\dot{m}_e < \frac{\dot{Q}_c(\text{fire})}{c_p(T_U - T_L)} \quad (22)$$

The 1.895 power used in the plume region can result in over-prediction of the plume flows far above the fire [20].

6. VENT FLOW

Mass flow is the dominant source term for the predictive equations because it fluctuates most rapidly and transfers the greatest amount of enthalpy on an instantaneous basis of all the source terms (except the fire). Also, it is most sensitive to changes in the environment. Both horizontal flow through vertical vents and vertical flow through horizontal vents are modelled in CFAST. Horizontal flow encompasses flow through doors, windows and so on. Vertical flow occurs in ceiling vents.

6.1 Horizontal Flow Through Vertical Vents

The general form for the velocity of the mass flow is given by:

$$v = C\left(\frac{2\Delta P}{\rho}\right)^{1/2} \quad (23)$$

where C is the flow coefficient (≈ 0.7), ρ is the gas density on the source side, and ΔP is the pressure across the interface.

The vent opening is partitioned into at most six slabs where each slab is bounded by a layer height, neutral plane, or vent boundary such as a soffit or sill. The mass flow for each slab is determined by:

$$\dot{m}_{i\to o} = \frac{1}{3} C(8\rho) A_{slab}\left(\frac{x^2 + xy + y^2}{x + y}\right) \quad (24)$$

where

$$x = |P_t|^{1/2}$$

and

$$y = |P_b|^{1/2}$$

P_t and P_b are the cross-vent pressure differential at the top and bottom of the slab respectively and A_{slab} is the cross-sectional area of the slab. The value of the density ρ is taken from the source compartment.

6.2 Vertical Flow Through Horizontal Vents

Cooper's algorithm is used in computing the mass flow through ceiling and floor vents. It is based on correlations to model the unsteady component of the flow. There are two components to the flow: a net flow due to pressure difference; and an exchange flow due to density difference of the gases. The overall flow is given by:

$$\dot{m} = Cf(\gamma, \varepsilon)\left(\frac{\delta P}{\bar{\rho}}\right)^{1/2} A_v \quad (25)$$

where $\gamma = c_p / c_v$ is the ratio of specific heat and

$$\varepsilon = \delta P / P$$

$$C = 0.68 + 0.17\varepsilon$$

f is a weak function of both γ and ε. When there is unstable flow, Cooper's correlations was applied to study the exchange flow:

$$\dot{m}_{ex} = 0.1\left(\frac{g\delta\rho A_v^{5/2}}{\rho_{av}}\right)\left(1.0 - \frac{2A_v^{2}\delta\rho}{S^2 g\delta\rho D^5}\right) \quad (26)$$

where $D = 2\sqrt{A_v/\pi}$ and S is taken as 0.754 or 0.942 for round or square openings, respectively.

7. HEAT TRANSFER

7.1 Radiation

The four wall algorithms for computing radiative heat exchange are based upon the equations developed by Siegel and Howell [21]. A modified form of net radiation equation is used as:

$$\Delta\hat{q}_k'' - \sum_{j=1}^{N}(1-\varepsilon_j)\Delta\hat{q}_j'' F_{k-j}\tau_{j-k}$$

$$= \sigma T_k^4 - \sum_{j=1}^{N}\sigma T_j^4 F_{k-j}\tau_{j-k} - \frac{c_k}{A_k} \qquad (27)$$

$$\Delta q_k'' = \varepsilon_k \Delta\hat{q}_k'' \qquad (28)$$

There are two reasons for solving this equation. First, since ε_k does not occur in the denominator, radiation exchange can be calculated when some of the wall segments have zero emissivity. Second and more importantly, the matrix corresponding to the linear system of equation is diagonally dominant. Iterative algorithms can be used to solve such systems more efficiently than direct methods such as Gaussian elimination. The more diagonally dominant a matrix (the closer the emissivities are to unity), the quicker the convergence when using iterative methods.

7.2 Convection

Convective heat flow is the enthalpy transfer across a thin boundary layer. The thickness of this layer is determined by the temperature difference between the gas zone and the wall or object being heated. In general, convective heat transfer $\dot{q}$ is defined as:

$$\dot{q} = hA_s(T_g - T_s) \qquad (29)$$

The convective heat transfer coefficient *h* is defined in terms of the Nusselt number, a dimensionless temperature gradient at the surface, which is defined as:

$$h = \frac{Nu_L k}{L} = CRa_L^n \qquad (30)$$

where the Rayleigh number

$$Ra_L = Gr_L Pr = \frac{g\beta(T_s - T_g)L^3}{v\alpha} \qquad (31)$$

is based on a characteristic length, L, of the geometry. The power n is typically 1/4 and 1/3 for laminar and turbulent flow, respectively. All properties are evaluated at the film temperature,

$$T_f = (T_s + T_g)/2$$

The thermal diffusivity α and thermal conductivity k of air are defined as a function of the film temperature:

$$\alpha = 1.0\times10^{-9} T_f^{7/4}, \quad k = \left(\frac{0.0209 + 2.33\times10^{-5} T_f}{1 - 0.000267 T_f}\right) \qquad (32)$$

These together with typical correlations of Nu_L applicable to the problem are picked out from the literature.

7.3 Conduction

Conduction transfers heat within the wall. Convection and radiative heat transfer calculations provide the boundary conditions for the conduction algorithm [22-24]. The partial differential equation which governs the heat transfer in solids is:

$$\partial T/\partial t = (k/\rho c)\nabla^2 T \qquad (33)$$

The coefficients k, ρ and c are considered as independent of temperature for all the materials. However, for some materials in fact, such as gypsum, the value of k may vary distinctly.

A finite difference approach using a non-uniform spatial mesh is used to advance the wall temperature solution. The heat equation is discretized using a second-order central difference for the spatial derivative and a backward difference for the time derivative. The resulting tri-diagonal system of equations is then solved to advance the temperature solution to time t + Δt. This process is repeated, using the work of Moss and Forney, until the heat flux striking the wall (calculated from the convection and radiation algorithms) is consistent with the wall temperature gradient at the surface via Fourier's law:

$$q'' = -k(dT/dx) \qquad (34)$$

7.4 Heating of Target Object

The net flux striking a target is used as a boundary condition for an associated heat conduction problem in order to compute the surface temperature of the target. This temperature can then be used to estimate the conditions at the target, i.e. whether the target will ignite. Alternatively, if the target is assumed to be thin, then its temperature quickly rises to a level where the net heat flux striking the target is zero, i.e. to a steady state. The calculation is done using the concept of net heat flux. The net heat flux $\Delta'' q_t$ striking a target t is given by:

$$\Delta'' q_t = q''_{rad}(in) + q''_{convec} - q''_{rad}(out) \tag{35}$$

where $q''_{rad}(in)$ is the incoming radiative flux, q''_{convec} is the convective flux and $q''_{rad}(out)$ is the outgoing radiative flux.

The modified version of heat flux equation is:

$$\begin{aligned}\Delta'' q_t &= \varepsilon_t q''_{rad}(in) + q''_{convec} - \varepsilon_t \sigma T_t^4 \\ &= \varepsilon_t \left(\sum_f q''_{f,t} + \sum_w q''_{w,t} + \sum_i q''_{g,t} \right) + q''_{convec} - \varepsilon_t \sigma T_t^4\end{aligned} \tag{36}$$

where ε_t is the emittance of the target and σ is the Stefan-Boltzman constant.

The heat flux $\Delta'' q_t$ can be used in estimating the surface temperature of the target or as a boundary condition to solve the heat conduction problem:

$$\left.\begin{aligned}&\frac{\partial T}{\partial t}(x,t) = \frac{k}{\rho c}\frac{\partial^2 T}{\partial x^2}(x,t) \\ &T(x,0) = T_0(x), -k\frac{\partial T}{\partial x}(0,t) = \Delta'' q_t, \\ &-k\frac{\partial T}{\partial x}(L,t) = 0\end{aligned}\right\} \tag{37}$$

For the target temperature profile T, k, ρ and c are the thermal conductivity, density and heat capacity of the target, L is the thickness of the target and T_o is the initial temperature profile of the target.

Alternatively, the target temperature is assumed as always at steady state, i.e. $\Delta'' q_t = 0$. T_t can then be found using Newton's method that will satisfy $\Delta'' q_t = 0$. To illustrate it, suppose that the convective flux is given by:

$$q''_{convec} = c(T_g - T_t) \tag{38}$$

where c is a convective heat transfer coefficient and T_g is the gas temperature adjacent to the target.

Then, the above heat flux equation can be simplified to:

$$f(T_t) = \varepsilon_t \sigma T_t^4 - c(T_g - T_t) - \varepsilon_t q''_{rad}(in) = -\Delta'' q_t \tag{39}$$

This non-linear eqation can be solved using Newton's method. There are three steps necessary to complete this calculation: First, calculate the heat transfer through the compartment; Second, calculate the heat flux to the target or object; and finally, compute the target temperature.

In order to calculate the radiation heat transfer from fires, gas layers and wall surfaces to targets, configuration factors, gas layer transmissivity and absorptance must be calculated first.

Configuration factors:

$$F_{1\to 2} \approx A_2 / A_{total} \tag{40}$$

where surface 1 is the target and 2 is a wall in a compartment, A_2 is the area of the wall and A_{total} is the total area of the surfaces 'seen' by the target.

Transmissivity: The transmissivity of a gas volume is the fraction of radiant energy that will pass through it unimpeded and is given by:

$$\tau(y) = e^{-ay} \tag{41}$$

where a is the absorptance per unit length of the gas volume and y is a characteristic path length.

Absorptivity: The absorptivity α of a gas volume is the fraction of radiant energy absorbed by that volume. For a grey gas:

$$\alpha + \tau = 1 \tag{42}$$

The absorptivity of the lower (upper) layer is denoted as $\alpha_L(\alpha_U)$.

7.5 Computing the Heat Flux to a Target

There are four components of heat flux to a target: fires, walls, gas layer radiation and gas layer convection.

- Heat flux from a fire to a target

  Let n_t be a unit vector perpendicular to the target , r be a vector from the fire to target and θ_t be the angle between the vector n_t and r. q_f is the radiative portion of the energy release rate of the fire. The heat flux on a sphere of radius r due to this fire is $q_f / (4\pi r^2)$ and on the target is $q_f \cos(\theta_t)/(4\pi r^2)$. Considering the transmissivity of gas layer, the heat flux to the target is:

$$q''_{f,t} = \tau_L(y_L)\tau_U(y_U)\, q_f \cos(\theta_t)/(4\pi r^2)$$
$$= -q_f\, \tau_L(y_L)\tau_U(y_U)\, n_t.r/(4\pi r^3) \quad (43)$$

- Radiative heat flux from a wall segment to a target

The flux $q''_{w,t}$ from a wall segment to a target can be computed using:

$$q''_{w,t} = q''_w(out)\, \tau_L(y_L)\tau_U(y_U)\, F_{w\to t} A_w/A_t \quad (44)$$

where $q''_w(out)$ is the flux leaving the wall segment, A_w and A_t are the areas of the wall segment and target respectively, $F_{w\to t}$ is a configuration factor denoting the fraction of radiant energy given off by the wall segment that is intercepted by the target. Accounting for symmetry relation $A_w F_{w\to t} = A_t F_{t\to w}$, the above equation can be simplified as:

$$q''_{w,t} = q''_w(out)\, \tau_L(y_L)\tau_U(y_U)\, F_{t\to w} \quad (45)$$

where

$$q''_w(out) = \sigma T^4 - \Delta q''_w(1-\varepsilon_w)/\varepsilon_w \quad (46)$$

and σ is radiative constant, T_w is the temperature of the wall segment, ε_w is the emissivity of the wall segment and $\Delta q''_w$ is the net flux striking the wall segment.

- Radiation from the gas layer to the target

The upper and lower gas layers in a room contribute to the heat flux striking the target if the layer absorptance is non-zero. Heat transfer does not occur to the target when $T_t = T_g = T_w$.

Let $\Delta q''_{w,t}(gas)$ denote the flux striking the target due to the gas g in the direction of wall segment w. Then the total radiation from the gas to the target is:

$$q''_{g,t} = \sum_w q''_{w,t}(gas) =$$
$$\sigma F_{t\to w}\left\{\left(\alpha_L \tau_U T_L^4 + \alpha_U T_U^4\right) + \left(\alpha_U \tau_L T_U^4 + \alpha_L T_L^4\right)\right\} \quad (47)$$

where two parts in the above equation denote the wall *w* in the lower or upper layer respectively.

7.6 Computing Target Temperature

The steady state target temperature T_t can be found by solving the equation $f(T_t) = 0$ where $f(T_t)$ is defined before. This can be done by using the Newton iteration:

$$T_{new} = T_{old} - f(T_{old})/f'(T_{old}) \quad (48)$$

where

$$f(T_t) = \varepsilon_t \sigma T_t^4 - c(T_g - T_t) - \varepsilon_t q''_{rad}(in) \quad (49)$$

$$f'(T_t) = \frac{df(T_t)}{dT_t} = 4\varepsilon_t \sigma T_t^3 + c - (T_g - T_t)\frac{dc}{dT_t} \quad (50)$$

8. CONCLUSION

Basic equations adopted in the fire model CFAST were reviewed. Many algorithms used here are based on empirical formula. Formulations are also based on assumptions which can give errors. Physical process modelled might have limits to their applicability. Some limitations are relatively obvious while others are not. The user should be familiar with fire dynamics and the numerical algorithms used.

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Q & A

No questions.