



Issues in Evaluation of Complex Fire Models

Richard D. Peacock,^a Paul A. Reneke,^a C. Lynn Forney^a
& Michael M. Kostreva^b

^aBuilding and Fire Research Laboratory, NIST, Gaithersburg, MD 20899, USA

^bDepartment of Mathematical Sciences, Clemson University, Clemson, SC 29634, USA

(Received 20 June 1996; revised version received 28 August 1997; accepted 8 September 1997)

ABSTRACT

Several methods of evaluation of the predictive capability have been applied to fire models, but with limited utility. These range from explicit evaluation of the equations used in simple models such as ASET to pointwise evaluation of complex models from numerous computer runs of a model. This paper presents a discussion of the issues involved in conducting an analysis of a complex room fire model. Examples using currently available room fire models are presented. For the models and test cases examined, heat release rate and heat transfer effects dominate the behavior of the models. For simple models like the ASET model, analytical techniques can be readily applied. For more complex fire models, obtaining an overall assessment of the model increases in complexity with the complexity of the model, requiring evaluation of numerous model inputs and outputs. Thus, more directed local investigations are currently the only tractable means of evaluation. Areas for additional research are identified. Published by Elsevier Science Ltd.

NOMENCLATURE

A	Room area
B	Matrix, defined in eqn (9)
H	Height of the room
J	Jacobian, defined in eqn (9)
L_c	Characteristic length, taken to be the height of the room
\dot{Q}	Heat release rate
\dot{Q}_0	Characteristic heat release rate, taken to be the same as \dot{Q} for the ASET analysis
S	Sensitivity equation vector in eqn (5)
T	Temperature
T_a	Ambient temperature

X	Discretization of the upper-layer temperature
Y	Discretization of layer interface height
Z	Elevation above fire
Z_i	Elevation of layer interface
c	Matrix, defined in eqn (9)
c_1, c_2	Dimensionless parameters in eqns (2) and (3)
c_p	Specific heat
g	Gravitational constant
h	Height of a vent
p	Arbitrary input parameter vector in eqn (1)
\dot{q}	Dimensionless heat release rate
t	Time
t_c	Characteristic time, taken to be 900 s for the ASET analysis
z	Arbitrary solution vector in eqn (1)
Δ	Height of the base of the fire above the floor
δ	Dimensionless value of Δ
λ_c	Conductive heat loss fraction
λ_r	Radiative heat loss fraction
ζ	Dimensionless layer interface height
ρ	Gas density
ρ_a	Ambient gas density
τ	Dimensionless time
φ	Dimensionless upper-layer temperature
ω	Arbitrary sensitivity variable in eqn (4)

1 INTRODUCTION

Analytical models for predicting fire behavior have been evolving since the 1960s. During this time, the completeness of the models has grown. In the beginning, the focus of these efforts was to describe in mathematical language the various phenomena which were observed in fire growth and spread. These separate representations have typically described only parts of a fire. When combined though, they can create a complex computer code capable of giving an estimate of the expected effects of a fire based upon given input parameters. Analytical models have progressed to the point of providing predictions of fire behavior with an accuracy suitable for most engineering applications. Two obvious questions arise concerning the use of these models for engineering calculations:

- How good do the inputs to the model need to be (How do changes in the model inputs affect the model outputs)?

- How good is the output of model (How close are the actual conditions to those predicted by the model)?

To address the former question, this paper presents a discussion of the issues involved in conducting a sensitivity analysis of a complex room fire model. Examples using one fire model are provided. For the latter question, some examples are presented illustrating comparisons for both simple correlations and complex fire models. More complete investigations are available.^{1,2} From the outset, it is important to note that this paper does not provide all the answers to the issues discussed. Rather, it is intended to highlight the strengths and weaknesses of the current level of understanding of evaluation of complex fire models and to promote further discussion of the topic.

1.1 Fire models

In a recent international survey,³ 62 actively supported models were identified. Of these, 31 predict the fire-generated environment (mainly temperature and smoke movement in some way). Twelve models predict fire endurance, eight address detector or sprinkler response, and four calculate evacuation times. The computer models now available vary considerably in scope, complexity, and purpose. Simple 'room filling' models such as the Available Safe Egress Time (ASET) model⁴ run quickly on almost any computer, and provide estimates of a few parameters of interest for a fire in a single compartment. A special purpose model can provide a single function. For example, COMPF2⁵ calculates post-flashover room temperatures and LAVENT⁶ includes the interaction of ceiling jets with fusible links in a room containing ceiling vents and draft curtains. More detailed zone models like the HARVARD 5 code⁷ or FIRST⁸ predict the burning behavior of multiple items in a room, along with the time-dependent conditions therein. In addition to the single-room models mentioned above, there are a smaller number of multi-room models which have been developed. These include the BRI transport model,⁹ the HARVARD 6 code¹⁰ (which is a multi-room version of HARVARD 5), FAST¹¹⁻¹³ CCFM¹⁴ and CFAST.¹⁵ In addition, 10 field models are identified which can provide detailed information on the environment within compartments.

Although the papers are several years old, Mitler¹⁶ and Jones¹⁷ reviewed the underlying physics in several of the fire models in detail. The models fall into two categories: those that start with the principles of conservation of mass, momentum, and energy; and those that typically utilize curve fits to particular experiments or series of experiments, used in order to try to understand the underlying relationship among a small set of parameters. In both cases, errors arise where a mathematical short cut was taken, a

simplifying assumption was made, or some important phenomenon was not included.

Once a mathematical representation of the underlying science has been developed, the conservation equations can be recast into predictive equations for temperature, smoke and gas concentration, and other parameters of interest, and are coded into a computer for solution. The environment in a fire is constantly changing. Thus, the equations are often in the form of *differential equations*. A complete set of equations can compute the conditions produced by the fire at a given time in a specified volume of air. Referred to as a *control volume*, the model assumes that the predicted conditions within this volume are uniform at any time. Thus, the control volume has one temperature, smoke density, gas concentration, etc.

Different models divide the building into different numbers of control volumes depending on the desired level of detail. The most common fire model, known as a *zone model*, generally uses two control volumes to describe a room—an upper layer and a lower layer. In the room with the fire, additional control volumes for the fire plume or the ceiling jet may be included to improve the accuracy of the prediction (see Fig. 1).

This two-layer approach has evolved from observation of such layering in real-scale fire experiments. Hot gases collect at the ceiling and fill the room from the top. While these experiments show some variation in conditions within the layer, these are small compared to the differences between the layers. Thus, the zone model can produce a useful simulation under most conditions.

Other types of models include *network models* and *field models*. The former use one element per room and are used to predict conditions in spaces far removed from the fire room, where temperatures are near ambient and layering does not occur. The field model goes to the other extreme, dividing

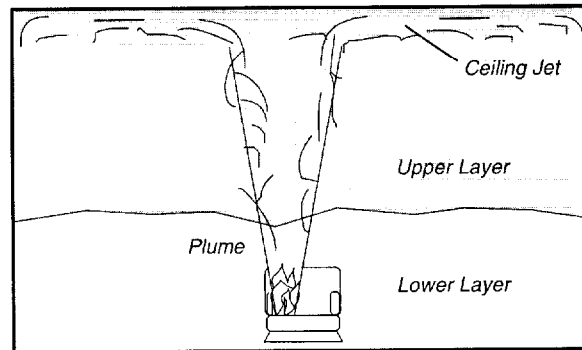


Fig. 1. Zone model terms.

the room into thousands or even hundreds of thousands of control volumes. Such models have less dependence on experimental correlations and can provide high resolution of conditions throughout the rooms, but typically require far longer run times than zone models. Thus, they are used when highly detailed calculations are essential.

1.2 Earlier research

The ASTM guide for evaluating the predictive capability of fire models¹⁸ identifies four areas important for fire model evaluation: (1) model and scenario definition, (2) theoretical basis and assumptions in the model, (3) mathematical and numerical robustness of the model, and (4) quantifying the uncertainty and accuracy of the model. The first two of these are largely documentation issues for the model developer. Additional guidance is available in the ASTM guide for fire-model documentation.¹⁹ The third area is outside the scope of this paper. The work of Forney²⁰ examines the numerical robustness of fire models using the CFAST model as an example. Sensitivity analysis and experimental comparisons are the primary focus of the final area. An overview of published literature related to these is presented below.

1.2.1 Sensitivity analysis

Although published literature is available which includes discussion of techniques for sensitivity analysis of predictive models,²¹ their primary focus is most often stochastic models of human behavior and rarely have been applied to deterministic fire models. This section provides a brief overview of some of the publications related to the evaluation of fire models. It is not an exhaustive review, rather, it is intended to give an appreciation for the current status of the topic as applied to fire modeling.

Clemson, *et al.*²² provide an overview of methods for sensitivity analysis of simulation models. Although not specific to fire modeling, they provide numerous references to additional research, present the advantages and disadvantages of different sampling techniques for experiment selection, and apply chosen methods to an example simulation model.

Khoudja²³ has studied the sensitivity of an early version of the FAST model with a fractional factorial design involving two levels of 16 different input parameters. The statistical design, taken from the texts by Box and Hunter²⁴ and Daniel,²⁵ reduced the necessary model runs from more than 65000 to 256 by studying the interactions of input parameters simultaneously. His choice of values for each input parameter represented a range for each parameter. His analysis of the FAST model (a precursor to the CFAST model used for this paper) showed a particular sensitivity to the inclusion of conduction in the

calculations and lesser, though consistent sensitivities to the number of compartments included in a simulation and the ambient temperature. Without the inclusion of surface thermophysical properties, this model treats surfaces as adiabatic for conductive heat transfer. Thus, this consistent sensitivity should be expected. Sensitivity to changes in thermal properties of the surfaces were not explored.

Iman and Helton²⁶ studied the sensitivity of complex computer models developed to simulate the risk of severe nuclear accidents which may include fire and other risks. Three approaches to uncertainty and sensitivity analysis were explored:

- response surface methodology, where the complex model is replaced by a series of simple linear models with inputs determined from a fractional factorial design,
- Latin hypercube sampling, where carefully chosen random sampling is used to determine model inputs, and
- differential analysis, used to evaluate sensitivity for small perturbations about a single set of model inputs.

These techniques were evaluated for three different models with respect to ease of implementation, flexibility, estimation of the cumulative distribution function of the output, and adaptability to different methods of sensitivity analysis. With respect to these criteria, the techniques using Latin hypercube sampling had the best overall performance. Programs to generate such samples are available.^{27,28}

For a steady-state model of a liquid pool fire, Ndubizu *et al.*²⁹ used a Fourier amplitude sensitivity test to study the relative importance of model inputs. With appropriate transformation of input parameters, the model outputs define a periodic function of the transformed inputs. This resulting function is then Fourier analyzed with the Fourier coefficients directly corresponding to the sensitivity of each input parameter.

1.2.2 Comparisons with experimental data

A number of researchers have studied the level of agreement between computer fire models and real-scale fires. These comparisons fall into two broad categories: fire reconstruction and comparison with laboratory experiments. Both categories provide a level of verification for the models used. Fire reconstruction, although often more qualitative, provides a higher degree of confidence for the user when the models successfully simulate real-life conditions. Comparisons with laboratory experiments, however, can yield detailed comparisons that can point out weaknesses in the individual phenomena included in the models. The comparisons made to date are mostly qualitative

in nature. The level of agreement between the models and experiment is typically reported as 'favorable', 'satisfactory', 'well predicted', 'successful', or 'reasonable'. Some of the comparisons in the literature are reviewed below.

Nelson³⁰ used simple computer fire models along with the existing experimental data to develop an analysis of a large high-rise building fire. This analysis showed the value of available analytical calculations in reconstructing the events involved in a multiple-story fire. Bukowski³¹⁻³³ has applied the FAST and CFAST models in several fatal fire reconstructions. Details of the fires including temperatures, vent flows, and gas concentrations were consistent with observed conditions and witness accounts. Emmons³⁴ applied computer fire modeling to the MGM Grand Hotel fire of 1980. Using the HARVARD 5 model, Prof. Emmons analyzed the relative contributions of booth seating, ceiling tiles, decorative beams, and the HVAC system on the outcome of the fire.

Several studies comparing model predictions with experimental measurements are available. Mitler and Rockett³⁵ utilized the Harvard Computer Fire Code V to model two in a series of eight well-instrumented full-scale room fires. They reported 'good to excellent' agreement for most of the model variables studied. Rockett *et al.*³⁶ used the HARVARD VI multi-room fire model to simulate the results of real-scale, multi-room fire experiments. While the model was generally found to provide 'favorable' simulations, several areas where improvements were needed were identified. They pointed out limitations in modeling of oxygen-limited burning, mixing of gases at vents, convective heat transfer, and plume entrainment. Deal³⁷ reviewed four computer fire models (CCFM, FIRST, FPETOOL³⁸ and FAST) to ascertain the relative performance of the models in simulating fire experiments in a small room. All the models simulated the experimental conditions including temperature, species generation, and vent flows, 'quite satisfactorily'. Duong³⁹ studied the predictions of several computer fire models (CCFM, FAST, FIRST, and BRI), comparing the models with one another and with large fires in an aircraft hanger. For a 4 MW fire size, he concluded that all the models are 'reasonably accurate'. At 36 MW, however, 'none of the models did well'. Beard^{2,40} evaluated four fire models (ASET, FAST, FIRST, and JASMINE⁴¹) by modeling three well-documented experimental fires, ranging in scope from the same tests used by Mitler and Rockett³⁵ to a large-department-store space with closed doors and windows. He provides both a qualitative and quantitative assessment of the models ability to predict temperature, smoke obscuration, CO concentration, and layer interface position (for the zone-based models). Peacock *et al.*¹ compared the CFAST model to a range of experimental fires. The model provided predictions of the magnitude and trends (time to critical conditions and general curve shape) for the experiments

studied which range in quality from within a few percent to a factor of two or three of the measured values.

2 SENSITIVITY ANALYSIS

A sensitivity analysis is a study of how changes in model parameters affect the results generated by the model. Model predictions may be sensitive to uncertainties in input data, to the level of rigor employed in modeling the relevant physics and chemistry, and to the accuracy of numerical treatment. Among the purposes for conducting a sensitivity analysis are to determine the following:

- the important input variables in the models (those which effect changes in important output variables,
- the required accuracy for input variables (particularly sensitive input variable may need to be known to a greater precision than insensitive ones), and
- the sensitivity of output variables to variations in input data (which inputs effect output variable of interest).

Conducting a sensitivity analysis of a complex fire model is a difficult task. Many models require extensive input data and generate predictions for numerous output variables over a period of simulated time. Several methods of sensitivity analysis have been applied to fire models, but most have had limited utility. These range from explicit evaluation of the equations used in simple models such as ASET⁴² to pointwise evaluation of complex models from numerous computer runs of the model.²³ The technique chosen for use will be dependent on the objectives of the study, the required results, the resources available and the complexity of the model being analyzed.

Fire growth models are typically based on a system of ordinary differential equations of the form

$$\frac{dz}{d\tau} = f(z, p, \tau), \quad z(\tau = 0) = z_0 \quad (1)$$

where z (z_1, z_2, \dots, z_m) is the solution vector for the system of equations (for example, mass, temperature, or volume) and p (p_1, p_2, \dots, p_n) is a vector of input parameters (for example, room area, room height, heat release rate) and τ is the time.⁴³ The solutions to these equations are, in general, not known explicitly and must be determined numerically. To study the sensitivity of such a set of equations, the partial derivatives of an output z_j with respect to an input p_i (for $j = 1, \dots, m$ and $i = 1, \dots, n$) are examined.

Two basic approaches exist for obtaining sensitivity information:

- *Local methods*—produce sensitivity measures for a particular set of input parameters and must be repeated for a range of input parameters to obtain information on the overall model performance. Finite-difference methods can be applied without modifying a model's equation set, but require careful selection of input parameters to obtain good estimates. Direct methods supplement the equation set solved by a model with sensitivity equations derived from the equation set solved by the model.²¹ The sensitivity equations are then solved in conjunction with the model's system of equations to obtain the sensitivities. Direct methods must be incorporated into the design of a fire model and are not often available for the already existing fire models.
- *Global methods*—produce sensitivity measures which are averaged over the entire range of input parameters. Global methods require knowledge of the probability density functions of the input parameters, which in the case of fire models, is generally unknown.

2.1 An example for a simple fire model

In 1985, Walton introduced ASET-B,⁴⁴ a BASIC program for personal computers based on the ASET mathematical model developed by Cooper and the ASET Fortran program written by Cooper and Stroup.⁴⁵ ASET-B is designed to simulate the development of a fire in a single room where any leakage from the room is assumed to occur near floor level. ASET-B is a single compartment, two-zone fire model with five input parameters and two time-dependent output variables. The relatively small size of this model makes the investigation of sensitivity analysis methods tractable.

2.1.1 ASET equations

The quantities estimated by ASET-B are the interface height (the height above the floor at which the upper layer of hot gases meets the lower layer of relatively cool air) and the average upper-layer temperature. The ASET equations derived by Cooper⁴ and used by ASET-B are defined in terms of a dimensionless time, τ , upper-layer temperature, ϕ , layer interface position, ζ , and heat release rate, \dot{q} , as follows:

$$\frac{d\zeta}{d\tau} = f_1(\zeta, \phi, c_1, c_2, \tau) = \begin{cases} -c_1\dot{q} - c_2\dot{q}^{1/3}\zeta^{5/3}, & 0 < \zeta \leq \zeta_0 \\ -c_1\dot{q}, & -\delta < \zeta \leq 0 \\ 0, & \zeta = -\delta \end{cases} \quad (2)$$

$$\frac{d\varphi}{d\tau} = f_2(\zeta, \varphi, c_1, c_2, \tau) = \begin{cases} \frac{\varphi(c_1\dot{q} - (\varphi - 1)c_2\dot{q}^{1/3}\zeta^{5/3})}{\zeta_0 - \zeta}, & 0 < \zeta < \zeta_0 \\ \frac{\varphi c_1\dot{q}}{\zeta_0 - \zeta}, & -\delta \leq \zeta \leq 0 \end{cases} \quad (3)$$

where the dimensionless variables are defined as $\tau = t/t_c$, $\zeta = Z_i/L_c$, $\varphi = T/T_a$, and $\dot{q} = \dot{Q}/\dot{Q}_0$. The constants c_1 and c_2 are defined as

$$c_1 = \frac{(1 - \lambda_c)\dot{Q}_0 t_c}{A L_c \rho_a c_p T_a} \quad \text{and} \quad c_2 = \frac{0.210 t_c}{A} \left(\frac{(1 - \lambda_r)\dot{Q}_0 g L_c^2}{\rho_a c_p T_a} \right)^{1/3}$$

For the purposes of this analysis, the initial conditions used by Cooper will be assumed, i.e.

$$\zeta_0 = \zeta(\tau = 0) = H - L_c, \quad \varphi(\tau = 0) = \varphi_0 = 1 + \frac{c_1}{c_2} \zeta_0^{5/3}$$

$$\lim_{\tau \rightarrow 0} \frac{d\varphi}{d\tau} = \frac{c_1 (2\dot{q}_0 \zeta_0 + 5(c_1 + c_2 \zeta_0^{5/3}))}{6c_2 \zeta_0^{8/3}} + o(\tau)$$

2.1.2 Sensitivity equations

Given a prediction by ASET-B of the upper-layer temperature, $\varphi(\tau_1)$, and the interface height, $\zeta(\tau_1)$, at time τ_1 , the following questions arise. If an input parameter is known with some degree of uncertainty, what degree of uncertainty will be associated with the outputs $\varphi(\tau_1)$ and $\zeta(\tau_1)$ or with the time to reach a particular upper-layer temperature or height? These types of questions can be addressed by performing a sensitivity analysis of the model. Since ASET-B is a simple system of ordinary differential equations, a direct method of sensitivity analysis can be applied. A decoupled direct method^{21,46} has been selected for illustration.

Sensitivity equations for the ordinary differential equation (ODE)

$$\frac{dz}{dt} = f(z, \omega, t) \quad (4)$$

can be derived by taking partial derivative of both sides of the ODE with respect to the desired parameter and using the chain rule for multi-variables. For the variable ω , we obtain

$$\frac{d}{dt} \left(\frac{\partial z}{\partial \omega} \right) = \frac{\partial f}{\partial \omega} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \omega} \quad (5)$$

Letting $S = \partial z / \partial \omega$, we then have an ODE for the sensitivity of the original eqn (4) to the parameter ω

$$\frac{dS}{d\tau} = \frac{\partial f}{\partial \omega} + \frac{\partial f}{\partial z} S \quad (6)$$

The sensitivity of the ASET eqns (2) and (3), to a parameter ω can be found in a similar way. In this study, we are interested in the parameters room surface area (A), height between the base of the fire and the ceiling ($H - \Delta$), and the conductive heat loss fraction λ_c . Rewriting eqns (2) and (3) in vector notation, we obtain

$$\frac{d}{d\tau} \begin{pmatrix} \zeta \\ \varphi \end{pmatrix} = \begin{pmatrix} f_1(\zeta, \varphi, c_1, c_2, \tau) \\ f_2(\zeta, \varphi, c_1, c_2, \tau) \end{pmatrix} \quad (7)$$

where f_1 and f_2 are defined previously. As before, take a partial derivative of both sides of eqn (7) with respect to ω and use the chain rule for multi-variables to obtain

$$\begin{aligned} \frac{d}{d\tau} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} &= \begin{pmatrix} \frac{\partial f_1}{\partial c_1} \frac{\partial c_1}{\partial \omega} + \frac{\partial f_1}{\partial c_2} \frac{\partial c_2}{\partial \omega} + \frac{\partial f_1}{\partial \zeta} \frac{\partial \zeta}{\partial \omega} + \frac{\partial f_1}{\partial \varphi} \frac{\partial \varphi}{\partial \omega} \\ \frac{\partial f_2}{\partial c_1} \frac{\partial c_1}{\partial \omega} + \frac{\partial f_2}{\partial c_2} \frac{\partial c_2}{\partial \omega} + \frac{\partial f_2}{\partial \zeta} \frac{\partial \zeta}{\partial \omega} + \frac{\partial f_2}{\partial \varphi} \frac{\partial \varphi}{\partial \omega} \end{pmatrix} \\ &= Bc + J \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} \\ &= Bc + JS \end{aligned} \quad (8)$$

where $S = (S_i)$. $S_1 = \partial \zeta / \partial \omega$, and $S_2 = \partial \varphi / \partial \omega$ are the sensitivities of ζ and φ with respect to ω . In addition,

$$B = \begin{pmatrix} \frac{\partial f_1}{\partial c_1} & \frac{\partial f_1}{\partial c_2} \\ \frac{\partial f_2}{\partial c_1} & \frac{\partial f_2}{\partial c_2} \end{pmatrix}, \quad J = \begin{pmatrix} \frac{\partial f_1}{\partial \zeta} & \frac{\partial f_1}{\partial \varphi} \\ \frac{\partial f_2}{\partial \zeta} & \frac{\partial f_2}{\partial \varphi} \end{pmatrix} \quad \text{and} \quad c = \begin{pmatrix} \frac{\partial c_1}{\partial \omega} \\ \frac{\partial c_2}{\partial \omega} \end{pmatrix} \quad (9)$$

The sensitivity equations for room surface area, A , for the range $0 < \zeta \leq \zeta_0$ is given by replacing ω with A in eqns (8) and (9) using the following definitions for B , J , and c with terms derived from the ASET eqns (2) and (3) with initial

conditions $S_1(\tau) = 0$ and $S_2(\tau) = 0$:

$$B = \begin{bmatrix} -\dot{q} & \frac{\dot{q}\varphi}{\zeta_0 - \varphi} \\ -\dot{q}^{1/3}\zeta^{5/3} & -\varphi \frac{(\varphi - 1)\dot{q}^{1/3}\zeta^{5/3}}{\zeta_0 - \zeta} \end{bmatrix}$$

$$J = \begin{bmatrix} -\frac{5c_2\zeta^{2/3}\dot{q}^{1/3}}{3} & -\frac{5\varphi(\varphi - 1)c_2\dot{q}^{1/3}\zeta^{2/3}}{3(\zeta_0 - \zeta)} + \frac{\varphi(c_1\dot{q} - (\varphi - 1)c_2\dot{q}^{1/3}\zeta^{5/3})}{(\zeta_0 - \zeta)^2} \\ 0 & \frac{c_1\dot{q} - (2\varphi - 1)c_2\dot{q}^{1/3}\zeta^{5/3}}{\zeta_0 - \zeta} \end{bmatrix} \quad (10)$$

$$c = \begin{bmatrix} -\frac{(1 - \lambda_c)\dot{Q}_0 t_c}{A^2 c_p \rho_a T_a L_c} \\ -\left(\frac{0.21 t_c}{A^2}\right) \left(\frac{(1 - \lambda_r)\dot{Q}_0 g L_c^2}{c_a \rho_a T_a}\right)^{1/3} \end{bmatrix}$$

The sensitivity differential equations for the other parameters can be done in an analogous manner. Note that the matrix J , the Jacobian of (f_1, f_2) with respect to the solution variables ζ and φ , remains the same for all of the sensitivity equations.

2.1.3 Solution procedure of the sensitivity equations

If we let $X(\tau_n)$ and $Y(\tau_n)$ represent the discretization of $\zeta(\tau_n)$ and $\varphi(\tau_n)$, respectively, and use the trapezoidal rule to approximate eqns (2) and (3), we obtain

$$X(\tau_n) = X(\tau_{n-1}) + \frac{(f_1(X(\tau_{n-1}), Y(\tau_{n-1}), c_1, c_2, \tau_{n-1}) + f_1(X(\tau_n), Y(\tau_n), c_1, c_2, \tau_n))(\tau_n - \tau_{n-1}))}{2} \quad (11)$$

$$Y(\tau_n) = Y(\tau_{n-1}) + \frac{(f_2(X(\tau_{n-1}), Y(\tau_{n-1}), c_1, c_2, \tau_{n-1}) + f_2(X(\tau_n), Y(\tau_n), c_1, c_2, \tau_n))(\tau_n - \tau_{n-1}))}{2} \quad (12)$$

Differentiating eqns (11) and (12) with respect to the room-surface area puts the sensitivity equation in finite-difference form:

$$\begin{aligned} \left(I - \frac{\tau_n - \tau_{n-1}}{2} J(\tau_n) \right) S(\tau_n) = & \left(I + \frac{\tau_n - \tau_{n-1}}{2} J(\tau_{n-1}) \right) S(\tau_{n-1}) \\ & + \frac{\tau_n - \tau_{n-1}}{2} \left(\frac{\partial}{\partial A} f(X(\tau_{n-1}), Y(\tau_{n-1}), c_1, c_2, \tau) + \frac{\partial}{\partial A} f(X(\tau_n), Y(\tau_n), c_1, c_2, \tau) \right) \end{aligned} \quad (13)$$

where $J(\tau_n)$ is the Jacobian of the original system of equations which is given as matrix J of eqn (10). Analogous equations can be developed for each of the ASET variables and the sensitivities, $S(\tau_n)$, solved using matrix techniques. The solution $S(\tau_n)$ represents the exact sensitivities of $X(\tau_n)$ and $Y(\tau_n)$, disregarding round-off and truncation errors, and an approximation to the sensitivities of $\zeta(\tau_n)$ and $\varphi(\tau_n)$.

In the decoupled direct method, the sensitivity coefficients are computed by solving eqns (11) and (12) at a particular time and then solving eqn (13) for that time. Specifically, given $X(\tau_{n-1})$ and $Y(\tau_{n-1})$ the values of $X(\tau_n)$ and $Y(\tau_n)$ are calculated using ASET-B. These values are then used in computing $S(\tau_n)$. Once $S(\tau_n)$ is computed, the time is advanced from τ_{n-1} to τ_n and the process is repeated.

For the ASET-B model, a factorial design (see, for example, Box *et al.*²⁴) was applied for the above sensitivity analysis in which area took on the values 8.9 and 26.8 m² (96 and 288 ft²), λ_c took on the values 0.6, 0.7, 0.8, and 0.9 and the height above the fire, H , took on the values 2.1 and 4.3 m (7 and 14 ft). The height of the fire measured from the floor, Δ , was set at 0.3 m (1 ft) and λ_r was fixed at 0.35. The energy release rate was 1 kW for the time period from 0 to 180 s and 25 kW from 180 to 1200 s. All other parameters were held at their nominal levels. When each run was made, the sensitivity measures were computed assuming a $\pm 10\%$ perturbation in each of the following parameters, floor area, λ_c , and height above the fire. Each run was terminated when the interface height had reached the floor and the upper-layer temperature had reached 100°C. Figure 2 presents the change in interface height resulting from a 10% change in floor area, λ_c , and height above the fire for the range of inputs above. From numerous plots made to study the effects of perturbations in the inputs on the interface height, upper-layer temperature and time to reach a particular height or temperature, an overall picture of the sensitivity of the ASET model can be obtained (Table 1).

ASET-B is fairly insensitive to the uncertainty in the room area and height above the fire, but can be quite sensitive to the uncertainty in the value of λ_c . Since the objective of ASET is to be able to determine the available safe egress

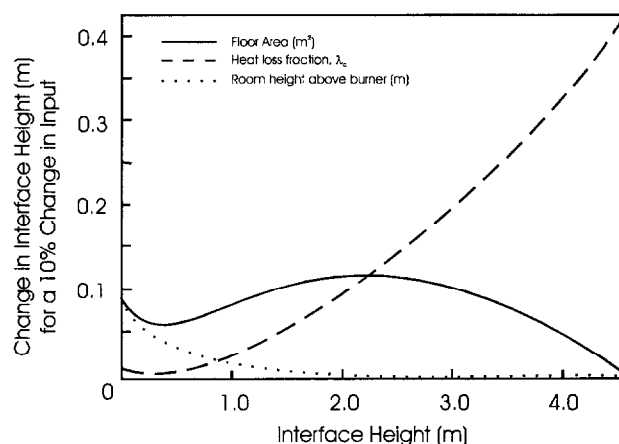


Fig. 2. Example of calculated sensitivity values for the ASET-B model.

time, conservative values of λ_c can be selected according to whether time of detection or time of hazardous conditions is desired. As Cooper⁴ suggests, select λ_c near 0.6 to obtain a conservative estimate of the time until hazardous conditions occur and 0.9 to obtain a conservative estimate of the time until detection (by occupants or detectors) occurs because the temperatures rise more quickly with smaller conductive losses (as λ_c becomes smaller). In general, if λ_c is thought to be within $x\%$ of λ , then choose λ_c to be $(1 - x/100)\lambda$ for a conservative estimate of the time of hazardous conditions and $(1 + x/100)\lambda$ for a conservative estimate of the time until detection.

The decoupled direct method seems to provide reasonable error bands on the ASET-B solution given a 10% change in area, λ_c , or height above the fire and also can provide error bands on the time to reach a particular temperature or height. The cost to provide these error bands is that of deriving the sensitivity equations and solving a matrix equation. For ASET-B, this effort was small compared to the information provided. For other models, it may be too difficult and complicated to derive the sensitivity differential equations

TABLE 1
Relative Range of Change in Outputs for a $\pm 10\%$ Change in Inputs to the ASET-B Model

$\downarrow \pm 10\%$ inputs/outputs \rightarrow	Interface height	Upper-layer temperature
$\pm 10\%$ room area	+2 to +5%	+10%
$\pm 10\%$ height above the fire	0 to +10%	-10 to -8%
$\pm 10\% \lambda_c$	+2 to +5%	-12 to -75%

analytically; however, it may be reasonable to compute the Jacobian of the function f and the partial derivatives of f with respect to the parameters numerically.

For a model even as simple as ASET-B, the evaluation of sensitivity adds considerably to the complexity of the solution. With more complex models, the task can become unmanageable. Thus, evaluation of sensitivity for specific sets of inputs (pointwise evaluation) becomes necessary. The remainder of this paper discusses the issues involved in such evaluations.

2.2 Sensitivity analysis for more complex fire models

For more complex fire models, obtaining an overall assessment of model sensitivity may become overly complex with numerous model inputs and outputs. Thus, more directed local sensitivity investigations are appropriate. Local methods produce sensitivity measures at a particular point of the parameter space of the model. There are several classes of local methods which are of interest. Using the nomenclature of eqn (1), these are outlined below.

- Finite-difference methods provide estimates of sensitivity functions by approximating the partial derivatives of an output z_i with respect to an input p_i as finite differences:

$$\frac{\partial z_j}{\partial p_m} = \frac{z_j(p_1, p_2, \dots, p_m + \Delta p_m, \dots, p_k) - z_j(p_1, p_2, \dots, p_m, \dots, p_k)}{\Delta p_m},$$

$$j = 1, 2, \dots, n, \quad m = 1, 2, \dots, k \quad (14)$$

This method is easy and straightforward to implement. However, as with any finite-difference method, the choice of Δp_m is pivotal in obtaining good estimates. To determine the $n \cdot k$ first-order sensitivity equations requires $k + 1$ runs of the model. These may be run simultaneously as a larger system or in parallel.

- Direct methods derive the sensitivity differential equations from the model's system of ordinary differential equations

$$\frac{d}{dt} \frac{\partial z_j}{\partial p_m} = \frac{\partial f_j}{\partial p_m} + \sum_i \frac{\partial f_j}{\partial z_i} \frac{\partial z_i}{\partial p_m}, \quad j = 1, 2, \dots, n, \quad m = 1, 2, \dots, k \quad (15)$$

These equations are then solved in conjunction with the model's system of differential equations to obtain the sensitivities. To compute the $n \cdot k$ first-order sensitivities requires 1 model run. These may be incorporated directly into the model and solved as a single, coupled set of $n + (n \cdot k)$ differential equations⁴⁷ or decoupled solving the model equations and the sensitivity equations iteratively using the model's solution and an

appropriate interpolation scheme.⁴⁶ This method was applied to the ASET earlier in this paper.

- Response surface methods fit an appropriate set of functions to selected model runs. The resulting functions are then assumed to behave in the same manner as the model. With appropriate choice for the set of functions (such that the sensitivity functions are easily calculable), the analysis of the behavior of the model is facilitated.

Even though it is possible to define the sensitivities and establish various methods for their computation, there are still difficulties associated with performing a sensitivity analysis. Iman and Helton²² note some of the properties of complex computer models which make analysis difficult:

- There are many input and output variables.
- The model is time consuming to run on a computer.
- Alterations to the model are difficult and time-consuming.
- It is difficult to reduce the model to a single system of equations.
- Discontinuities may exist in the behavior of the model.
- Correlations may exist among the input variables and the associated marginal probability distributions are often nonnormal.
- Model predictions are nonlinear, multivariate, time-dependent functions of the input variables.
- The relative importance of individual input variables is a function of time.

Many of these comments are applicable to current room fire models. In addition, the sensitivity equations have similar properties. For a given model output and a given model input, there may be regions of time where the model output is sensitive to the input and also regions where the model output is insensitive to the same parameter.

2.2.1 *Selecting inputs and outputs for sensitivity analysis*

At least two broad questions can be addressed with a sensitivity analysis of a fire model. First, the more general question, 'How sensitive is the model to a specific input?' is an attempt to gain an overall appreciation of the importance of an input relative to all other inputs. For this question, the range of model inputs could be chosen as broad as possible representing the range of applicability of the model. A subsequent analysis of model outputs for such broad changes would then provide insight into the relative importance of a given input variable on selected outputs. Such an analysis provides an overall picture of model behavior.

The second question, 'How closely must a specific input be specified?' is more focused than the first question. Rather than understanding the overall

behavior of the model, it is an effort to obtain an understanding of the effect on the model outputs of uncertainties in selected inputs. For this question, small perturbations in the inputs could be examined. If a specific scenario is of interest, perturbations of the inputs for this scenario could be examined.

For either question, several topics are of interest:

- What input and output variables are of interest?
- How should specific models runs be selected to study these variables?
- How can the results be quantified?

2.2.2 Model inputs and outputs

Current zone-type fire models have numerous inputs (Table 2) and outputs (Table 3) which may be of interest in a sensitivity analysis. The inputs and outputs for the CFAST model are typical of a complex zone-based room fire model.

Most studies of modeling related to fire hazard and fire reconstruction present a consistent set of variables of interest to the model user,^{34, 38–40} gas temperature, gas species concentrations, and layer interface position. To assess the accuracy of the physical basis of the models, additional variables must be included. Pressure drives the movement of gases through openings. The pyrolysis rate, and heat release rate of the fire in turn, produces the gases

TABLE 2
Typical Inputs for a Two-Zone Fire Model

Ambient conditions	Inside temperature and pressure Outside temperature and pressure Wind speed Relative humidity (0–100%)
Building geometry	Compartment width, depth, height , and surface material properties (conductivity, heat capacity, density, thickness) Horizontal flow vents: Height of soffit above floor, height of sill above floor, width of vent, angle of wind to vent, time history of vent openings and closings Vertical flow vents: Area of vent , shape of vent Mechanical ventilation, Orientation of vent, center height of vent, area of vent, length of ducts, diameter of ducts, duct roughness, duct flow coefficients, fan flow characteristics
Fire specification	Fire room, X, Y, Z position in room, fire area Fire chemistry: Molar weight, lower oxygen limit, heat of combustion, initial fuel temperature, gaseous ignition temperature, radiative fraction Fire history: Mass loss rate, heat release rate , species yields for HCN, HCl, Ct, H/C, O₂/C, C/CO₂, CO/CO₂

Items in bold are inputs that may vary due to error in measurements.

TABLE 3
Typical Outputs for a Two-Zone Fire Model

Compartment Environment	For each compartment	Compartment pressure and layer interface height
	For each layer and compartment	Temperature, layer mass density, layer volume, heat release rate, gas concentrations (N_2 , O_2 , CO_2 , CO , H_2O , HCl , HCN , soot optical density), radiative heat into layer, convective heat into layer, heat release rate in layer
	For each vent and layer	Mass flow, entrainment, vent jet fire
	For each fire	Heat release rate of fire, mass flow from plume to upper layer, plume entrainment, pyrolysis rate of fire
	For each compartment surface	Surface temperatures
Tenability		Temperature
		Fractional Exposure Dose (FED)

Values are typically time histories.

of interest to be moved. For sensitivity analysis it is appropriate to consider all these variables for evaluation:

- upper- and lower-layer gas temperature,
- layer interface position,
- gas-species concentration,
- fire pyrolysis and heat release rate,
- room pressure, and
- vent flow.

Although there are certainly other comparisons of interest, these will provide evidence of the sensitivity of the model to most model inputs.

2.2.3 *Selecting specific model simulations*

With a sensitivity analysis of any model, numerous scenarios must be tested with the model. Usually, this implies some sort of statistical design for the experiments to be conducted. Techniques are readily available^{23,28} which can be used to select appropriate sets of model inputs and which have been applied to the analysis of fire models. With current computer capabilities, the efficiency of a particular design may not be as important as it has been in the past as considerably more model simulations can be conducted within a reasonable time frame.

Efficient choice of model inputs and outputs is further complicated by functional dependencies and redundancy in model inputs and outputs. For

example, suppose two parameters, say a and b , occur in an unsimplified form of a model, always as the product $a \cdot b$. Comparing outputs of calculations which double the parameter a while halving the parameter b will produce the same result as the base case in which both are unchanged. For example, Cooper⁴ simplified the ASET model from 12-dimensional physical parameters to four dimensionless parameters. In addition, even these can be further simplified to only two dimensionless groups.⁴² Choice of inputs to vary such a set of core parameters over the entire range of applicability of the inputs provides for a more complete assessment of the model's behavior.

2.2.4 Calculating and interpreting sensitivity functions for a complex fire model

In this section, some examples of model sensitivity are presented using the CFAST model¹⁵ for the simulations. Although numerous scenarios could be chosen for study, a single one was used in this paper to illustrate the analysis of a complex fire model. To obtain a complete picture of a model's sensitivity, a number of scenarios representing the entire range of the model would have to be studied. The scenario chosen includes a range of phenomena which can be simulated with this model. The building geometry (Fig. 3) includes four rooms on two floors with horizontal, vertical, and mechanical vents connecting the rooms and venting to the outdoors. The fire source in one of the rooms on the lower floor is a medium growth rate t^2 fire⁴⁸ chosen to simulate a mattress fire⁴⁹ (Fig. 4).

2.2.5 Sensitivity to small changes in model inputs

To investigate the sensitivity of the model, a number of simulations were conducted varying the input parameters for CFAST about this base scenario. Both small ($\pm 10\%$) and larger (up to an order of magnitude) variations for selected inputs were studied. Varying most of the inputs by small amounts had

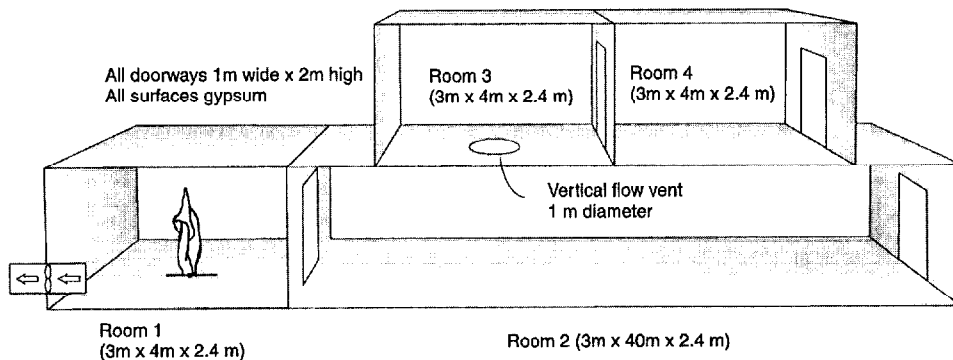


Fig. 3. Building geometry for base case scenario.

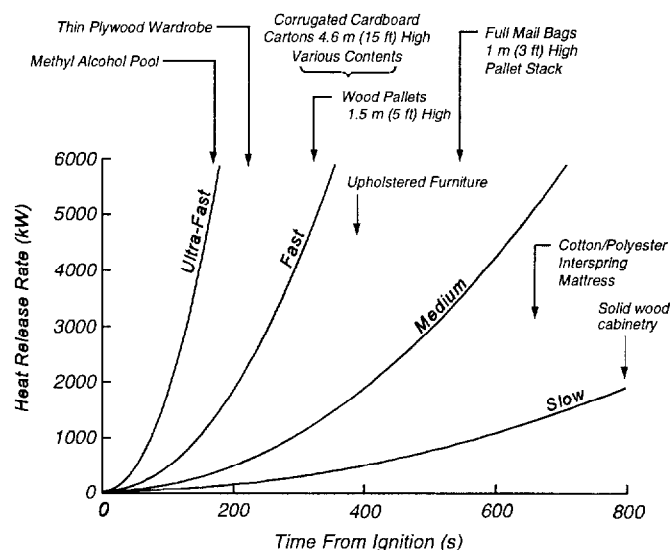


Fig. 4. Characterization of heat release rate of growing fires as t^2 fires

little effect on the model outputs. Figure 5 presents an example of the time-dependent sensitivity of several outputs to a 10% change in room volume for the fire compartment in the scenario described above. For example, the pair of dotted-line curves labeled 'Upper-layer volume' were created by comparing the base-case scenario with a scenario whose compartment volume was increased and decreased by 10%. The resulting curves presented on the graph are the relative difference between the variant cases and the base case defined by $(\text{variant value} - \text{base value})/\text{base value}$ for each time point. The graph shows that temperature and pressure are insensitive to changes in the volume of the fire room since the 10% change in room volume led to smaller relative changes in layer temperature and room pressure for all times. Upper-layer volume can be considered neutrally sensitive (a 10% change in room volume led to about a 10% change in layer volume). Further, this implies that there is negligible effect on layer interface height. This is consistent with both experimental observations in open-compartment room fires⁵⁰ and analytical solutions for single-compartment steady-state fires.⁵¹ In essence, this implies that reasonable uncertainties in room dimensions would have little effect on the results predicted by the model for this scenario.

In addition, Fig. 5 shows a somewhat constant relative difference for the changes as a function of time. As suggested by Iman and Helton,²⁵ an average relative difference could thus be used to characterize the model sensitivity for comparing individual inputs and outputs.

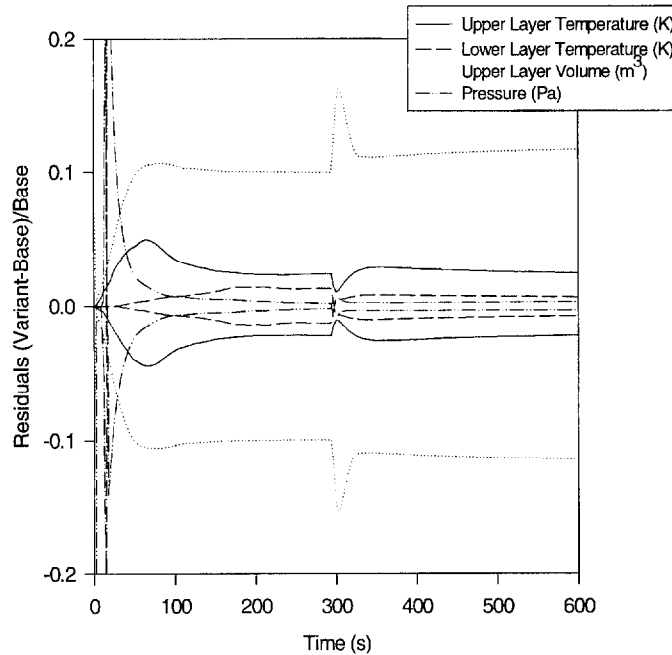


Fig. 5. An example of time dependent sensitivity of fire model outputs to a 10% change in room volume for the fire compartment.

2.2.6 Sensitivity to larger changes in model inputs

To investigate the effects of much larger changes in the inputs, a series of simulations where the inputs were varied from 0.1 to 4.0 times the base value was conducted. Simulations by changing the heat release rate (*HRR*) inputs are shown in Fig. 6. Each set appears as families of curves with similar functional forms. This indicates that multiples of the *HRR* have a simple monotonic effect on the layer temperatures. Again, it may be possible to describe the sensitivity with a single characteristic number. The choice of heat release is particularly interesting since it appears to be one of the inputs to the model which has a greater effect on the model outputs than other inputs. In the majority of fire cases, the most crucial question that can be asked by the person responsible for fire protection is: 'How big is the fire?' Put in quantitative terms, this translates to: 'What is the *HRR* of this fire?' Recently, the National Institute of Standards and Technology (NIST) examined the pivotal nature of *HRR* measurements in detail.⁵² Not only is *HRR* seen as the key indicator of real-scale fire performance of a material or construction, *HRR* is, in fact, the single most important variable in characterizing the 'flammability' of products and their consequent fire hazard. Much of the remainder of this paper focuses on *HRR* as an example for examining sensitivity analysis.

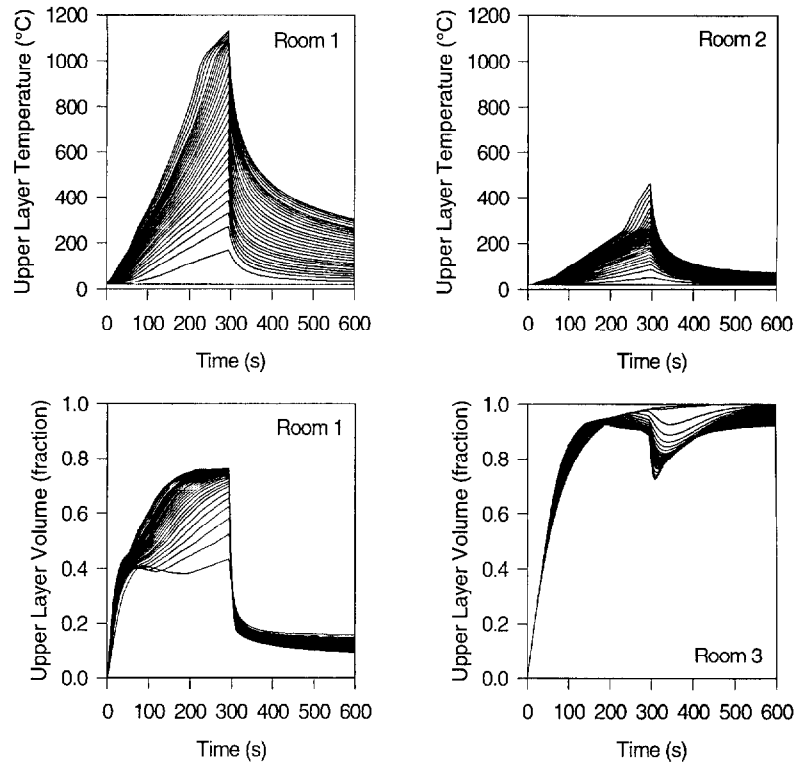


Fig. 6. Layer temperatures and volumes in several rooms resulting from variation in heat release rate for a four-room growing fire scenario.

2.2.7 Simple ‘response-surface’ correlations

A next step beyond the simple time-history plots presented in Fig. 6 is a cross-plot of outputs of interest. Figure 7 presents plots of the upper (presented in Fig. 6) and lower-layer temperatures plotted against the heat release rate for the simulations shown in Fig. 6. The shaded areas in Fig. 7 show the locus of all the individual data points (the layer temperature at time t of a particular simulation plotted against the HRR at the same t). For this example, only the data up to the time the fires became oxygen-limited were included—the latter data would complicate the functional relationship between HRR and layer temperature unnecessarily for this sample presentation. For each room, a regression fit to the data for each room overlays the locus. For the simple geometry and fire in this example, the curves for both upper- and lower-layer temperature in all four rooms (Fig. 7) show a strong functional dependence on HRR . Even for the wide variation in inputs, the HRR provides a simple predictor of the temperature in the rooms. In addition, this relationship allows calculation of the sensitivity of the temperature outputs to the HRR inputs as

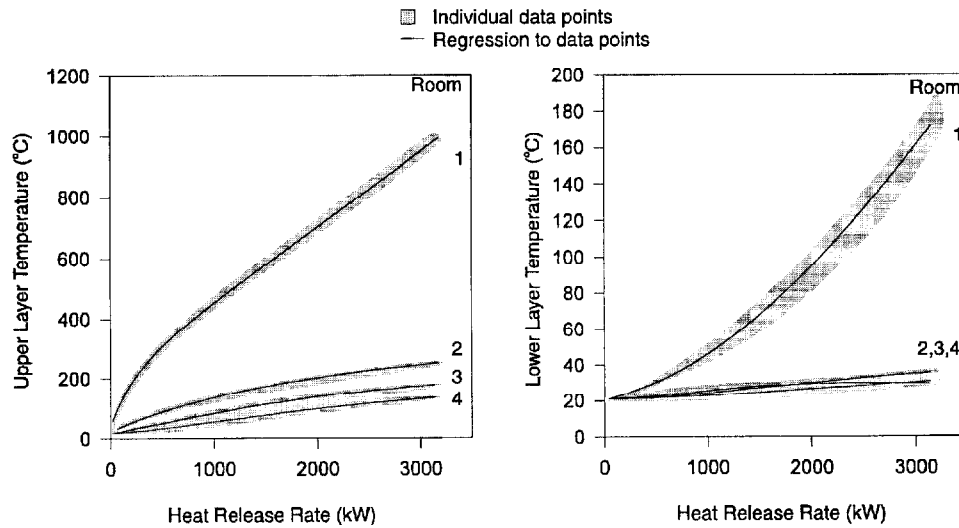


Fig. 7. Upper- and lower-layer temperature in rooms.

a simple slope of the resulting correlation between HRR and temperature. Similar analysis could be applied to the oxygen-limited burning period or other model outputs of interest.

Figure 8, simply a plot of the slope of the curves in Fig. 7, shows this sensitivity, $\partial(T)/\partial(HRR)$, for the four-room scenarios studied and represents

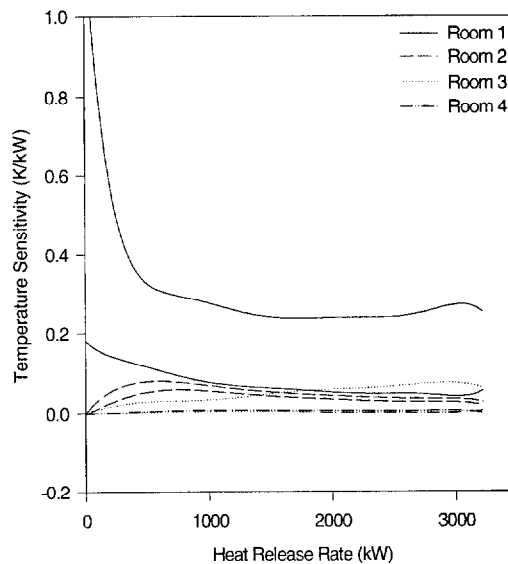


Fig. 8. Sensitivity of temperature to heat release rate for a four-room growing fire scenario.

all time points in all the simulations in which the peak *HRR* was varied from 0.1 to 4.0 times the base value. Except for relatively low *HRR*, the upper-layer-temperature sensitivity is less than 1 K/kW and usually below 0.2 K/kW. Not surprisingly, the layer that the fire feeds directly is most sensitive to changes. The lower layer in the fire room and all layers in other rooms have sensitivities less than 0.2 K/kW. This implies, for example, that if the *HRR* for a 1 MW fire is known to within 100 kW, the resulting uncertainty in the calculation of upper-layer temperature in the fire room is about ± 30 K.

For upper-layer volumes (Fig. 9) of both rooms 1 and 2, it is again a simple correlation between *HRR* and volume fraction (upper-layer volume expressed as a fraction of the total-room volume). The correlations for the upper-layer volumes of rooms 1 and 2 could also be differentiated as was done for the temperature correlations to obtain sensitivities for the upper-layer volume. For rooms 3 and 4, the relationship is not as clear. The flow into the layers of these rooms is more complicated than for rooms 1 and 2, resulting from flow from the first floor through a vent in the floor of room 3 and from a vent to the outside in room 4. However, even these rooms approach a constant value for higher *HRR* values, implying near zero sensitivity for high *HRR*.

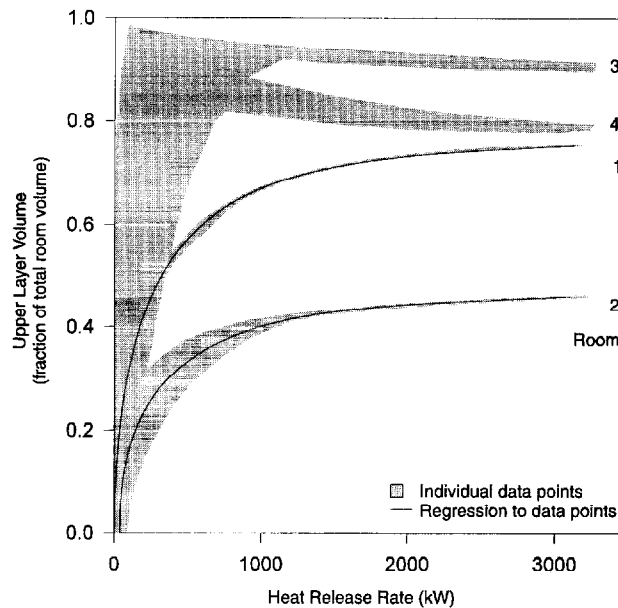


Fig. 9. Comparison of heat release rate and upper-layer volume in several rooms for a four-room growing fire scenario.

2.2.8 Evaluating sensitivity by single values

Many phenomena of interest in fire modeling are transient events that are best represented as time-history curves. Examples are *HRR*, gas temperature, smoke density, and CO concentration. To evaluate the sensitivity of multiple outputs, it would be desirable to have a single number to characterize each output. For the example scenario used in this paper, several choices are available. From Fig. 5, an average relative difference could be used. From Fig. 8, the average sensitivity calculated from a simpler model (in this case, a simple correlation) could be used. Other possibilities include time to critical events (for example, flashover), average value, or peak value. Figure 10 shows the peak *HRR* and peak upper-layer temperature normalized relative to the values at corresponding times from the base scenario for the base scenario and $\pm 50\%$ of the base *HRR*.

Although there is some scatter in the data, most of this comes at early times in the fire. From Fig. 10, this is apparent by choosing a single temperature. For ease of discussion and obvious interest, we will focus on peak values for *HRR* and temperature.

Figure 11 presents the effect of both peak *HRR* and vent opening (in the fire room) on the peak upper-layer temperature. In this figure, actual model

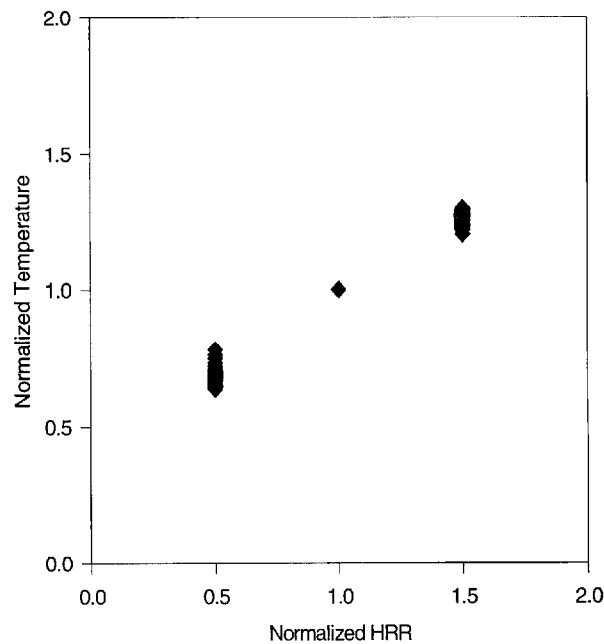


Fig. 10. Comparison of normalized peak temperature to normalized heat release rate for a series of four-room growing fire scenarios.

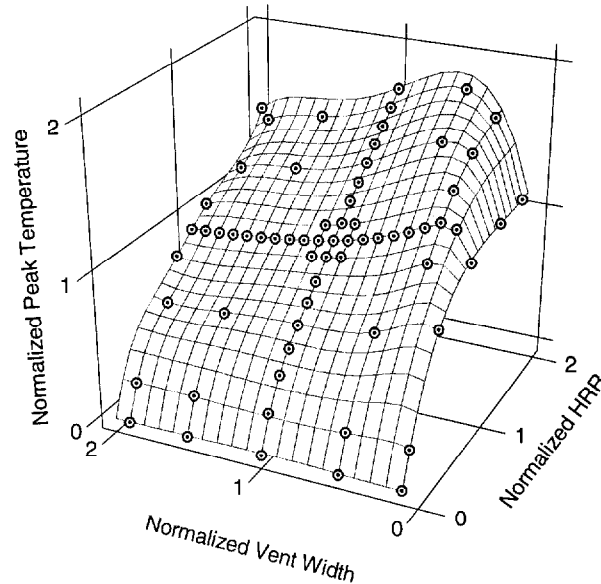


Fig. 11. Effect of both heat release rate and vent opening size on upper-layer temperature for a four-room growing fire scenario.

calculations, normalized to the base scenario values are indicated by circles overlaid on a surface grid generated by a spline interpolation between the data points. At high *HRR* and small vent openings, the fire becomes oxygen-limited and the temperature trails off accordingly, but for the most part, the behavior of the model is monotonic in nature. Although more laborious, the approaches used to calculate sensitivities for single-variable dependencies illustrated earlier are thus equally applicable to multivariate analyses.

From the surface, it is clear that *HRR* has more of an effect on the peak temperature than does the vent width. Until the fire becomes oxygen-limited, the trends evident in the surface are consistent with expectations—temperature goes up with rising *HRR* and down with rising vent width. The effects are not, of course, linear with either *HRR* or vent opening. Plume theory and typically used calculations for estimating upper-layer temperature in a single room with a fire^{53,54} suggest that the dependence is of the order of $\dot{q}^{2/3}$ for *HRR* and $A\sqrt{h}$ for the vent opening where *A* is the area of the vent and *h* is the height of the vent. Although these correlations are based on a simple analysis of a single-room fire, the dependence suggested is similar to that illustrated in Fig. 11.

3 COMPARISON WITH EXPERIMENTAL MEASUREMENTS

Several researchers have studied the level of agreement between computer fire models and real-scale fires¹. These range from comparisons using simple correlations⁵⁵ to intricate field models². The comparisons made to date are mostly qualitative in nature. The level of agreement between the models and experiment is typically reported as 'favorable', 'satisfactory', 'well predicted', 'successful', or 'reasonable'. This section provides an overview of some comparisons made as part of a program to better understand the evaluation process in concert with research to provide a level of quantification to the comparisons.

3.1 Prediction of flashover

A number of simple correlations and the CFAST model were used to simulate a range of geometries and fire conditions to predict the development of the fire up to the point of flashover. The simulation represent a range of compartment sizes from 8 to 1327 m³, with ceiling height varying from 2.4 to 12.2 m and vent openings from 10 to 100% of the length of the short wall (plus a 'standard' door, 0.76 m in width). For most of the simulations, the surface-lining material was gypsum wallboard, 12.7 mm in thickness, consistent with the values used in the correlations. A simple constant fire size was varied until the calculated upper-layer temperature reached 600°C at the end of the simulation. For some simulations, the surface linings ranged from aluminum to a highly insulating foam and the fire source diverged from the simple steady-state fire to more complex shapes.

The important test of all these prediction methods is in the comparison of the predictions with actual fire observations. Figure 12 presents estimates of the minimum energy required to achieve flashover for a range of room and vent sizes. This figure is an extension of the earlier work of Babrauskas⁵⁴ and includes additional experimental measurements from a variety of sources, most notably the work of Deal and Beyler.⁵⁵ In addition, it includes predictions from the CFAST model.

As with some of the experimental data defining flashover as an upper-layer temperature reaching 600°C, many experimental measures were reported as peak values rather than minimum values necessary to achieve flashover. Thus, ideally all the predictions should provide a lower bound for the experimental data. Indeed, this is consistent with the graph—the vast majority of the experimental observations lie above the correlations and model predictions. For a considerable range in the ratio $A_T/A\sqrt{h}$, the correlations of Babrauskas,⁵⁴ Thomas,⁵⁶ and McCaffrey et al.⁵³ provide nearly identical estimates of the minimum energy required to produce flashover. The estimates of

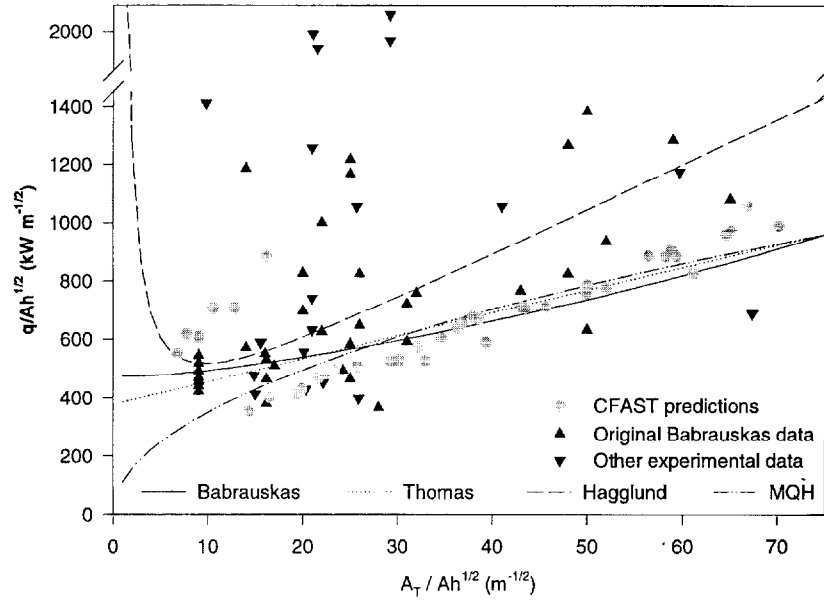


Fig. 12. Comparison of correlations, CFAST predictions, and experimental data for the prediction of flashover in a compartment fire.

Hägglund⁵⁷ yield somewhat higher estimates for values of $A_T/A\sqrt{h}$ greater than 20.

The results from the CFAST model for this single-compartment scenario provide similar results to the experiments and the correlations for most of the range of $A_T/A\sqrt{h}$. For small values of $A_T/A\sqrt{h}$, the CFAST values rise somewhat above the values from the correlations. These small values of $A_T/A\sqrt{h}$ result from either very small compartments (small A_T) or very large openings (large $A\sqrt{h}$), both of which stretch the limits of the assumptions inherent in the model. For very small compartments, radiation from the fire to the compartment surfaces becomes more important, enhancing the conductive heat losses through the walls. However, the basic two-zone assumption may break down as the room becomes very small. For very large openings, the calculation of vent flow via an orifice flow coefficient approach is likely inaccurate. Indeed, for such openings, this limitation has been observed experimentally.⁵⁴ Still, the estimates are close to the ranges provided by the correlations which also diverge at very small values of $A_T/A\sqrt{h}$.

Perhaps most significant in these comparisons is that all the simple correlations provide estimates similar to the CFAST model and all the models are consistent with a wide range of experimental data independent of the correlations. For this simple scenario, little is gained with the use of the more

complex models. For more complicated scenarios, the comparison may not be as simple.

3.2 Other comparisons

Arguably, the most frequent question asked about a fire is ‘How hot did it become’? Temperature in the rooms of a structure is an obvious indicator to answer this question. Peak temperature, time to peak temperature, or time to reach a chosen temperature tenability limit are typical values of interest. Papers by Peacock *et al.*¹ Beard,² Deal and Beyler,⁵⁵ and Reneke *et al.*⁵⁸ are illustrative.

Figure 13 shows a comparison of measured and predicted upper-layer temperature for several tests studied. For the single-room tests, predicted temperatures show obvious similarities to the measured values. Peak values occur at similar times with comparable rise and fall for most comparisons. Peak values are typically higher for upper-layer temperature and lower for lower-layer temperature and layer interface position. For all the tests, including the single-room tests, times for peak values and times for 100°C predicted by the model average within 25 s of experimentally measured values.

Systematic deviations exist for the remaining three data sets. Differences between model predictions and experimental measurements change monotonically over time (rising for the three-room test and falling for the four-rooms tests. Modeling of heat conduction (losing too much or too little heat to the surfaces) or lack of modeling of leakage (rooms are presumed perfectly sealed unless vents are included to simulate leakage) may account for the trends.

In general, upper-layer temperatures predicted by the model are higher than experimental measurements, with the differences ranging from -46 to 230°C . Conversely, the lower-layer temperature is somewhat lower for the model than for the experiments (-60 to 5°C). Presuming conservation of energy (an underlying assumption in *all* fire models), these observations are consistent. Limitations inherent in the model also account partially for these trends. In the current version of CFAST, energy exchange in the lower layer is *only* by mixing or convection from surfaces. Adding radiative exchange to the lower layer would reduce the upper-layer temperature and increase the lower-layer temperature. Layer interface position is primarily affected by entrainment by the fire or at vents. Underestimation of the conduction would also account for the effect. Plume entrainment in CFAST is based on the work of McCaffrey on circular plumes in relatively small spaces. For large fires in small spaces where the fire impinges on the ceiling (such as the single-room tests with wall burning) or very small fires in large spaces (such as atria), these correlations may not be as valid.

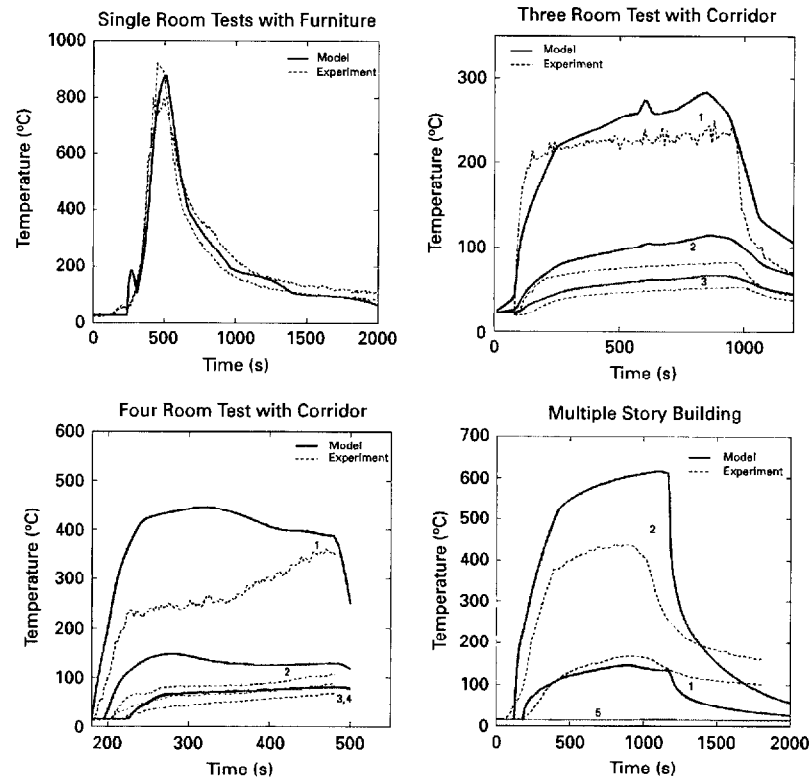


Fig. 13. Comparison of measured and predicted upper-layer temperatures for several tests. (Numbers indicate comparable rooms in the test structure.)

4 CONCLUSIONS

This paper has presented a number of alternatives for evaluating both simple and complex room fire models. For the models and test cases examined, heat release rate and heat transfer effects are the dominant factors in determining the behavior of the models. For simple models like the ASET model, analytical techniques can be readily applied. For more complex fire models, obtaining an overall assessment of model sensitivity increases with the complexity of the model, requiring evaluation of numerous model inputs and outputs. Thus, more directed local investigations are appropriate.

In the past, sensitivity analysis has been applied with limited success to fire models. In this paper, both analytical and numerical techniques were applied to obtain limited estimates of model sensitivity. Several areas which need additional research are apparent in order to be able to perform broader

analyses:

- *Presenting the results of a sensitivity analysis*—For a complex fire model with m inputs and n outputs, a complete sensitivity analysis will result in a matrix of $m \cdot n$ time series. It is unlikely that this much information will be of general use. It may be appropriate to develop threshold values for important outputs to alert the model user of particularly sensitive effects for a given test case.
- *Range of applicability for fire model inputs*—Little guidance is available in documentation for any of the current generation of room fire models on the range of applicability of the inputs to the models. For example, for different scenarios of interest, compartment size could range from small residential rooms to large industrial plants. Such information is important in order to obtain an overall picture of model performance and allow the models to be studied over the entire range of applicability.
- *Selecting specific model inputs for study*—With a sensitivity analysis of any model, numerous scenarios must be tested with the model. Although current computer capabilities allow far more simulations to be conducted than in earlier studies, the scope of room fire models continues to expand. Suitability of particular statistical designs to the selection of specific scenarios to be simulated should be included in future studies of fire model sensitivity.
- *Calculating sensitivity functions for a complex fire model*—In order to apply analytical techniques for sensitivity analysis of a complex fire model, the sensitivity equations need to be included in the equation set solved directly by the model. Even though it is desirable to obtain an overall picture of model performance, the broad range of application of current models demonstrates that whatever range of study is chosen, applications outside this envisioned range will continue to be of interest.

Comparisons of model predictions with experimental measurements to date have been largely subjective in nature. Areas of additional research which would address the need for more quantitative comparisons include the following.

- *Statistical treatment of the data*—Presentation of the differences between model predictions and experimental data in this paper are intentionally simple. With a significant base of data to study, appropriate statistical techniques to provide a true measure of the ‘goodness of fit’ should be investigated.
- *Experimental measurements*—Measurement of leakage rates, room pressure, or profiles of gas concentration are atypical in experimental data. These measurements are critical to assessing the accuracy of the

underlying physics of the models or of the models ability to predict toxic gas hazard.

- *Uncertainty*—Uncertainty in model predictions can be estimated by a sensitivity analysis. Estimation of uncertainty in experimental measurements by performing replicate experiments is uncommon in real-scale fire experiments. Such estimates for both model and experiment would place the resulting comparisons in better context.

REFERENCES

1. Peacock, R. D., Jones, W. W. & Bukowski, R. W., Verification of a model of fire and smoke transport. *Fire Safety J.*, **21** (1993) 89–129.
2. Beard, A., Evaluation of fire models: Part I—introduction. *Fire Safety J.* **19** (1992) 295–306.
3. Friedman, R., Survey of computer models for fire and smoke. *J. Fire Protection Engng.* **4** (1992) 81–92.
4. Cooper, L. Y., A mathematical model for estimating available safe egress time in fires. *Fire Mater.*, **6** (1982) 135–44.
5. Babrauskas, V., COMPF2—a program for calculating post-flashover fire temperatures. Natl. Bur. Stand. (US), Tech. Note 991, 1979, 76 pp.
6. Davis, W. D. & Cooper, L. Y., Computer model for estimating the response of sprinkler links to compartment fires with draft curtains and fusible link-actuated ceiling vents. *Fire Technol.* **27** (1991) 113–27.
7. Mitler, H. E. & Emmons, H. W., Documentation for CFCV, the fifth Harvard computer fire code. Nat. Bur. Stand. (US), NBS GCR 81-344, 1981, 187 pp.
8. Mitler, H. E. & Rockett, J., A user's guide for FIRST, a comprehensive single room fire model. Natl. Bur. Stand. (US), NBSIR 87-3595, 1987.
9. Tanaka, T., A model of multiroom fire spread. Nat. Bur. Stand. (US), NBSIR 83-2718, 1983, 175 pp.
10. Gahm, J. B., Computer fire code VI, vol. I. Nat. Bur. Stand. (US), NBS GCR 83-451, 1983, 116 pp.
11. Jones, W. W., A multicompartment model for the spread of fire, smoke and toxic gases, *Fire Safety J.*, **9** (1985) 55.
12. Jones, W. W. & Peacock, R. D., Refinement and experimental verification of a model for fire growth and smoke transport. In *Proc. 2nd Int. Symp. on Fire Safety Science*, Tokyo, 1989.
13. Jones, W. W. & Peacock, R. D., Technical reference guide for FAST version 18. Natl. Inst. Stand. Technol. Tech. Note 1262, 1989.
14. Forney, G. P. & Cooper, L. Y., The consolidated compartment fire model (CCFM) computer application CCFM. VENTS—Part II: software reference guide. Nat. Inst. Stand. Technol. NISTIR 90-4343, 1990.
15. Peacock, R. D., Forney, G. P., Reneke, P. A., Portier, R. W. & Jones, W. W., CFAST, the consolidated model of fire and smoke transport. Natl. Inst. Stand. Technol. Tech. Note 1299, 1993, 104 pp.
16. Mitler, H. E. Comparison of several compartment fire models: an interim report. Natl. Bur. Stand. (US), NBSIR 85-3233, 1985, 33 pp.

17. Jones, W. W., A review of compartment fire models. Natl. Bur. Stand. (US), NBSIR 83-2684, 1983, 41 pp.
18. Standard Guide for Evaluating the Predictive Capability of Fire Models, ASTM E 1355, Annual Book of ASTM Standards, Vol. 04.07. American Society for Testing and Materials, Philadelphia, 1995.
19. Standard Guide for Documenting Computer Software for Fire Models, ASTM E 1472, Annual Book of ASTM Standards, Vol. 04.07. American Society for Testing and Materials, Philadelphia, 1995.
20. Forney, G. P., & Moss, W. F., Analyzing and exploiting numerical characteristics of zone fire models. *Fire Sci. Technol.*, **14** (1994) 49–60.
21. Wierzbicki, A., *Models and Sensitivity of Control Systems*. Wiley, New York, 1984.
22. Clemson, B., Tang, Y., Pyne, J. & Unal, R., Efficient methods for sensitivity analysis. *System Dyn. Rev.*, **11** (1995) 31–49.
23. Khoudja, N., Procedures for quantitative sensitivity and performance validation of a deterministic fire safety model. Ph.D. Dissertation, Texas A&M University, Natl. Inst. Stand. Technol., NBS-GCR-88-544, 1988.
24. Box, G. E. P., Hunter, W. G. & Hunter, J. S., *Statistics for Experimenters, An Introduction to Design, Data Analysis and Model Building*. Wiley, New York, 1978.
25. Daniel, C., *Applications of Statistics to Industrial Experimentation*. Wiley, New York, 1976.
26. Iman, R. L. & Helton, J. C., An investigation of uncertainty and sensitivity analysis techniques for computer models. *Risk Analysis*, **8** (1988) 71–90.
27. Iman, R. L. & Conover, W. J., A distribution-free approach to inducing rank correlation among input variables. *Commun. Statist.* **B11** (1982) 331–4.
28. Iman, R. L. & Shortencarier, A FORTRAN 77 program and user's guide for the generation of Latin hypercube and random samples for use with computer models. NUREG/CR-3624, SAND83-2365, Sandia National Laboratories, Albuquerque, NM, 1984.
29. Ndubizu, C. C., Ramaker, D. E., Tatem, P. A. & Williams, F. W., The sensitivity of various physical parameters upon fire model predictions. In *Proc. Chemical and Physical Processes in Combustion*, 1982 Technical Meeting, The Eastern Section of the Combustion Institute, 14–16 December, Atlantic City, NJ 1982.
30. Nelson, H. E., An engineering view of the fire of May 4, 1988 in the first Interstate Bank Building, Los Angeles, California. Natl. Inst. Stand. Technol., NISTIR 89-4061, 1989, 39 pp.
31. Bukowski, R. W., Reconstruction of a fatal residential fire at Ft. Hood, Texas. In *Proc. 1st HAZARD I Users' Conf.*, National Institute of Standards and Technology, Gaithersburg, MD, 5–6 June 1990.
32. Bukowski, R. W., Analysis of the Happyland Social Club Fire With HAZARD I. *Fire Arson Investigator*, **42** (1992) 36–47.
33. Bukowski, R. W., Modeling a backdraft: the fire at 62 Watts Street. *NFPA J.*, **89** (1995) 85–9.
34. Emmons, H. W., Why fire model? The MGM fire and toxicity testing. *Fire Safety J.*, **13** (1988) 77–85.
35. Mitler, H. E. & Rockett, J. A., How accurate is mathematical fire modeling? Natl. Bur. Stand. (US), NBSIR 86-3459, 1986, 50 pp.
36. Rockett, J. A., Morita, M. & Cooper, L. Y., Comparisons of NBS/HARVARD VI simulations and data from all runs of a full-scale multi-room fire test program. *Fire Safety J.*, **15** (1989) 115–69.

37. Deal, S., A review of four compartment fires with four compartment fire models. In *Fire Safety Developments and Testing, Proc. Annual Meeting of the Fire Retardant Chemicals Association*, Ponte Verde Beach, FL, 21–24 October, 1990, pp. 33–51.
38. Nelson, H. E., FPETOOL: Fire protection engineering tools for hazard estimation. Natl. Inst. Stand. Technol., NISTIR 4380, 1990, 120 pp.
39. Duong, D. Q., The accuracy of computer fire models: some comparisons with experimental data from Australia. *Fire Safety J.*, **16** (1990) 415–31.
40. Beard, A., Evaluation of fire models: overview. Unit of Fire Safety Engineering, University of Edinburgh, Edinburgh, UK, 1990.
41. Cox, G. & Kumar, S., Field modeling of fire in forced ventilated enclosures. *Combust. Sci. Technol.*, **52** (1987) 7–23.
42. Jarvis, J. P., Kostreva, M. M. & Forney, C. L., Tools for validation and analysis of fire models, Combustion Institute/Eastern States Section. Chemical and Physical Processes in Combustion. 20th Fall Technical Meeting. Abstracts., Gaithersburg, MD, 2–5 November 1987, 103/1–4pp.
43. Forney, G. P. & Moss, W. F., Analyzing and exploiting numerical characteristics of zone fire models. Natl. Inst. Stand. Technol., NISTIR 4763, 1992.
44. Walton, W. D., ASET-B: A room fire program for personal computers. NBSIR 85-3144-1, 1985.
45. Cooper, L. Y. & Stroup, D. W. Calculating safe egress time (ASET)—a computer program and user's guide. NBSIR 82-2578, 1982.
46. Dunker, A. M., The decoupled direct method for calculating sensitivity coefficients in chemical kinetics. *J. Chem. Phys.*, **81** (1984) 2385–93.
47. Dickinson, R. P. & Gelinas, R. J., Sensitivity analysis of ordinary differential equation systems—a direct method. *J. Comput. Phys.*, **21** (1976) 123–43.
48. NFPA 72, National Fire Alarm Code, National Fire Protection Association, Quincy, Massachusetts, 1993.
49. Babrauskas, V. & Krasny J. F., Fire behavior of upholstered furniture. Natl. Bur. Stand. (US), Monograph 173, 1985.
50. Peacock, R. D., Davis, S. & Babrauskas, V., Data for room fire model comparisons. *J. Res. Natl. Inst. Stand. Technol.* **96** (1991) 411–62.
51. Drysdale, D., *An Introduction to Fire Dynamics*. Wiley, New York, 1985, p. 310.
52. Babrauskas, V. & Peacock, R. D., Heat release rate: The single most important variable in fire hazard. *Fire Safety J.*, **18** (1992) 255–72.
53. McCaffrey, B. J., Quintiere, J. G. & Harkleroad, M. F., Estimating room temperatures and the likelihood of flashover using fire tests data correlations. *Fire Technol.*, **17** (1981) 98–119.
54. Babrauskas, V., Upholstered furniture room fires—measurements, comparisons with furniture calorimeter data, and flashover predictions. *J. Fire Sci.*, **2** (1984) 5–19.
55. Deal, S. & Beyler, C., Correlating preflashover room fire temperatures. *J. Fire. Prot. Engng*, **2** (1990) 33–48.
56. Thomas, P. H., Testing products and materials for their contribution to flashover in rooms. *Fire Mater.*, **5** (1981) 103–11.
57. Häggglund, B., Estimating flashover potential in residential rooms. FOA Rapport C 20369-A3, Forsvarets Forskningsanstalt, Stockholm, 1980.
58. Reneke, P. A., Peatross, M. J., Jones, W. W., Beyler, C. L. & Richards, B., A Comparison of CFAST predictions to USCG real-scale fire tests, to be published.