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# EVALUATION OF COMPLEX FIRE MODELS

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## ABSTRACT

Several methods for studying predictive capability and sensitivity 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 evaluation of complex models from numerous computer runs of a model along with usually quantitative comparison to laboratory experiments. This paper presents a discussion of the issues involved in conducting an evaluation of a complex room fire model. Examples using currently available room fire models are presented.

Analytical models for predicting fire behavior have been evolving since the 1960's. 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 summary 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. Both of these discussion highlight the strengths and weaknesses of our current level of understanding of evaluation of complex fire models. More complete investigations are available[1,2].

## 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 important variables in the models,
- the computationally valid range of values for each input variable, and
- the sensitivity of output variables to variations in input data.

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 ASET[3] to pointwise evaluation of complex models from numerous computer runs of the model[4]. 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.

*Earlier efforts:* Khoudja[4] 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 Hunter[5], and Daniel[6] 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.

For a steady-state model of a liquid pool fire, Ndubizu[7], et. al. 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.

The ASTM guide for evaluating the predictive capability of fire models[8] identifies model sensitivity analysis as an important part of model evaluation and identifies two methods which may be applied to perform a sensitivity analysis – a partial differential method and a response surface method. Further details are left to other sources.

*Application to a current fire model:* Fire growth models are typically based on a system of ordinary differential equations of the form

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

where z $(z_1, z_2, ..., z_m)$ is the solution vector for the system of equations (for example, mass, temperature, or volume) and p $(p_1, p_2, ... p_n)$ is a vector of input parameters (for example, room area, room height, heat release rate) and $\tau$ is time[9]. 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,...,m and I=1,...,n) are examined.

Although numerous scenarios could be chosen for study, a single one was used in this paper to illustrate the analysis of a single complex fire model, CFAST[10]. 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 included 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 $t^2$ fire[11] chosen to simulate a mattress fire[12].

*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 (±10%) and larger (up to an order of magnitude) variations for selected inputs were studied. Varying most of the inputs by small amounts had little effect on the model outputs.

An example, figure (1), shows the results of a 10% change in room volume (effected by changing the floor area) on several model outputs. The figure shows a somewhat constant relative difference for the changes as a function of time. Ignoring the effects at very early times where upper layer volume and pressure are very nearly zero, the graph shows that temperature and pressure are less sensitive 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 fires[13] and analytical solutions for single compartment steady-state fires[14]. In essence, this implies that reasonable uncertainties in room dimensions would have little effect on the results predicted by the model for this scenario. As suggested by Iman and Helton[15], an average relative difference could be used to characterize the model sensitivity for comparing individual inputs and outputs.

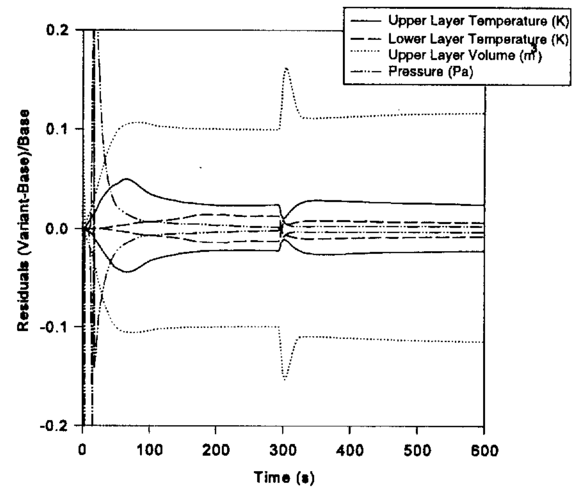


Figure 1. An example of time dependent sensitivity of fire model outputs to a 10% change in room volume for a single room fire scenario

*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 changing the heat release rate (HRR) inputs are shown in figure 1. 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.

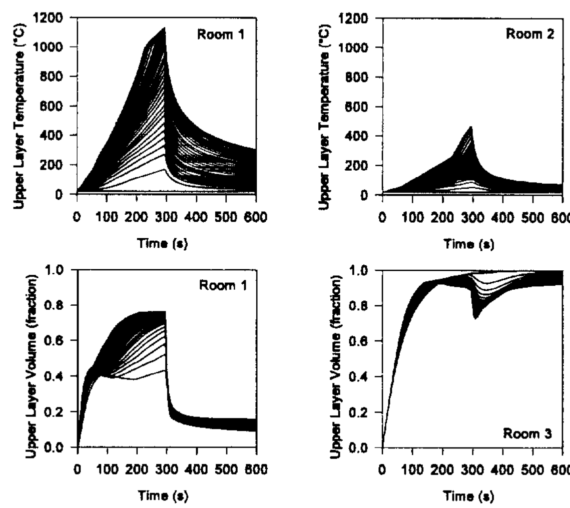


Figure 2. Layer temperatures and volumes in several rooms resulting from variation in heat release rate for a four-room growing fire scenario

*Simple "response-surface "correlations:* A next step beyond the simple plots presented in figure 1 is a cross-plot of outputs of interest against HRR. The shaded areas on figure 2 shows the locus of individual data points representing more than 100,000 single-time values for layer temperature. For each room, a regression fit to all the data for that room overlays the locus. The temperature curves for both upper and lower layer temperature in all four rooms (figure 2) 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 a simple slope of the resulting correlation between HRR and temperature. Figure 4 shows this sensitivity for the four-room scenario studied. 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.

*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 figure (1), an average relative difference could be used. Again from figure 4, an 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.

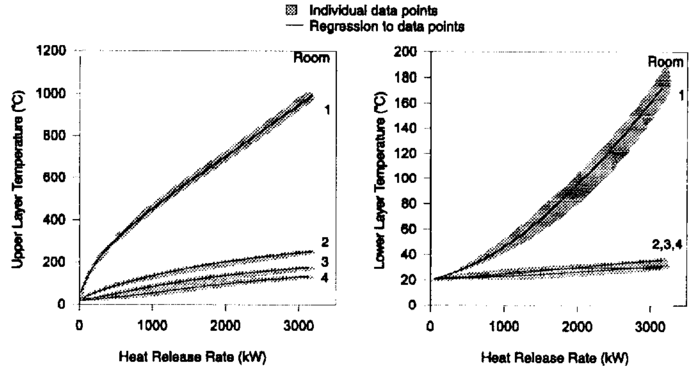


Figure 3. Comparison of heat release rate and layer temperature in several rooms for a four-room growing fire scenario

Figure 4 presents the effect of both HRR and vent opening (in the fire room) on the upper layer temperature. In this figure, actual model 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.

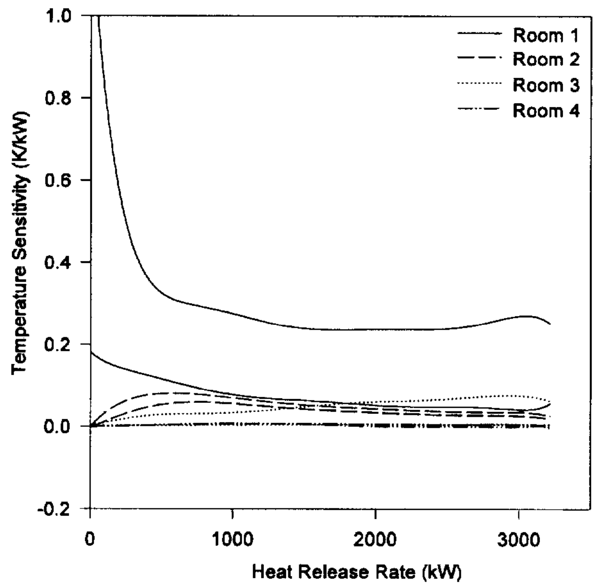


Figure 4. Sensitivity of temperature to heat release rate for a four-room growing fire scenario

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[16,17] suggest that the dependence is on the order of $q^{2/3}$ 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 figure 4.

## EVALUATION OF THE PREDICTIVE CAPABILITY OF FIRE MODELS

Several researchers have studied the level of agreement between computer fire models and real-scale fires[2]. These range from comparisons using simple correlations[18] to intricate field models[19,]. 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.

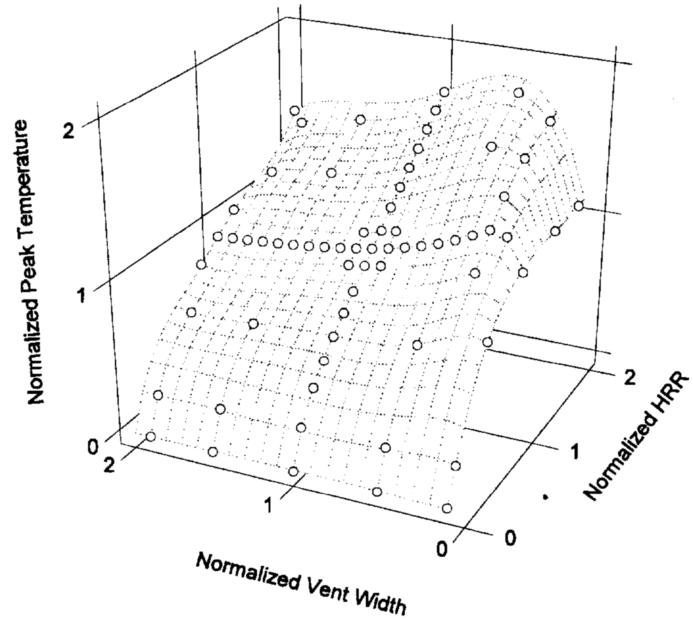


Figure 5. Effect of both heat release rate and vent opening size on upper layer temperature for a four-room growing fire scenario.

*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 $m^3$ to 1327 $m^3$, with ceiling height varying from 2.4 m 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 6 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 Babrauskas[17] and includes additional experimental measurements from a variety of sources, most notably the work of Deal and Beyler[18]. In addition, it includes predictions from a current generation zone fire model, CFAST that will be discussed in more detail below.

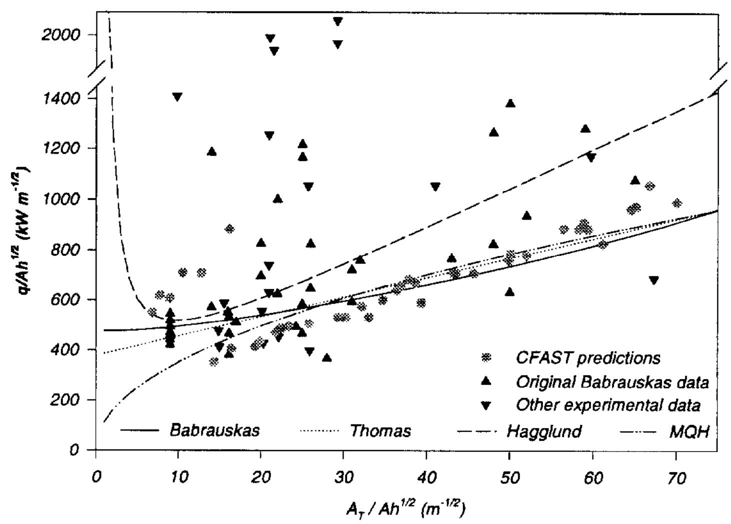


Figure 6. Comparison of correlations, CFAST predictions, and experimental data for the prediction of flashover in a compartment fire.

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, Thomas, and McCaffrey, Quintiere, and Harkelroad provide nearly identical estimates of the minimum energy required to produce flashover. The estimates of Hägglund yields 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[17]. 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. 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.

*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, Jones, and Bukowski[2], Beard[19], Deal and Beyler[18], and Reneke et.al.[20] are illustrative.

Figure 7 shows a comparison of measured and predicted upper layer temperature for several tests studied[2]. 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 to peak values and times to 100 °C predicted by the model average within 25 s of experimentally measured values.

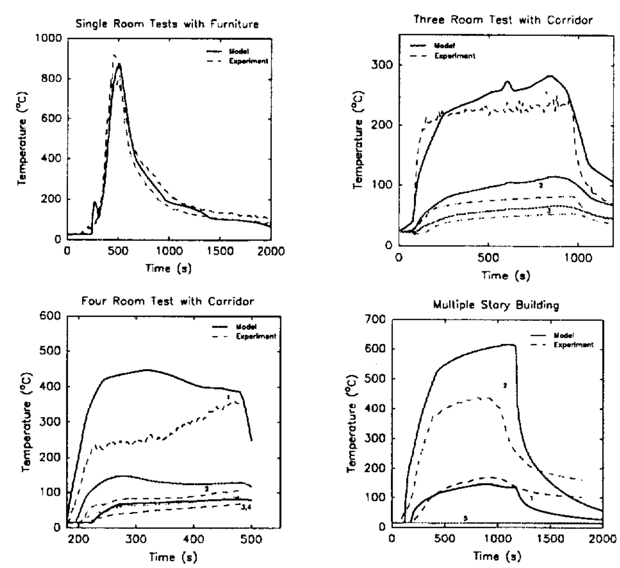


Figure 7. Comparison of measured and predicted upper layer temperatures for several tests. (Numbers indicate comparable rooms in the test structure.)

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 °C 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. 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.

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 *mxn* 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.

- *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.

- *Statistical treatment of the data* – presentation of the differences between model predictions and experimental data to date have been 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* – Most interest in applying current generation models is in a non-residential setting. Little experimental data is available for these scenarios. 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.

## 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, the heat release rate is dominant in determining the behavior of the models. Other model inputs, including room volume and vent size have lesser effects on a range of predicted ouputs.

Comparison of model prediction with available experimental measurements show agreement and differences which are understandable given the limitations inherent in the models and experiments. Although a range of applications have been reported in the literature, to use the models with assurance for any purpose, the user must understand the underlying science, assumptions, and limitations inherent in the models and from this decide the applicability for a particular application. Such an understanding allows the trained professional to assure use of the models where applicable does not exceed the capabilities of a particular model.

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***Discussion***

Patrick Pagni: We decided that comparison with data was the major task for the computational models for this meeting. While sensitivity analyses are interesting, I don't think they accomplish that goal. Let me give you a negative comparison since you didn't think there were any out there. We have compared the results of CFAST for the temperature in the upper layer in a long, steady heat release rate experiment and we find consistent overprediction of the upper layer temperature. In the comparisons you showed us today, I think I saw the same trend. I cannot be sure since you didn't dwell on the temperature comparison, but could you tell me if that was the case?

Richard Peacock: Overprediction of temperature by CFAST is fairly classic. We are aware of that and need to look at it. We suspect it's related to two things: one is plume entrainment, which drives practically everything else in the model; and the second is mixing between the layers, because going along with this overprediction of upper layer temperature is an underprediction of lower layer temperature. That's somewhat forced by the mass balance. The dichotomy of overprediction of upper layer temperature and underprediction of lower layer temperature is somewhat forced by mass and energy balance in a compartment. It's something that we are addressing.

Patrick Pagni: I am very happy that you agree with the phenomenon. Let me give you another mechanism. We think there may be something wrong with the heat transfer algorithm at the wall. By running several different programs, we thought we were able to determine that the plume entrainment was correct, but there was something wrong with the wall heat transfer. The paper will appear in the forthcoming issue of the Fire Safety Journal.

Walter Jones: I asked Nick to send the data along when the paper's published. We are certainly interested in finding problems in the model. That's a general request which I will make later today in talking about the database for comparison of models and data. In order to fix problems in models of that sort, one has to have the relevant data sets which show the discrepancies.

John Hall: As a statistician, I tend to think first of all of statistical checks for goodness of fit of mean squared deviation. I'm wondering what you might have done to pursue that concept's applicability here.

Richard Peacock: We have looked at it. The catch is not so much what technique do I use for a specific problem, but rather the fact that I have roughly an infinite amount of data that I'd like to look at and from the offset, don't know what that data looks like. So if we would like to look at an arbitrary problem, before we know what that problem looks like, we'd like to know what appropriate statistical treatment to use. It's sort of a problem of the cart following the horse: I can choose an appropriate technique if I know the problem I'm interested in but not necessarily vice versa.