

Quantitative Determination of Smoke Toxicity Hazard—A Practical Approach for Current Use

RICHARD W. BUKOWSKI

Hazard Analysis

Center for Fire Research

National Bureau of Standards

Gaithersburg, Maryland 20899, USA

ABSTRACT

The concepts of fire hazard assessment are discussed. The development of these concepts into the framework for a hazard assessment model is described. This model, which is actually a group of interacting models, is presented in terms of the component functions and the interactions necessary to accomplish a hazard analysis. The most critical research issues which must be resolved in order to use this hazard analysis model for practical problems are identified. Preliminary results of experiments to assess the predictive accuracy of the multi-compartment transport model used within the hazard model are presented. A simple, engineering approach to toxicity evaluation included in the current model is also discussed.

INTRODUCTION

Over the past decade, the field of fire modeling has progressed to the point that quantitative predictions of fire in buildings can be made to an accuracy which is useful for engineering purposes. Over the past two years, the Center for Fire Research (CFR), National Bureau of Standards (NBS), has been working on the application of fire modeling techniques to the prediction of the hazard to occupants from building fires. Hazard assessment is a logical extension of fire modeling. Its development has been driven primarily by the need to evaluate the role of combustion product toxicity in relation to other hazards associated with fire.

This paper presents a framework for using fire models for hazard assessment and focuses on the progress made with two critical components: the assessment of the transport model's (FAST) predictive accuracy and the prediction of occupant response to toxic combustion products.

HAZARD MODELING

Fire models consist of sets of equations which describe the physical processes associated with fires in buildings. They describe the evolution and distribution over time, of energy and mass released by a burning material. Thus, with the proper model or combination of models, the environment in each compartment in the building is described in terms of the temperature, smoke density and gas concentrations. These time-varying conditions represent the exposure of the building occupants as a function of their location during the fire. Hazard analysis requires that this predicted exposure be evaluated in

terms of the expected response of the occupants to it. Thus, exposure-response is translated into the consequences of the exposure in terms of incapacitation, injury, or death. The ability to assess the exposure-response represents a critical step in moving from fire models to hazard models.

But there are many scenario dependent factors which influence the exposure and the likelihood of an injury or fatality. In the simplest terms, these factors all relate to one common denominator - time. As so aptly put by Cooper [1], we need to know whether the time available for occupant escape is greater than the time needed. The former encompasses all the environmental conditions (e.g., temperature, radiant flux, smoke obscuration) which may delay or prevent successful escape and the latter includes the occupants' awareness and physical ability to reach a refuge or exit the building.

FRAMEWORK

Figure 1 presents a block diagram of the major components of a fire hazard analysis method. Each block represents a model or calculation method which describes a general process, or a data input which is specific to the scenario being evaluated. Within this modular framework the most appropriate model or data is used for each element and improved techniques can be easily substituted as they develop. The calculation begins with a specified fire or combustion model. The specified fire is described in the form of total energy and mass release rates deduced from data from small or large scale calorimeter measurements or experiments. The combustion model (a limited version is contained in the Harvard Computer Fire Code [2]) predicts the total energy and mass release rates taking into account the thermochemical properties of the burning material and the thermophysical properties of the enclosure. If a suppression system is present, its effect on the total release rates of energy and mass is taken into account. A transport model, such as the computer code FAST [3], then takes these total release rates and predicts the distribution of temperature and combustion products throughout the structure, accounting for the influences of building geometry, construction materials, HVAC (including any smoke control system), stack effect and wind. This results in a description of the time varying environment within each compartment to which any occupants therein would be exposed. This information is also used to predict detection or suppression system actuation.

The response of each occupant to this exposure based on a set of prescribed tenability limits is then evaluated (see example later) as a function of location and time of exposure. Location is provided by an evacuation model which begins with a specified, initial occupant distribution and predicts their movement, accounting for notification delays and their capabilities, either inherent or as they might change as a result of exposure to fire products. The eventual result is a prediction of the expected consequences of the fire scenario in terms of injuries or fatalities, and the time, location, and factor(s) related to each.

CALCULATING SMOKE TOXICITY HAZARD

Determining the Exposure-Dose

The procedure for estimating smoke toxicity hazard involves four steps: (1) determining fuel mass loss rate, (2) calculating mass concentration, (3) calculating exposure-dose, and (4) fixing the time at which the exposure begins. Consider an arbitrary compartment containing a growing fire and an occupant exposed to the combustion products. The measured heat release rate of an item of upholstered furniture can be approximated by a triangle as shown in

Figure 1 - Hazard Model Framework

INTERRELATIONSHIPS OF MAJOR COMPONENTS OF A FIRE HAZARD MODEL

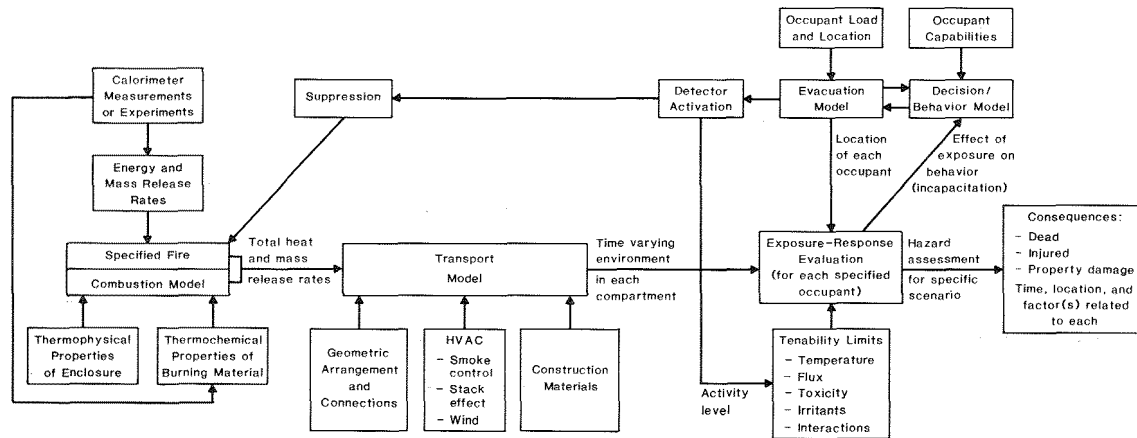


Figure 2a using a method described by Babrauskas [4]. By assuming that the effective heat of combustion is a constant, the mass loss rate of the fuel (burning item) can be calculated.

By also assuming that all of the fuel mass lost goes to "combustion products", and that all of these combustion products are contained within the occupied volume, then the increase over time of the mass concentration of combustion products in the space and the resulting exposure to the occupants can be calculated as shown below. Note that both the concentrations and the resultant exposures (Figures 2b and c) vary, depending on whether it is assumed that the combustion products entering the occupied volume are fully mixed or stratified.

For the fully mixed case, the concentration and exposure as a function of time are simply given by equations (1) and (2) below.

$$C(t) = \frac{1}{V} \int_0^t \dot{m} dt \quad (1)$$

$$E(t) = \int_0^t C(t) dt \quad (2)$$

where: $C(t)$ is the combustion products mass concentration
 V is the volume of the space
 \dot{m} is the fuel mass loss rate
 $E(t)$ is the exposure dose [5]

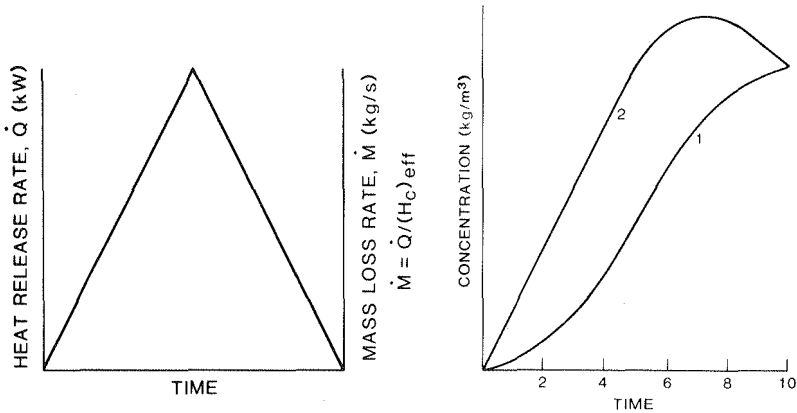
For the stratified case, the volume into which the combustion products are distributed (the upper layer) changes with time, and the exposure only begins when the occupant is immersed in the upper layer. Thus, for this case, equations (3) and (4) would apply.

$$C(t) = \frac{\int_0^t \dot{m} dt}{AD(t)} \quad (3)$$

$$E(t) = \int_{t'}^t C(t) dt \quad (4)$$

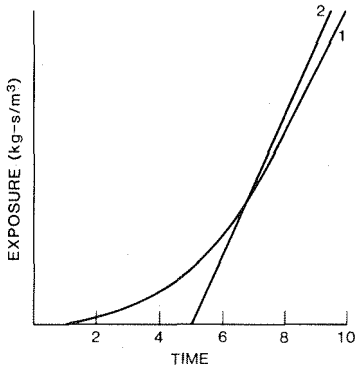
where: $D(t)$ is the upper layer depth at a time t
 A is the compartment floor area
 t' is the time that the layer interface reaches the level of the occupant

For equation (4), the quantity t' , i.e., the time at which the interface reaches the level of the occupant must be estimated. Simple filling models such as ASET [6] can be used to determine a value for t' . Otherwise, when the difference in height between the assumed occupant position and the level (base) of the fire is less than about 10% of the compartment ceiling height, a crude approximation for t' can be made from a family of curves (Fig. 2(d)) based on

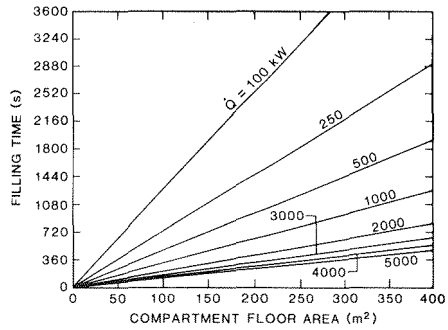


(a) Triangular approximation for upholstered furniture heat release rate

(b) Concentration of "combustion products" vs. time, assuming (1) fully mixed and (2) stratified (linear filling rate)



(c) Exposure of occupant, assuming (1) fully mixed and (2) stratified (linear filling rate)



(d) Time to fill to the level of the fire

Figure 2 - Procedure For Hazard Estimation

the work of Cooper [7]. These curves give estimated time to fill an enclosure to the level of the fire as a function of compartment floor area for various levels of heat release rate. This time is approximately t' .

The above described procedure for determining exposure-dose for the stratified case has been incorporated into FAST version 17 [3] by treating the product of concentration and time as a transportable species called CT.

It represents an interim implementation of a smoke toxicity dose calculation. For each fire interval, the fraction of fuel mass which is converted to "toxic" combustion products is calculated. In the NBS protocol [8], the lethal concentration, the LC_{50} , is defined as the total fuel mass loaded into the furnace divided by the exposure chamber volume. Thus, where NBS protocol data is used for analysis, this conversion fraction is defined as unity.

The species CT calculated by the model then represents the mass concentration of combustion products in the upper layer of each compartment integrated over time. The units are $mg\text{-min/liter} = \text{gram-min/m}^3$.

Quantifying Hazard

This method enables easy correction of the predicted value of CT to allow for the actual time to start of exposure (t'). If, for example, it is assumed that the exposure begins when the interface reaches 5 feet (1.5 m) from the floor (nose level of a standing person), it is only necessary to determine the value of CT at this time, and subtract this value from all subsequent values of CT to provide the corrected results. To determine a critical value for CT (called CT^*), the LC_{50} for the fuel material is multiplied by the exposure time over which the LC_{50} was determined. For example, if the fuel is PVC undergoing flaming combustion, the $LC_{50} = 17 \text{ mg/l}$ for a 30 min. exposure. Thus, $CT^* = 17 \times 30 = 510 \text{ mg-min/l} = 510 \text{ g-min/m}^3$. When $CT = CT^*$ for the fuel, a lethal condition is considered to exist. Note that, since the 30 min. LC_{50} for most common fuels is in the range 20-40 mg/l , a CT^* value of approximately 900 $mg\text{-min/l}$ could be generally applied for estimating purposes where a specific value for the fuel is unknown. Likewise, since CT^* values for incapacitation are often of the order of 1/2 the value for lethality [9], a value of 450 $mg\text{-min/l}$ might be used.

It should be noted that this evaluation procedure (but not the model calculation) assumes the CT product which causes a biological effect is a constant (referred to as Haber's Law [10]). Recent data indicate that this is not generally true, but is the best approximation which can currently be made with available toxicity data. If LC_{50} data are available for different exposure times for the material in question, the Fractional Effective Dose (FED) procedure described by Hartzell, et al. [11], can be used to correct the CT^* estimate.

Where the fuel (burning item) consists of a mixture of materials for which the LC_{50} data are available for each, an effective LC_{50} (and thus an effective CT^*) can be estimated by the following equation [12].

$$\frac{1}{LC_{50}} = \sum_i \frac{f_i}{LC_{50_i}}$$

where f_i is the fraction of total fuel mass represented by material i and, LC_{50_i} is the LC_{50} (generally for a 30 min. exposure) of material i

Then $\overline{CT^*} = \overline{LC}_{50} \times 30 \text{ min}$

If IC_{50} (concentration necessary to incapacitate), or EC_{50} (concentration necessary to produce any specified effect) data are available, they would be used in exactly the same way to produce a CT^* and predict time to incapacitation or other effect.

Progress on Assessing the Accuracy of FAST

Initial work on the development of techniques for assessing the accuracy of fire models has used the transport model FAST as an example; but the techniques are intended to be generally applicable to any model. This work has shown the value of coordinated experiments both to establish the statistical accuracy of predicted quantities and to identify the sensitivity of results to model assumptions.

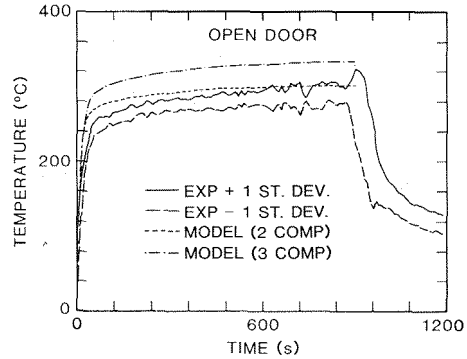
The criterion used for comparison of model predictions and experiments was that, for a given parameter, the model prediction must lie within the normal variation for a set of replicate experiments. Thus, a set of experiments (generally 5) was conducted and the derived parameters were statistically analyzed to produce an envelope of \pm one standard deviation about the mean value for the set. This requires that the prediction be within a range covered by 68% of the experimental values. The preliminary results of this exercise with FAST version 17 [3] are presented in the next section.

Experiments

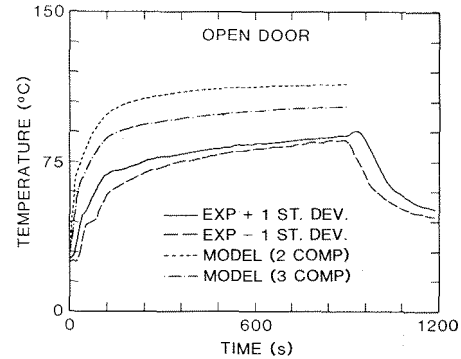
The facility constructed for the study consisted of a 2.4 m (8 ft) cubic burn room at one end of a 10 m (30 ft) corridor. For some experiments, a target room of the same size as the burn room was included near the far end of the corridor. The fire source was a natural gas burner where about 15% acetylene was mixed with the natural gas to produce visible smoke. The door at the far end of the corridor from the burn room was below a collector hood equipped for oxygen consumption measurements as a check on heat release rate in the effluent flow. In some experiments, this door was closed except for a 20 mm undercut. Complete details on the facility and experimental results will be published in a separate report by Peacock, et al. [13].

Some of the results for two sets of experiments (five open door and five closed door) with a 100 kW fire strength are presented in Figures 3 and 4. In each case, the experimental results are presented as two curves, representing plus and minus one standard deviation for a series of five experiments. The predictions by the model treating the facility as a two room arrangement are shown. On some plots, the effect of including the short corridor-like space between the burn room and corridor as a third compartment in the model is also shown. The level of agreement varies from excellent to fair, although the reasons for disagreement are not always indicative of problems with the model. This is demonstrated by the comparisons with corridor interface height.

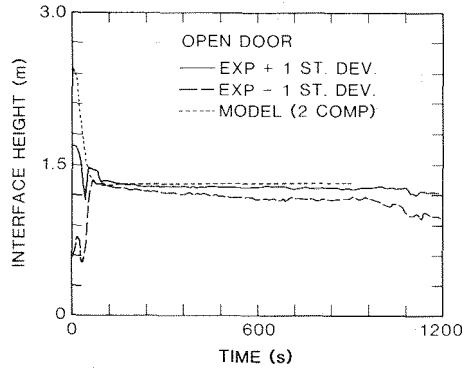
The interface position is derived from experimental data in two ways: a temperature method similar to one proposed by Cooper, et al. [14] and a new smoke method. The temperature method estimates the temperature at the interface at 10% to 20% of the temperature rise on the top thermocouple in a tree (15% was used for the data presented). The vertical location of this tempera-



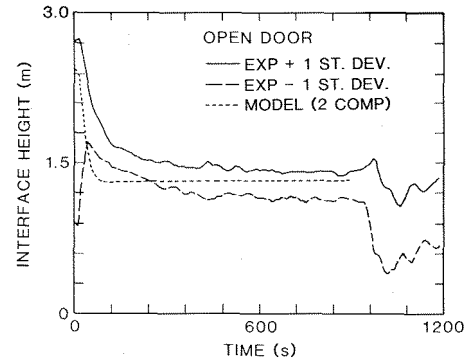
(a) Burn room upper layer temperature



(b) Corridor upper layer temperature

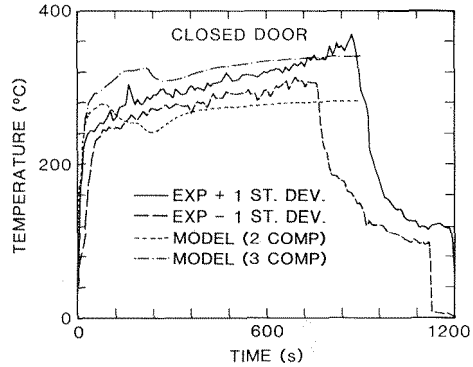


(c) Corridor interface position - temperature method

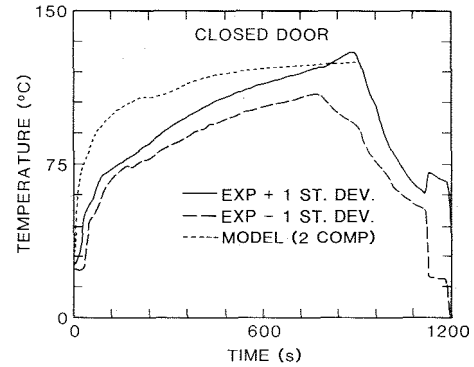


(d) Corridor interface position - smoke method

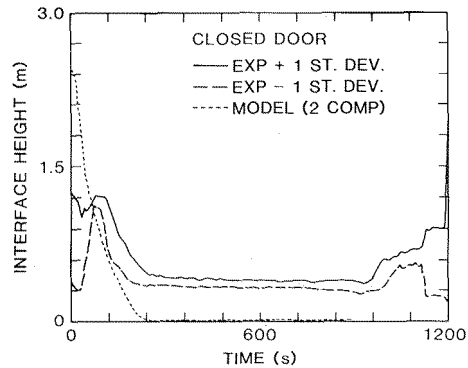
Figure 3 - Comparison Of Experiments To Model - Open Door



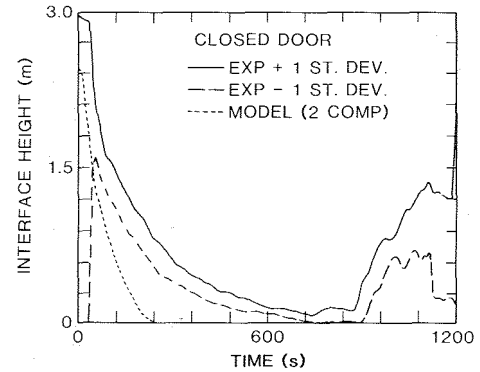
(a) Burn room upper layer temperature



(b) Corridor upper layer temperature



(c) Corridor interface position - temperature method



(d) Corridor interface position - smoke method

Figure 4 - Comparison of Experiments To Model - Closed Door

ture is then calculated by linear interpolation between the thermocouples in the tree. This method is thus bounded by the physical location of the top and bottom thermocouples - in this case 15 cm (6 in) below the ceiling and above the floor.

The smoke method employs a horizontal smoke meter located near the ceiling and a vertical smoke meter from the floor to ceiling (actually built into the floor and ceiling so that the path length is full room height). From the horizontal meter, the optical density (OD) per unit path length in the upper layer is obtained. This value is then set equal to the OD per unit path for the vertical meter, and the "effective path length" which produces this result is obtained. This is the upper layer thickness. This technique makes the same assumption as the zone model - that the upper layer is uniform and the lower layer is relatively clean. If there is significant contamination in the lower layer, it can be accounted for with another horizontal meter in the lower layer; although this was not necessary in these tests.

Both methods were employed to measure the corridor interface position in these experiments. Only the temperature method was used within the burn room. Comparison of the two methods to each other and to visual observations indicates that the results are comparable for the open door experiments where the layer stabilized at about mid level. Both showed the same major features including the rise in interface position after the burner was turned off at 900 s. The temperature method shows the layer beginning below the top thermocouple at zero time due to a small thermal layer from the burner pilot. The smoke method shows the layer beginning at the ceiling since the pilot did not have the acetylene feed. For the closed door tests, however, the smoke method shows the layer goes to the floor which agrees with visual observations, while the temperature method shows it stopping at the bottom thermocouple for the reasons explained previously.

IMPLICATIONS OF EXPERIMENTAL RESULTS FOR ASSUMPTIONS IN FAST

The data from the experiments were used to identify potential improvements in FAST. These improvements relate to conduction through layered walls, the door jet, and leakage.

The experimental facility surfaces are kaowool over brick in the burn room and calcium silicate board over gypsum board in the corridor. In the model an attempt was made to treat this multilayered wall as a single layer of material with composite properties. Poorer agreement between the model prediction and experiments and the difficulty of estimating composite properties indicate this approximation should not be used. Thus a conduction routine which accounts for up to three layers in a wall has been developed.

As most models do, FAST assumes the door jet is a horizontal plume, with a circular cross section; when, in fact, the cross section is rectangular due to flow through the door opening. This different geometry effects the entrainment. The effect of a rectangular geometry in the model was examined and some improvement in agreement was seen. This feature will be included in the next generation transport model.

The effect of leakage at the wall/ceiling junction was also investigated. In the experiments, visual observations identified that leaks occurred, and the mass flows at the corridor door showed more flow in than out. If this difference in corridor door mass flow rates were included in the model as a leak from the upper layer, the agreement with experimental conditions should improve

substantially. Thus, care must be taken to either eliminate leaks in the test, or to include them in the model.

SUMMARY

A framework for fire hazard assessment which describes the major components and their interactions was presented. Specific models or techniques which might be used within this framework may vary depending on the level of accuracy required by the application.

An engineering approach to smoke toxicity evaluation was then presented within the context of this framework. The easily used approach utilizes data produced by currently available toxicity test methods.

Finally, an example of the use of validation experiments to provide an understanding of the predictive accuracy of the transport model FAST was described. The importance of some of the assumptions used in FAST was indicated by the experiments. Considerably more work has been completed than is reported here, and a complete report is in preparation [13].

REFERENCES

- [1] Cooper, L.Y. and Nelson, H.E., Life Safety Through Designed Safe Egress - A Framework for Research, Development and Implementation, Proceedings of the 6th UJNR, Tokyo, Japan, 1982.
- [2] Mitler, H.E. and Emmons, H.W., Documentation for CFC V, The Fifth Harvard Computer Fire Code, National Bureau of Standards, NBS-GCR-81-344, Oct. 1981.
- [3] Jones, W.W., A Multicompartment Model for the Spread of Fire, Smoke, and Toxic Gases, Fire Safety Journal, Vol. 19, Nos. 1 and 2, May/July 1985.
- [4] Babrauskas, V. and Krasny, J.F., Fire Behavior of Upholstered Furniture, NBS Monograph MN-173, in press.
- [5] Huggett, C., Combustion Conditions and Exposure Conditions for Combustion Product Toxicity Testing, J. of Fire Sciences, 2, 328-347, Sept/Oct 1984.
- [6] Cooper, L.Y., A Mathematical Model for Estimating Available Safe Egress Time in Fires, Fire and Materials, Vol. 16, Nos. 3 and 4, 135-144, 1983.
- [7] Cooper, L.Y., The Development of Hazardous Conditions in Enclosures with Growing Fires, NBSIR 82-2622, NBS, Gaithersburg, MD 20899, December 1982.
- [8] Levin, B.C., Fowell, A.J., Birky, M.M., Paabo, J., Stolte, A., and Malek, D., Further Development of a Test Method for the Assessment of the Acute Inhalation Toxicity of Combustion Products, NBSIR 82-2532, NBS, Gaithersburg, MD 20899, June 1982.
- [9] Kaplan, H.L. and Hartzell, G.E., Modeling of Toxicological Effects of Fire Gases: I. Incapacitating Effects of Narcotic Fire Gases, J. of Fire Sciences, Vol. 2, No. 4, 286-305 (1984).
- [10] Kaplan, H.L., Grand, A.F., and Hartzell, G.E., Combustion Toxicology Principles and Methods, Technomic Publishing Co., Inc., Lancaster, Pa., p. 25.

- [11] Hartzell, G.E., Priest, D.N., and Switzer, W.G., Mathematical Modeling of Toxicological Effects of Fire Gases, Proceedings of the 8th UJNR, Tokyo, Japan, in press.
- [12] Bukowski, R.W., Evaluation of Furniture Fire Hazard Using a Hazard Assessment Computer Model, Fire and Materials, in press.
- [13] Peacock, R.D., Davis, S., and Lee, B.T., Experimental Data for Model Validation, NBSIR, in press.
- [14] Cooper, L.Y., Harkleroad, M., Quintiere, J., and Rinkinen, W., An Experimental Study of Upper Hot Layer Stratification in Full-Scale Multiroom Fire Scenarios, J. Heat Transfer, 104, 741-749.