The Development of a Method for Assessing Toxic Hazard

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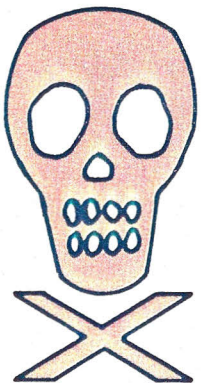

We have known for many years that most fire victims die from the effects of smoke and toxic gases rather than from burns. This knowledge has been the primary motivation for research into fire toxicology, and has led to the development of a number of tests that can be used to assess the toxicity of the combustion products of various materials.

Most of these toxicity tests measure the acute toxicity of a given material's combustion products. That is, they measure the harmful effects that a single, short exposure to the combustion products generated by a burning material has under specified laboratory conditions.

Unfortunately, such tests do not give a true picture of a material's relative hazard because they do not reveal the entire hazard the material represents when it is used in a specific application. This larger toxic hazard is defined as the environmental conditions a material presents which increase the probability that a fire will produce a toxic atmosphere and result in injury.

A toxic hazard evaluation must take into account not only acute toxicity, but several other factors, as well.[1] Among these are:

- The quantity of material present.
- The configuration of the material.

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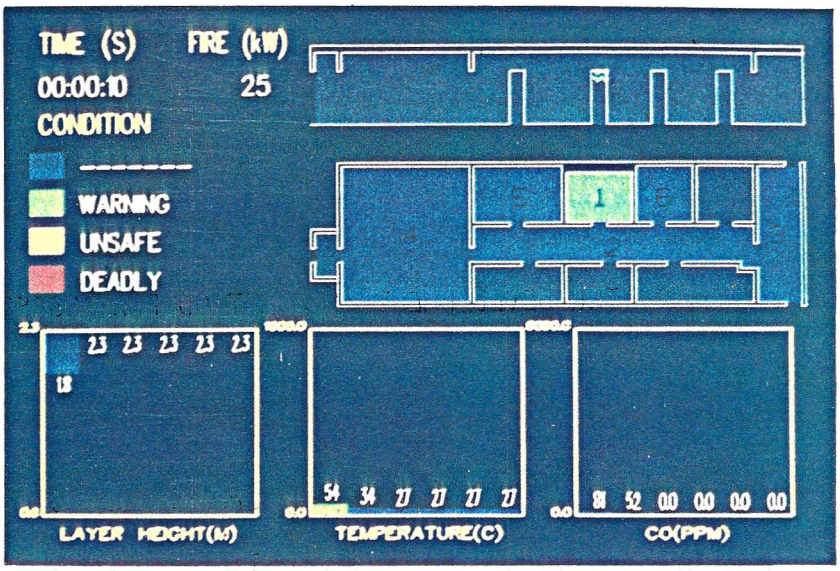
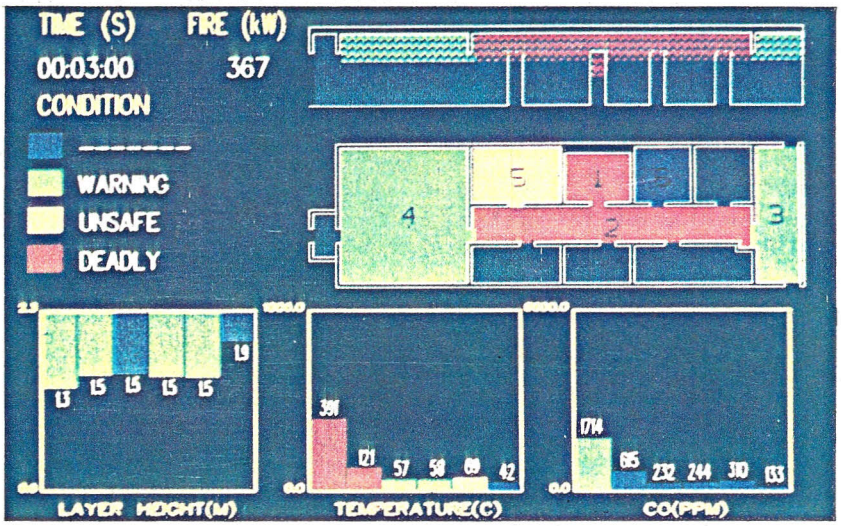
[1] B. C. Levin, et al., *Further Development of a Test Method for the Assessment of the Acute Inhalation Toxicity of Combustion Products*, NBSIR 82-2532, National Bureau of Standards, Gaithersburg, Md., 1982.

- The proximity of the material to other combustibles.
- The volume of the compartments to which combustion products may spread.
- Ventilation conditions within the building.
- The ignition and combustion properties of the material.
- The presence of ignition sources.
- The density of the smoke the material will produce.
- Irritants present in the smoke.
- The presence of fire protection systems in the building.
- Building occupancy, including its size and design.
- The expected ability of building occupants to escape a fire.

It is not enough to rank a material simply on the basis of its acute toxicity test results because large differences in the other factors listed can easily overwhelm the differences in acute toxicity that the tests reveal. Thus, any meaningful assessment of fire hazard must integrate the results of a number of material fire property tests, while taking into account in a realistic way the quantity and use of the material. It is for this reason that the Center for Fire Research at the National Bureau of Standards (NBS) has begun to develop a rigorous toxic hazard assessment methodology based on computer fire modeling techniques.



Above is a frame of computer graphic film taken 10 seconds into a toxic hazard assessment model simulation. This early in the test, the burn room is the only area that exhibits any sign of toxic hazard. Below is another frame of film taken 3 minutes into the same simulation. By this time, conditions in the burn room and the corridor are deadly and the rest of the test area is becoming unsafe.



The NBS Project

The toxic hazard assessment project at NBS was started in early 1983. Its goal was to develop methods that could be used to assess how much the toxicity of a material's combustion products contributes to the overall fire hazard the material presents to human beings when it is used in a specific context. These methods will eventually provide designers and code officials with a means of determining how effective their designs and code provisions are likely to be in reducing the toxic hazard within a building.

To determine the contribution of combustion products to overall fire hazard, we must be able to make quantitative predictions about the evolution and transport over time of the heat, smoke, and toxic products a specific material used in a specific fashion within a specific building generates when it burns. We must also take into account the impact of fire protection features provided in the building, as well as the effect the occupants' location and any physical restraints they face have on their ability to escape.

Thus, the NBS model was designed to examine three major elements.[2] These are product generation, product transport, and occupant response.

The product generation portion of the model consists of a fire growth

[2] W. W. Jones, *A Model for the Transport of Smoke, Fire, and Toxic Gases (FAST)*, NBSIR 84-2934, National Bureau of Standards, Gaithersburg, Md., 1984.

model which predicts the development and spread of fire in the compartment of origin and the evolution over time of energy, smoke, and gas species. For input, this fire growth model uses the results of material property tests and toxicity tests that have already been conducted on the materials being examined. The model can also be used to define the range of exposure conditions under which these material property and toxicity tests should have been conducted.

The second major element, the smoke transport model, is used to predict the spread over time of the energy, smoke, and gases generated by the fire through all of the interconnected compartments of the building. This transport model is a zone model. It divides each compartment into upper and lower zones in a way that is consistent with the stratified flows observed in real fires. Unlike many earlier zone models, in which the lower zone or layer was assumed to remain at ambient temperatures throughout the fire, this model allows for mixing between the zones at each of the vents between the compartments so that the lower layer is contaminated by energy and mass. As a result, agreement between this model and experimental data has been vastly improved.

The final major element, occupant response, measures the effect the predicted conditions at any location will have on a building occupant at that location. This element includes a prediction of the physiological impact of heat, smoke, and gases over the time of the exposure. The result is a quantitative assessment of the overall hazard to occupants of the building.

Contrast this test methodology with that used to determine acute toxicity, and it becomes clear why acute toxicity tests alone cannot adequately measure toxic hazard. Generally, acute toxicity tests involve burning a material and exposing an animal to the combustion products the material gives off. They then measure the impact of these products in terms of their lethality or the time it takes them to produce an effect on the animal. Results of the NBS test methodology are much more detailed and sophisticated than results obtained in an acute toxicity test.

The First Order Model

Early in the project, the NBS decided to produce a complete "first order" model which could be tested and used with restrictions while various refinements were being developed. The refinements could then be added to the model when they were completed. Figure 1 shows the major elements of each portion of the model and the way in which they relate to each other. The items below each portion in the figure represent refinements that will be made to the model as the project continues.

The first, or generation, portion of this first order model is currently designed to accept heat release, mass loss, and smoke and gas production data for a single burning item. This information can be obtained with the NBS furniture calorimeter.[3] The model can then predict the generation of energy, smoke, and gases the item will produce when it burns in a specific compartment.

The generation portion of the model is also designed to accept an effective LC_{50} value for an item. As defined in the NBS test method,[4] an LC_{50} value is the concentration of combustion products which results in the death of 50 percent of the animals exposed to it over a specified time period. For items made of more than one material, it is a "mass weighted average" value and is obtained from data on the material or materials produced by the NBS toxicity test. This "effective" LC_{50} value is used to calculate a fractional lethal dose of its combustion products in the second portion of the model.

The second, or transport, part of the model, which predicts the distri-

[3] V. Babrauskas, et al., *Upholstered Furniture Heat Release Rates Measured with a Furniture Calorimeter*, NBSIR 82-2604, National Bureau of Standards, Gaithersburg, Md., 1982.

[4] B. C. Levin, et al., op. cit.

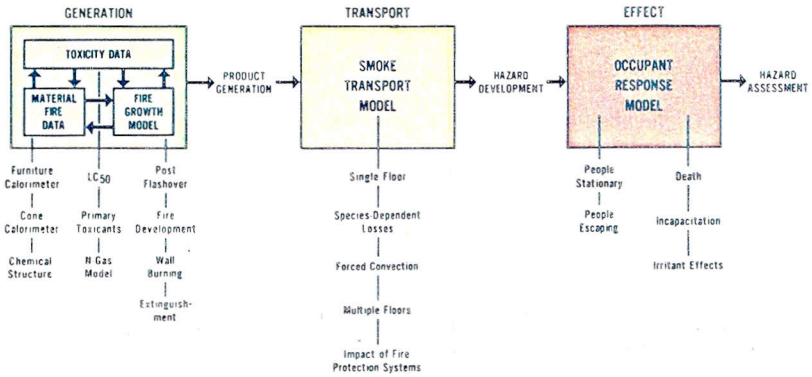


Figure 1.

These are the major elements of each portion of the toxic hazard assessment test model. The refinements represented by the items listed below each box will be made as work on the project continues.

bution of energy and mass in the interconnected compartments as a function of time, is currently used to compute the temperature, smoke density, and gas concentrations, as well as a fractional lethal dose, for the upper and lower layers in each compartment. It can also determine the location of the interface between the two layers as a function of time. This model can be run with as many as eleven interconnected compartments on a single floor.

Finally, the occupant response portion of the model is currently used to compare the conditions in each compartment against a mathematical description of the physiological impact these conditions would have on anyone in those compartments. In this way, the model can determine the level of hazard which exists at any time during the simulation.

Refinement of the first order model is ongoing. Eventually, the model will be able to describe the firespread and involvement of multiple items, as well as the spread of smoke and gases up stairwells and shafts to a number of floors. The model will also be able to use material property data from small-scale test methods, such as the cone calorimeter. An evacuation submodel will be included to reflect the changing exposure to occupants during their escape and to take into account the effects of incapacitation and irritants on the occupants.

One example of a refinement that is being incorporated into the first order model is the N-gas model for toxicity. As was stated earlier, determination of toxicity involves the calculation of a fractional lethal dose based on a mass weighted LC_{50} value from the NBS toxicity test method. But an LC_{50} value is a biological measure of an effect; it does not identify the cause of the effect.

At present, there is no mechanism for determining whether LC_{50}s are additive, antagonistic, or synergistic. For modeling purposes, NBS has hypothesized that, for most materials, the toxic effect is largely the product of a small group of primary toxicants. If one knows the concentration of each primary toxicant produced by the material in question as a function of time and has data on the biological effect of the toxicants both individually and in combination, one can estimate the combined biological effect they will have reasonably accurately for most materials. Since NBS researchers do not yet know how many gases will have to be included in the model to provide reasonable estimates of toxic effect for most common materials, they refer to the model as the N-gas model.

The initial group of primary toxicants NBS researchers selected for the N-gas model consists of carbon monoxide, carbon dioxide, hydrogen chloride, and hydrogen cyanide. Also included in this group are the effects of reduced oxygen. While oxygen itself is not toxic, depletion of oxygen by the combustion process affects the oxygen level in the blood and this lower level, especially when combined with the carbon monoxide and hydrogen cyanide present in the atmosphere, accelerates the onset of anoxia.

Pure gas studies conducted by NBS to quantify the impact of these primary toxicants examined all of the toxicants individually and in most combinations, with the exception of hydrogen chloride.[5] The resulting inter-relationships are being tested against data obtained during the development of the NBS toxicity test method, and researchers are now incorporating an initial form of the N-gas model into the toxic hazard model along with the fractional lethal dose calculation using LC_{50} data. In this way, comparisons can be made between the toxic effect predicted by the N-gas model and that predicted by the LC_{50} approach.

[5] B. C. Levin, private communication to author, 1984.

If the N-gas model approach proves valid, it would greatly reduce the number of different materials that would have to be examined in a toxicity test method. Researchers would only need to identify classes of materials which produce toxicants not included in the model. The animal test for acute toxicity would then become just a screen, since much of the needed data would be provided by analytical testing.

Comparing Model Results With Experiment Results

How well do the results of the model compare with the results of full-scale experiments? Allowing for some discrepancies, the answer seems to be "Quite well."

The full-scale experiments which served as a data base and control for this analysis were a two-room fire test conducted by L. Y. Cooper and associates[6] and a continuing series of full-scale validation tests conducted by the NBS.[7] The two-room fire tests, known as the Nike Site experiments, involved a 10-by-12-foot burn, or fire, room and a corridor which was varied in length from 30 to 60 feet (see Figure 2). The full-scale validation test series involved three rooms, one an 8-by-8-foot burn room, another a 30-foot corridor, and the third an 8-by-8-foot target room (see Figure 3). Both the experiments and the model predictions used 100-kW fires.

The results of the actual two-room fire test and the model predictions for that test are remarkably similar for both upper-layer temperatures produced in the burn room and corridor (see Figure 4) and the height of the boundary between the two layers or zones in the corridor (see Figure 5).

[6] L. Y. Cooper, et al., *An Experimental Study of Hot Layer Stratification in Full Scale Multiroom Fire Scenarios*, ASME 81-HT-9, Milwaukee, Wis., 1981.

[7] B. Lee, private communication to author, 1984.

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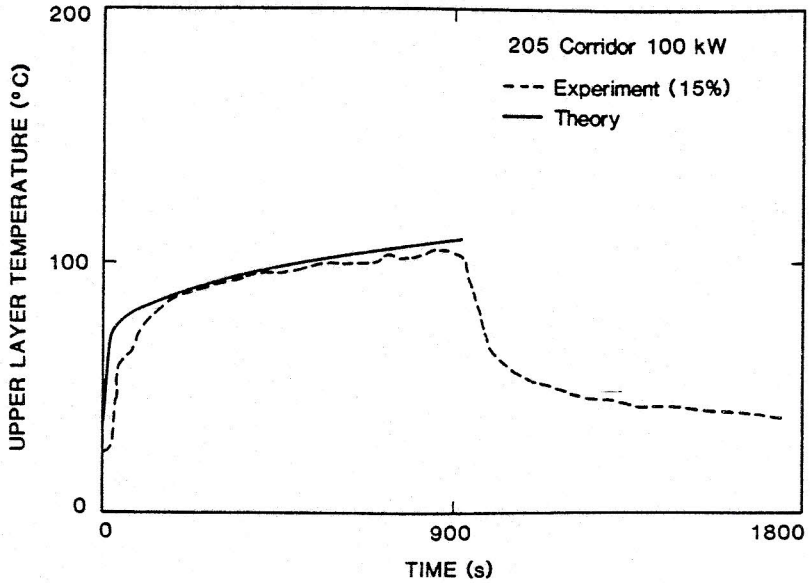
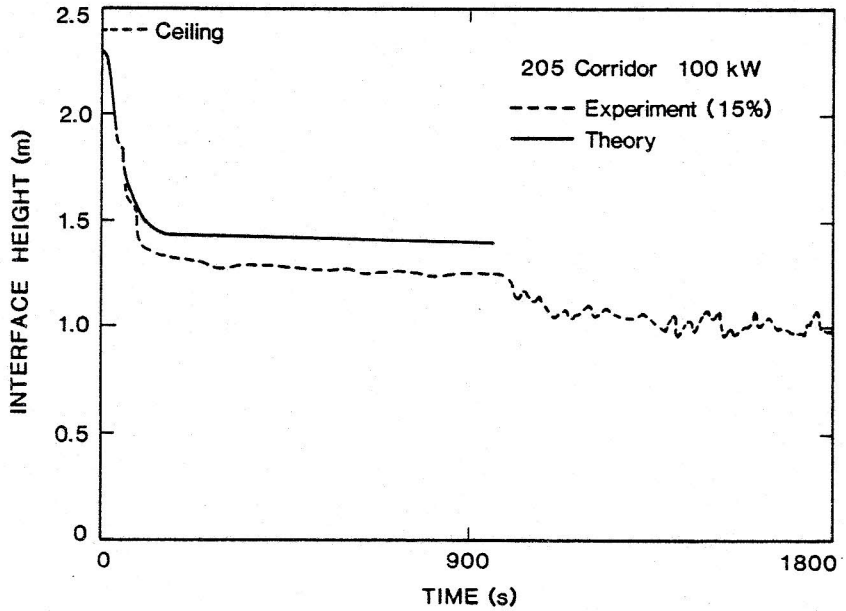


Figure 6.

The upper-layer temperatures produced in the three rooms of the full-scale validation tests are also very close to the results predicted by the model.

Figure 7.

The height of the boundary between the two zones in the corridor of the three-room full-scale validation tests is very similar to the boundary height predicted by the model.



Effort is also being made to streamline the model's input. Researchers will soon start using a large-size digitizing table to enter building geometry data into the model. By placing a building's floor plans on a digitizing table and tracing the drawing into the computer, the configuration of the entire building, as well as such factors as room dimensions and doorway locations, will be entered into the program automatically.

A computer data base of the "standard" items found in a building, along with their associated fire properties, will be developed so that the user can "furnish" the room of origin by selecting items from a list and placing them in the proper room on the floor plan. After selecting an ignition source from another list, the user will then be able to begin the simulation. In the same way, the location and status of building occupants will eventually be specified as the building design is being entered into the computer.

In Conclusion

There you have the NBS toxic hazard assessment test model. It is available now, and is capable of measuring the toxic hazard of a single burning item in a specific building or section of a building consisting of several compartments on a single floor. In a year's time, this model should be capable of predicting the spread and involvement of a number of items in the room of origin. Some time later, it will be able to predict the spread of heat, gases, and smoke to several floors of a building. And within five years' time, it will include egress actions, the incapacitating and irritant effects of combustion products on occupants, and the impact of fixed fire protection systems. This model will provide a means of answering most of those "what if?" questions we face all too frequently in the fire protection field. △