NIST Technical Note 1763

Smoke Component Yields from Benchscale Fire Tests: 4. Comparison with Room Fire Results

Nathan D. Marsh Richard G. Gann

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Fire Research Division Engineering Laboratory

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U.S. Department of Commerce *Penny Pritzker, Secretary*

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ABSTRACT

A standard procedure is needed for obtaining smoke toxic potency data for use in fire hazard and risk analyses. Room fire testing of finished products is impractical, directing attention to the use of apparatus that can obtain the needed data quickly and at affordable cost. In this work we compare yields of toxic gases generated by four bench scale apparatus to previously conducted room-scale fires. The bench scale apparatus are the radiant apparatus in NFPA 269 and ASTM E 1678, the smoke density chamber in ISO 5659-2, a controlled-atmosphere version of the cone calorimeter (ASTM E 1354), and the tube furnace in ISO/TS 19700. In the bench scale experiments, the test specimens were cut from finished products that were also burned in the room-scale tests: a sofa made of upholstered cushions on a steel frame, particleboard bookcases with a laminated finish, and household electric cable. The yields of CO₂ CO, HCl, and HCN were determined. The yields of other toxicants (NO, NO₂, formaldehyde, and acrolein) were below the detection limits, but volume fractions at the detection limits were shown to be of limited toxicological importance relative to the detected toxicants. The bench scale and room scale yields are compared, and the bench scale apparatus are assessed for the degree to which they accurately predict room scale yields. The results of this study provide a better basis for obtaining toxic potency input data for fire modeling than currently exists.

Keywords: fire, fire research, smoke, room fire tests, fire toxicity, smoke toxicity

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EXECUTIVE SUMMARY

Estimation of the times that building occupants will have to escape, find a place of refuge, or survive in place in the event of a fire is a principal component in the fire hazard or risk assessment of a facility. An accurate assessment enables public officials and facility owners to provide a selected or mandated degree of fire safety with confidence. Without this confidence, regulators and/or designers tend to apply large safety factors to lengthen the tenable time. This can increase the cost in the form of additional fire protection measures and can eliminate the consideration of otherwise desirable facility designs and construction products. Error in the other direction is also risky, in that if the time estimates are incorrectly long, the consequences of a fire could be unexpectedly high.

Such fire safety assessments now rely on some form of computation that takes into account multiple, diverse factors, including the facility design, the capabilities of the occupants, the potential growth rate of a design fire, the spread rates of the heat and smoke, and the impact of the fire effluent (toxic gases, aerosols, and heat) on people who are in or moving through the fire vicinity. The toolkit for these assessments includes computer models of the movement and distribution of fire effluent throughout a facility, laboratory devices which are routinely used to generate information on the rate of heat release as a commercial product burns, and a number of standards from ISO TC92 SC3 that provide support for the generation and use of fire effluent information in fire hazard and risk analyses. Of particular importance is ISO 13571, which provides consensus equations for estimating the human incapacitating exposures to the narcotic gases, irritant gases, heat, and smoke generated in fires.

More problematic are the sources of data for the production of these harmful products of combustion. Different materials can generate fire effluent with a wide range of toxic potencies. Most furnishing and interior finish products are composed of multiple materials assembled in a variety of geometries, and there is as of yet no methodology for predicting the evolved products from these complex assemblies.

An analysis of the U.S. fire fatality data showed that postflashover fires comprise the leading scenario for life loss from smoke inhalation. Thus, it is most important to obtain data regarding the generation of harmful species under postflashover (or otherwise underventilated) combustion conditions. Data for preflashover (well-ventilated) flaming conditions have value for ascertaining the importance of prolonged exposure to "ordinary" fire effluent and to short exposures to effluent of high potency.

The universal metric for the generation of a toxic species from a burning specimen is the yield of that species, defined as the mass of the species generated divided by the consumed mass of the specimen. These yields are input to the calculations used to estimate fire hazard.

A base set of the most prevalent harmful species is given in ISO 13571. To obtain an indicator of whether the base list of toxic species needs to be enhanced, living organisms should also be exposed to the fire effluent. However, it is recognized that animal testing is not always possible. In these cases, it is important to identify, from elemental analysis of the fuel and its degradation chemistry, a reasonable list of the combustion products that might be harmful to people.

Typically, the overall effluent from a harmful fire is determined by the large combustibles, such as a bed or a row of auditorium seats. The ideal fire test specimen for obtaining the yields of effluent components is the complete combustible item, with the test being conducted in an

enclosure of appropriate size. Unfortunately, reliance on real-scale testing of commercial products is impractical, both for its expense per test and for the vast number of commercial products used in buildings. Such testing *is* practical for forensic investigations in which there is knowledge of the specific items that combusted.

A more feasible approach for obtaining toxic gas yields for facility design involves the use of a physical fire model – a small-scale combustor that captures the essence of the combustible and of the burning environment of interest. The test specimen is an appropriate cutting from the full combustible. To have confidence in the accuracy of the effluent yields from this physical fire model, it must be demonstrated:

- How to obtain, from the full combustible, a representative cutting that can be accommodated and burned in the physical fire model;
- That the combustion conditions in the combustor (with the test specimen in place) are related to the combustion conditions in the fire of interest;
- How well, for a diverse set of combustible items, the yields from the small-scale combustor relate to the yields from real-scale burning of the full combustible items; and
- How sensitive the effluent yields are to the combustor conditions and to the manner in which the test specimen was obtained from the actual combustible item.

There have been numerous bench-scale devices that were intended for measuring the components of the combustion effluent, and at least three of these are under current scrutiny in the standards arena. Thus, before too long there may well be diverse (and perhaps conflicting) data on fire effluent component yields available for any given product. This situation does not support either assured fire safety or marketplace stability.

The National Institute of Standards and Technology (NIST) has completed a project to establish a technically sound protocol for assessing the accuracy of bench-scale device(s) for use in generating fire effluent yield data for fire hazard and risk evaluation. A related intent was to identify the most appropriate bench-scale device(s), in their current stage(s) of development, for obtaining accurate toxic gas yields.

In this protocol, the yields of harmful effluent components were determined for the real-scale burning of complete finished products during three fire stages: preflashover conditions, postflashover conditions, and underventilated burning in a closed room. These fuels were selected for diversity of physical form, combustion behavior, and the nature and yields of toxicants produced. They included "sofas" made of up to 14 upholstered cushions supported by a steel frame, particleboard bookcases with a laminated finish, and household wiring cable.

In each of these tests, the "preflashover" data were for an approximately two-minute period after flaming was established, but before the flames accelerated in intensity toward flashover. The "postflashover" data were for a period of similar length after flames filled the test room. Two of the sofa tests were performed with the test room door sealed, a replication of ventilation limited fire that did not proceed to room flashover.

Subsequently, NIST conducted bench-scale experiments with specimens cut from these combustibles and tested in four standard apparatus: (A) the radiant apparatus in NFPA 269 and NFPA E 1678, (B) the smoke density chamber in ISO 5659-2, (C) the tube furnace in ISO/TS 19700, and (D) a controlled-atmosphere version of the cone calorimeter (ASTM E 1354).

Each apparatus was operated according to the procedure in its Standard. In addition, the operating conditions in each apparatus were varied to determine the sensitivity of the test results to the test conditions and whether improved agreement with the room test results was possible. The variation included: cutting the test specimen into small pieces, varying the initial oxygen volume fraction, varying the added heat flux. For the tube furnace, some of the tests included varying the mass combusted and the air flow, while preserving the same fuel/air equivalence ratio. The standard for Apparatus C includes protocols for both well ventilated and underventilated combustion. The standards for the other three apparatus more closely replicate well ventilated burning. Varying the initial oxygen level was intend to examine the utility of the apparatus for burning in a vitiated environment.

The concentrations of CO₂, CO, and O₂ were monitored using species-specific analyzers. Fourier transform infrared (FTIR) spectroscopy was used to monitor CO₂, CO, HCN, HCl, NO, NO₂, H₂CO (formaldehyde), and C₃H₄O (CH₂=CH-CH=O, acrolein). For all the gases except CO₂ and CO, many or all of the measurements were below or close to the limits of detection. The upper limits to the gas yields were calculated using the detection limits.

The equations in ISO 13571 were used to estimate the relative contributions of these gases to the tenability of the fire environment. The results for each of the test series are presented in referenced individual reports. Not surprisingly, the contribution of some of these gases to compromised tenability was of second order. This unimportance of secondary toxicants is consistent with the results of the animal experiments used to establish the N-gas hypothesis that attributes fire effluent lethality to a small number of gases.

The test specimens in the apparatus A, B, and D were similar. The specimens of the same layout as in the finished product and were exposed to similar levels of thermal irradiation from above. The air flow to the burning zone was determined by natural convection. The tube dimensions in apparatus C necessitated using a long, narrow test specimen, and the specimen was heated on all sides. A preselected stream of air flowed to and over the specimen.

It was necessary to develop criteria to characterize the degree of agreement between the gas yields from the bench-scale apparatus and the room tests. In practice, the needed accuracy is appropriately defined in terms of the acceptable uncertainty in the calculated times at which survival in a burning building is compromised. For the current study, it was decided that the calculation of the two markers of toxic potency, the fractional effective dose (FED) due to inhalation of narcotic gases and the fractional effective concentration (FEC) due to exposure to sensory irritants, each be sufficiently accurate to identify significant deviations from "ordinary" toxic hazard. Given the current state of the art in fire modeling and the limits of precision of the IC₅₀ data, it was deemed reasonable that the accuracy be within a factor of two.

The accuracies of the yields of the toxic gases are not equally important. Due to the prevalence of fire deaths due to smoke being from postflashover fires, a greater importance was attached to the postflashover gas yields. The yield of CO₂ affects the carbon balance, and thus the relationship between the gas yields and the heat release. This, in turn, affects the calculated room temperatures and the burning rates of combustibles. It also exponentially increases a person's breathing rate and thus the volume of inhaled smoke. CO is an important toxicant in virtually all fires. When nitrogen is present in the fuel, it can also be a significant contributor to the FED. All three fuels in this study were nitrogen-containing, but HCN was only a contributor to the FED from the sofa materials. The cable was the only fuel that contained a high mass

fraction of Cl, and HCl dominated the FEC. For the other two fuels, all the irritant concentrations were low, and tenability was dominated by the narcotic gases.

The findings regarding the comparison between the gas yields from the room-scale tests and the bench-scale apparatus were as follows.

- CO₂: The yields from apparatus A, B, and D were within experimental uncertainty of the postflashover room test yield and within a factor of 2 of the preflashover yield.
 - The underventilated yield from apparatus C was low compared to the postflashover room value, and the well ventilated value was in agreement with the preflashover room value.
 - The CO₂ yields from all four apparatus agreed with the sofa material yield from the closed room tests to within a factor of 2.
- CO: None of the apparatus generated CO volume fractions comparable to the 0.2 value compiled from multiple series of postflashover room tests. This is because the postflashover CO yields result from room conditions that are not readily replicated in a simple bench-scale device. The yield value of 0.2 should be used in hazard calculations.
 - The yields from Apparatus A and D agreed with the preflashover room yield within a factor of 2. Decreasing the oxygen volume fraction to 0.16 in Apparatus D appears to have improved the agreement.
 - A decrease in the oxygen volume fraction to 0.18 in Apparatus D led to agreement with the closed room yield.
- HCl: For the cable, the yields from Apparatus A and D were within experimental uncertainty of the postflashover room yield. Decreasing the oxygen volume fraction in Apparatus D degraded the agreement, but it was still well within a factor of 2. The yields from Apparatus B and C were within a factor of 2 of the room test yield.
 - The yields from all four apparatus were very high compared to the preflashover room test yield, which was a very low value.
 - The upper limits of the HCl yields from the bench-scale tests of the sofa materials were too high for quantitative comparison with the very low yield from the closed room tests.
- HCN: The underventilated yield from Apparatus C tests of the sofa materials was within a factor of 2 of the postflashover room yield. The value from Apparatus D at an oxygen volume fraction of 0.21 was very low, but at a volume fraction of 0.16, the agreement was within experimental error. The values from the other apparatus were very low.
 - The values for the sofa materials from Apparatus A, C, and D agreed with the preflashover room value within experimental uncertainty.
 - The yields from the bench-scale tests of the sofa materials were within a factor of 2 of the closed room values for Apparatus A and D. The yield from Apparatus C operated at underventilated conditions was very high.

The CO₂ yields for underventilated burning of all three types of test specimens burned in the tube furnace were notably very low. We were unable to account for approximately two-thirds of the carbon. Qualitatively, there was no evidence in the FTIR spectra of large concentrations of gasified organic material, nor was there unusual residue in the downstream portion of the tube or

in the collection chamber. The mass losses from the test specimens were close to the mass losses in the other three bench-scale apparatus. This an issue that merits further research.

It should not be surprising that physical fire models, being imperfect approximations of some stage of real-scale burning, did not precisely predict the yields of multiple toxic gases from a set of diverse, non-homogeneous products that burned quite differently from each other. It should also not be surprising that under certain test conditions, the yields from both the room tests and the physical fire models showed large uncertainties. Nonetheless, one of the purposes of this project was to identify the more promising physical fire models to use for obtaining input data for fire hazard and risk analysis. The data indicate the following choices:

Underventilated fires:

• The cone calorimeter operated at 50 kW/m² and a reduced oxygen volume fraction in the range of 0.16 to 0.18.

Well ventilated fires:

• The cone calorimeter operated at 50 kW/m² and an oxygen volume fraction of 0.21. None of the apparatus predict the HCl yield within a factor of two.

There are some recommendations regarding modifications to the standard operating conditions for these physical fire models.

- In all cases, the CO yields from the physical fire model should be adjusted to 0.2.
- In the radiant furnace, the shutter isolating the combustion chamber from the collection chamber should be closed immediately following the cessation of flaming.
- For the products examined, there was no sizable effect of cutting the specimens into small pieces. However, it is likely that the effect would be significant if some or all of the combustible mass were intentionally being protected by a fire barrier.
- The extensive ongoing research using various designs of the cone calorimeter with variable oxygen volume fraction and total inflow should include measurement of toxic species. This would further refine the operating conditions that provide the broadest agreement with the gas yields from room fire tests.

Further investigation of the tube furnace is warranted. It is important to understand why the CO₂ yields for the underventilated condition are low and why the yields from the well ventilated condition are in agreement with the postflashover fire stages of the room fires for all three combustibles. It would also be helpful to understand the observed changes in some yields when the same equivalence ratio was achieved with different combinations of mass and air flow.

The results of this study provide a better basis for obtaining toxic potency input data for fire modeling than currently exists. A more robust basis for future engineering assessments of fire safety designs would result from the performance of

- Room-scale tests with more combustibles and room placements.
- Parametric runs of a zone or field fire model in order to define better the effect of input data accuracy and variability on the times to threats to building occupant life safety.

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I. INTRODUCTION

A. CONTEXT OF THE RESEARCH

Estimation of the times that building occupants will have to escape, find a place of refuge, or survive in place in the event of a fire is a principal component in the fire hazard or risk assessment of a facility. An accurate assessment enables public officials and facility owners to provide a selected or mandated degree of fire safety with confidence. Without this confidence, regulators and/or designers tend to apply large safety factors to lengthen the tenable time. This can increase the cost in the form of additional fire protection measures and can eliminate the consideration of otherwise desirable facility designs and construction products. Error in the other direction is also risky, in that if the time estimates are incorrectly long, the consequences of a fire could be unexpectedly high.

Such fire safety assessments now rely on some form of computation that takes into account multiple, diverse factors, including the facility design, the capabilities of the occupants, the potential growth rate of a design fire, the spread rates of the heat and smoke, and the impact of the fire effluent (toxic gases, aerosols, and heat) on people who are in or moving through the fire vicinity.¹ The toolkit for these assessments, while still evolving, has achieved some degree of maturity and quality. The kit includes such tools as:

- Computer models of the movement and distribution of fire effluent throughout a facility.
 - O Zone models, such as CFAST², have been in use for over two decades. This model takes little computational time, a benefit achieved by simplifying the air space in each room into two zones. A number of laboratory programs, validation studies,³ and reconstructions of actual fires have given credence to the predictions.⁴
 - O Computational fluid dynamics (CFD) models, such as the Fire Dynamics Simulator (FDS)⁵, have seen increased use over the past decade. FDS is more computationally intense than CFAST in order to provide three-dimensional temperature and species concentration profiles. There has been extensive verification and validation of FDS predictions.⁵

These models calculate the temperatures and combustion product concentrations as the fire develops. These profiles can be used for estimating when a person would die or be incapacitated, *i.e.*, is no longer able to effect his/her own escape.

- Devices such as the cone calorimeter⁶ and larger scale apparatus⁷, which are routinely used to generate information on the rate of heat release as a commercial product burns.
- A number of standards from ISO TC92 SC3 that provide support for the generation and use of fire effluent information in fire hazard and risk analyses. Of particular importance is ISO 13571, which provides consensus equations for estimating the human incapacitating exposures to the narcotic gases, irritant gases, heat, and smoke generated in fires 9

More problematic are the sources of data for the production of the harmful products of combustion. Different materials can generate fire effluent with a wide range of toxic potencies. Most furnishing and interior finish products are composed of multiple materials assembled in a variety of geometries, and there is as of yet no methodology for predicting the evolved products

from these complex assemblies. Furthermore, the generation of carbon monoxide (CO), the most common toxicant, can vary by orders of magnitudes, depending on the fire conditions. ¹⁰

An analysis of the U.S. fire fatality data¹¹ showed that postflashover fires comprise the leading scenarios for life loss from smoke inhalation. Thus, it is most important to obtain data regarding the generation of harmful species under postflashover (or otherwise underventilated) combustion conditions. Data for preflashover (well-ventilated) flaming conditions have value for ascertaining the importance of prolonged exposure to "ordinary" fire effluent and to short exposures to effluent of high potency.

B. OBTAINING INPUT DATA

The universal metric for the generation of a toxic species from a burning specimen is the yield of that species, defined as the mass of the species generated divided by the consumed mass of the specimen.¹² If both the mass of the test specimen and the mass of the evolved species are measured continuously during a test, then it is possible to obtain the yields of the evolved species as the burning process, and any chemical change within the specimen, proceeds. If continuous measurements are not possible, there is still value in obtaining a yield for each species integrated over the burning history of the test specimen.

The concentrations of the gases (resulting from the yields and the prevalent dilution air) are combined using the equations in ISO 13571 for a base set of the most prevalent toxic species. Additional species may be needed to account for the toxic potency of the fire-generated environment.

To obtain an indicator of whether the base list of toxic species needs to be enhanced, living organisms should also be exposed to the fire effluent. The effluent exposure that generates an effect on the organisms is compared to the effect of exposure to mixtures of the principal toxic gases. Disagreement between the effluent exposure and the mixed gas exposure is an indicator of effluent components not included in the mixed gas data or the existence of synergisms or antagonisms among the effluent components. This procedure has been standardized, based on data developed using laboratory rats. ^{13,14} However, it is recognized that animal testing is not always possible. In these cases, it is important to identify, from the elemental analysis of the fuel and its degradation chemistry, a reasonable list of the combustion products that might be harmful to people.

Typically, the overall effluent from a harmful fire is determined by the large combustibles, such as a bed or a row of auditorium seats. The ideal fire test specimen for obtaining the yields of effluent components is the complete combustible item, with the test being conducted in an enclosure of appropriate size. Unfortunately, reliance on real-scale testing of commercial products is impractical, both for its expense per test and for the vast number of commercial products used in buildings. Such testing *is* practical for forensic investigations in which there is knowledge of the specific items that combusted.

A more feasible approach for obtaining toxic gas yields for facility design involves the use of a physical fire model – a small-scale combustor that captures the essence of the combustible and of the burning environment of interest. The test specimen is an appropriate cutting from the full combustible. To have confidence in the accuracy of the effluent yields from this physical fire model, it must be demonstrated:

- How to obtain, from the full combustible, a representative cutting that can be accommodated and burned in the physical fire model;
- That the combustion conditions in the combustor (with the test specimen in place) are related to the combustion conditions in the fire of interest, generally preflashover flaming (well ventilated or underventilated), postflashover flaming, pyrolysis, or smoldering;
- How well, for a diverse set of combustible items, the yields from the small-scale combustor relate to the yields from real-scale burning of the full combustible items; and
- How sensitive the effluent yields are to the combustor conditions and to the manner in which the test specimen was obtained from the actual combustible item.

Historically, there have been numerous bench-scale devices that were intended for measuring the components of the combustion effluent. The combustion conditions and test specimen configuration in the devices vary widely, and some devices have flexibility in setting those conditions. Currently, ISO TC92 SC3 (Fire Threat to People and the Environment) is proceeding toward standardization of one of these devices, a tube furnace (ISO/TS 19700¹⁷) and is considering standardization of another, the cone calorimeter (ISO 5660-1⁶) with a controlled combustion environment. There are concurrent efforts in Europe and ISO to upgrade the chemical analytical capability for a closed box test (ISO 5659-2¹⁸). Thus, before too long there may well be diverse (and perhaps conflicting) data on fire effluent component yields available for any given product. This situation does not support either assured fire safety or marketplace stability.

Only one device, used in both NFPA 269¹³ and ASTM E1678¹⁴, has been validated with animal exposure and gas measurement data against real-scale fire test data for the same materials, and then only for postflashover yields of the principal toxicants.¹⁹ The three, relatively homogeneous materials were Douglas fir, a rigid polyurethane foam, and an unplasticized PVC. The toxicology of the combustion products varied significantly among the three materials. Laboratory rats were exposed to the combustion effluent for 30 min and then observed for 14 days. The times of any animal deaths were recorded. The yields of the principal toxicants were also determined.

The validation was conducted according to five hypotheses:

- 1. The equal LC₅₀ hypothesis: LC₅₀ valuesⁱ, as measured in the bench-scale test and in the real scale, agree to within the acceptable uncertainty.
- 2. The primary toxic gas hypothesis: The bench-scale test shows the same primary toxic gases as the real-scale test.
- 3. The equal yields hypothesis: The yields of the measured toxic gases are the same, to within the acceptable uncertainty, in the bench-scale and in the real-scale tests.
- 4. The N-gas hypothesis: The real-scale and the bench-scale results agree, to with the acceptable uncertainty, with predictions based on measured gas concentration and computations made according to the N-gas Model.ⁱⁱ

ⁱ The LC₅₀ is the concentration of a species or of smoke that leads to the death of half (50 %) of the test animals within a specified time interval. An analogous metric is the IC₅₀, where the observed response is incapacitation.

5. The type-of-death hypothesis: The type of death (within- or post-exposure) is similar for the bench-scale and for the real-scale tests.

The agreement between the bench-scale results and the real-scale results was deemed to be within a factor of three, based on the hypothesis with the *worst* agreement. The LC₅₀ values agreed within approximately \pm 50 %.

At some point, there will be sufficient data to imbue confidence that testing of further combustibles in a particular physical fire model will generate yields of effluent components with a consistent degree of accuracy.

ⁱⁱ When polymeric materials are thermally decomposed and burned, there are hundreds of species in the effluent. The N-gas model postulates that the toxic potency of the effluent can be substantially explained using a small number, N, of these species. Typically, N is fewer than 10.

II. TESTING IN THIS PROJECT

A. APPROACH

The National Institute of Standards and Technology (NIST) has completed a project to establish a technically sound protocol for assessing the accuracy of bench-scale device(s) for use in generating fire effluent yield data for fire hazard and risk evaluation. In this protocol, the yields of harmful effluent components were determined for the real-scale burning of complete finished products during both preflashover and postflashover conditions. Specimens cut from these products were then burned in various types of bench-scale combustors using their standard test protocols. These test protocols were then varied within the range of the combustion conditions related to these fire stages to determine the sensitivity of the test results to the test conditions and to provide a basis for improving the degree of agreement with the yields from the room-scale tests.

This project did not explicitly include the nonflaming fire stages. While there is evidence that people can experience lethal exposures to the smoke from smoldering fires, it was apparent that none of the bench-scale devices were intended for repeatable creation of this form of combustion. The nature and yields of pyrolysis products are sensitive to the geometry of the location of the heating source, its interaction with the test specimen, and the volume fraction of oxygen in the air. Therefore, study of these fire stages was reserved for future consideration.

B. ROOM-SCALE TESTS

Initially, NIST conducted room-scale fire tests of three combustible items.²⁰ These fuels were selected for diversity of physical form, combustion behavior, and the nature and yields of toxicants produced.

- "Sofas" made of up to 14 upholstered cushions supported by a steel frame. The cushions consisted of a zippered cotton-polyester fabric over a block of a flexible polyurethane (FPU) foam. The fire retardant in the cushion padding contains chlorine atoms. Thus, this fuel would be a source of CO₂, CO, HCN, HCl, and partially combusted organics. The ignition source was the California TB133 propane ignition burner²¹ faced downward, centered over the center of the row of seat cushions. The sofa was centered along the rear wall of the burn room facing the doorway. Two of the sofa tests were conducted in a closed room to examine the effect of vitiation on fire effluent generation. In these, an electric "match" was used to initiate the fires.
- Particleboard (ground wood with a urea formaldehyde binder) bookcases with a laminated polyvinylchloride (PVC) finish. This fuel would be a source of CO₂, CO, partially combusted organics, HCN, and HCl. To sustain burning, two bookcases were placed in a "V" formation, with the TB133 burner facing upward under the lower shelves.

• Household wiring cable, consisting of two 14 gauge copper conductors insulated with nylon and polyvinyl chloride (PVC), an uninsulated ground conductor, two paper filler strips, and an outer jacket of plasticized PVC. This fuel would be a source of CO₂, CO, HCl, and partially combusted organics. Two cable racks containing 3 trays each supported approximately 30 kg of cable in each of the bottom two trays and approximately 17 kg in each of the middle and top trays. The cable trays were placed parallel to the rear of the burn room. Twin propane ignition burners were centered under the bottom tray of each rack.

Data on these fuels are included as Appendix A.

In each of these tests, the "preflashover" data were for an approximately two-minute period after flaming was established, but before the flames accelerated in intensity toward flashover. The "postflashover" data were for a period of similar length after flames filled the test room.

Two sofa tests were performed with the test room door sealed. The effluent was sampled from the upper layer of the burn room. In both tests, the oxygen volume fraction declined to approximately 0.11 near 300 s into the test. At 500s, the oxygen volume fraction had stabilized at 0.12, indicating that any continuing combustion was minimal and that the gas mixing in the room was nominally complete. Thus, the calculated gas yields at 500 s were used for comparison with the bench-scale data described next.

B. BENCH-SCALE TESTS

Subsequently, NIST conducted bench-scale experiments with specimens cut from these combustibles and tested in four standard apparatus.

- The radiant apparatus in NFPA 269¹³ and NFPA E 1678¹⁴, with the NIST testing described in Reference 22.
- The smoke density chamber in ISO 5659-2¹⁸, with the NIST testing described in Reference 23.
- A controlled-atmosphere version of the cone calorimeter (ASTM E 1354⁶), with the NIST testing described in Reference 24.
- The tube furnace in ISO/TS 19700¹⁷, with the NIST testing described in Reference 25.

The test specimens for the bookcase and cable tests were pieces of the actual combustible -a slab of the laminated particle board and lengths of the cable, respectively. The sofa material specimens in the first three apparatus were a layer of fabric over a slab of the foam. A similar array was cut to shape to fit in the tube furnace.

Each apparatus was operated according to the procedure in its Standard. In addition, the operating conditions in each apparatus were varied to determine whether improved agreement with the room test results was possible. One of the variations, common to all the bench-scale tests but the cone calorimeter, was to cut the test specimen into small pieces. This increased the surface area for burning. For the cable, this also increased the direct exposure of the nylon jacketing to air and the external flux field. Diced specimens were not tested in the cone calorimeter because data from the other three apparatus, all of which also involved radiative exposure of the test specimens, showed little to no effect of this variation.

The other variations were:

- Radiant apparatus. The initial oxygen volume fraction was reduced to 0.17.
- Smoke density chamber. This was operated at three of the prescribed conditions: 50 kW/m² irradiance with and without a pilot flame, and 25 kW/m² irradiance with a pilot flame.
- Cone calorimeter. All tests were performed with a housing encasing the load cell and radiant source and sealed to the collection hood. The oxygen volume percent in the incoming air was reduced to as low as 14 %. The specimen irradiance was either 50 kW/m² or 25 kW/m². In some tests, the air flow past the specimen was reduced by half to 12.5 L/s.
- Tube furnace. This was operated at the two prescribed temperatures, 650 °C and 825 °C, to generate well ventilated and underventilated conditions, respectively. In some tests, the air flow was increased or decreased by 30 %, the mass of the specimen was doubled, or the feed rate of the specimen through the furnace was increased by 50 %. In some of these combinations, the same fuel/air equivalence ratio was achieved under different combustion conditions.

During each test, except for those in the tube furnace, the mass of the test specimen was monitored continuously. Each tube furnace specimen was weighed at the beginning and end of a test. The concentrations of CO₂, CO, and O₂ were monitored using species-specific analyzers. Fourier transform infrared (FTIR) spectroscopy was used to monitor CO₂, CO, HCN, HCl, NO, NO₂, H₂CO (formaldehyde), and C₃H₄O (CH₂=CH-CH=O, acrolein). The uncertainties in the measurements are discussed in the cited reports. For all the gases except CO₂ and CO, many measurements were below or close to the limits of detection. The upper limits to the gas yields were calculated using the detection limits.

The equations in ISO 13571 were used to estimate the relative contributions of these gases to the tenability of the fire environment. The results for each of the test series are presented in the individual reports. Further discussion is presented later in this report. Not surprisingly, the contribution of some of these gases to compromised tenability was of second order. This unimportance of secondary toxicants is consistent with the results of the animal experiments used to establish the N-gas hypothesis that attributes fire effluent lethality to a small number of gases. ²⁶

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III. COMPILED DATA FROM ROOM- AND BENCH-SCALE TESTS

As reported in each of the four testing reports, the gases for which yield data were analyzed were CO₂, CO, HCl, HCN, NO₂, NO, acrolein, and formaldehyde. The data for the last four gases were always below the limits of detection, and it is not possible to perform a quantitative comparison between the data from the combustible objects and specimens cut from them. Furthermore, their contributions to tenability were secondary to the contributions of the first four gases. (This takes into account the authors' position that incapacitating exposure to acrolein is properly reflected by the baboon smoke exposure data from the Southwest Research Institute.²⁷) These results are not included in the compiled data tables below.

Table 1 presents the notional, or maximum possible, yields of the four toxic gases for the room-scale and bench-scale tests. These were calculated as follows:

- CO₂: Assume all the carbon in the test specimen is converted to CO₂. Multiply the mass fraction of C in the test specimen (Appendix A) by the ratio of the molecular mass of CO₂ to the atomic mass of carbon.
- CO: Assume all the carbon in the test specimen is converted to CO. Multiply the mass fraction of C by the ratio of the molecular mass of CO to the atomic mass of carbon.
- HCN: Assume all the nitrogen in the test specimen is converted to HCN. Multiply the mass fraction of N by the ratio of the molecular mass of HCN to the atomic mass of nitrogen.
- HCl: Assume all the chlorine in the test specimen is converted to HCl. Multiply the mass fraction of Cl by the ratio of the molecular mass of HCl to the atomic mass of Cl.

The notional yields from the bookcase and cable specimens were assumed to be the same as the yields from the intact combustibles. The sofa specimen tests contained slightly different relative masses of fabric and foam.

| Table 1. | Calculated Notional | Yields of Toxic | Products from the | Test Specimens. |
|----------|---------------------|------------------------|-------------------|-----------------|
|----------|---------------------|------------------------|-------------------|-----------------|

| | | Notional Yields | | | | | | | | | | | | |
|--------|-------------------|------------------|--------------------|--------------------|--|--|--|--|--|--|--|--|--|--|
| | | | Sofa | | | | | | | | | | | |
| Gas | Bookcase | Cable | Room tests | Bench-scale tests | | | | | | | | | | |
| CO_2 | $1.72 \pm 1 \%$ | 2.11 ± 1 % | 2.00 ± 4 % | $1.95 \pm 4 \%$ | | | | | | | | | | |
| CO | $1.09 \pm 1 \%$ | $1.33 \pm 1 \%$ | $1.27 \pm 4 \%$ | $1.24 \pm 4 \%$ | | | | | | | | | | |
| HCN | $0.057 \pm 13 \%$ | $0.040 \pm 6 \%$ | $0.193 \pm 4 \%$ | $0.193 \pm 4 \%$ | | | | | | | | | | |
| HC1 | $0.0026 \pm 4 \%$ | $0.332 \pm 1 \%$ | $0.0070 \pm 19 \%$ | $0.0069 \pm 19 \%$ | | | | | | | | | | |

The uncertainty in the notional yield values is determined by the uncertainty in the prevalence of the central element (in the bullets just above) in the combustible. For the cuttings from the sofas, the uncertainty in the notional yields was increased by the small variability, estimated at 3 percent, in the relative masses of the fabric and padding materials in the test specimen.

Table 2 through Table 4 report the yields of these four gases as compiled from References 20 and 22 through 25. Table 5 through Table 7 present the calculated fractions of the notional yields of the gases for the three types of specimens. The numbers in parentheses are the percent uncertainties.

Table 2. Yields of Combustion Products from Bookcase Specimens

| | Yields | | | | | | | | elds | S | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|---------|------------------------------------|-----------------------------|-----------------------------|-----------------------------|--|
| Test Type | | Tes | t Variables | | | | CO_2 | СО | HCl | HCN | |
| Room | Ventilation | | | | | | | | | | |
| | Preflashover | | | | | 0.50 | | 2.4 x 10 ⁻² (55) | 2.2 x 10 ⁻³ (75) | 4.6 x 10 ⁻⁴ (10) | |
| | Postflashover | | | | | 1.89 (5 | :0) | 4.6 x 10 ⁻² (30) | 2.2 x 10 ⁻³ (65) | 2.5 x 10 ⁻³ (45) | |
| | Closed room | | | | | (7 | (5) | | | | |
| Radiant | O ₂ initial | Specimen | | | | (, | 3) | | | | |
| furnace | 0.21 | intact | | | | 0.88 | (8) | 1.8 x 10 ⁻² (40) | 3 x 10 ⁻⁴ (x 3) | < 2 x 10 ⁻⁴ | |
| | 0.21 | diced | | | | 0.91 | (8) | 1.7 x 10 ⁻² (15) | 6 x 10 ⁻⁴ (45) | < 1 x 10 ⁻⁴ | |
| | 0.17 | Intact | | | | 0.84 | (8) | 1.8 x 10 ⁻² (8) | < 2 x 10 ⁻⁴ | < 2 x 10 ⁻⁴ | |
| | 0.17 | diced | | | | 0.76 | (8) | 2.1 x 10 ⁻² (14) | < 8 x 10 ⁻⁴ | < 1 x 10 ⁻⁴ | |
| Smoke | Irradiance (kW/m²) | Pilot | | | | | | | | | |
| density | 50 | unpiloted | | | | 0.20 | (48) | 7.3 x 10 ⁻² (40) | < 5 x 10 ⁻⁴ | < 6 x 10 ⁻⁴ | |
| chamber | 50 | piloted | | | | 1.06 | (12) | $< 4 \times 10^{-4}$ | < 5 x 10 ⁻⁴ | $< 6 \times 10^{-4}$ | |
| | 25 | piloted | | | | | | | | | |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | | | |
| | 650 °C | intact | 1 | 1 | 1 | 1.43 | (3) | $< 1 \times 10^{-3}$ | < 1 x 10 ⁻³ | < 2 x 10 ⁻³ | |
| | (well ventilated) | diced | 1 | 1 | 1 | 1.49 | (5) (5) | $< 1 \times 10^{-3}$ | < 2 x 10 ⁻³ | < 2 x 10 ⁻³ | |
| | | intact | x 1.3 | 1 | 1 | 1.66 | (1) | < 1 x 10 ⁻³ | < 2 x 10 ⁻³ | < 2 x 10 ⁻³ | |
| | | intact | x2 | x 2 | 1 | 1.58 | | $< 6 \times 10^{-4}$ | < 1 x 10 ⁻³ | $< 1 \times 10^{-3}$ | |
| | | intact | x1.5 | 1 | x 1.5 | 0.83 | (7) (11) | < 8 x 10 ⁻⁴ | < 1 x 10 ⁻³ | < 1 x 10 ⁻³ | |
| | 825 °C | intact | 1 | 1 | 1 | 0.36 | (38) | 6.2 x 10 ⁻² (45) | < 2 x 10 ⁻³ | $< 2 \times 10^{-3}$ | |
| | (underventilated) | diced | 1 | 1 | 1 | 0.29 | (2) | 4.0 x 10 ⁻² (21) | < 2 x 10 ⁻³ | $< 2 \times 10^{-3}$ | |
| | | intact | x 0.7 | 1 | 1 | 0.21 | (2) (9) | 6.3 x 10 ⁻² (21) | $< 2 \times 10^{-3}$ | $< 2 \times 10^{-3}$ | |
| | | intact | x2 | x 2 | 1 | 0.31 | (10) | 5.7 x 10 ⁻² (16) | < 1 x 10 ⁻³ | $< 1 \times 10^{-3}$ | |
| | | intact | x1.5 | 1 | x 1.5 | 0.28 | (8) | $5.0 \times 10^{-2} $ (9) | $< 1 \times 10^{-3}$ | $< 1 \times 10^{-3}$ | |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | | (0) | | | | |
| calorimeter | 50 | 25 | 21 | | | 1.11 | (2) | 1.0 x 10 ⁻² (8) | $< 7 \times 10^{-3}$ | < 9 x 10 ⁻³ | |
| | | | 18 | | | 1.10 | (0.1) | 1.3 x 10 ⁻² (3) | $< 7 \times 10^{-3}$ | $< 9 \times 10^{-3}$ | |
| | | | 16 | | | 1.06 | (4) | 1.9 x 10 ⁻² (7) | $< 7 \times 10^{-3}$ | < 8 x 10 ⁻³ | |
| | 50 | 12.5 | 21 | | | 1.02 | (1) | 0.6×10^{-2} (3) | $< 4 \times 10^{-3}$ | $< 4 \times 10^{-3}$ | |
| | | | 16 | | | 1.03 | (0.5) | $0.9 \times 10^{-2} $ (9) | $< 4 \times 10^{-3}$ | $< 5 \times 10^{-3}$ | |
| | | | 14 | | | 0.93 | (0.3) | 3.2×10^{-2} (1) | $< 4 \times 10^{-3}$ | $< 5 \times 10^{-3}$ | |
| | 25 | 25 | 21 | | | 1.14 | (1) | 1.9 x 10 ⁻² (20) | | | |
| | | | 18 | | | 0.89 | (4) | 2.3 x 10 ⁻² (17) | | | |
| | | | 16 | | | 0.85 | (1) | 2.7 x 10 ⁻² (1) | | | |

Table 3. Yields of Combustion Products from Sofa Specimens

| | Yields | | | | | | | | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|-----------------------------|------------------------------|-----------------------------|------------------------------|
| Test Type | | Tes | t Variables | | | CO ₂ | СО | HCl | HCN |
| Room | Ventilation | | | | | | | | |
| | Preflashover | | | | | 1.59 | 1.4 x 10 ⁻² (35) | 1.8 x 10 ⁻² (30) | 3.5 x 10 ⁻³ (50) |
| | Postflashover | | | | | 1.13 (25) | 5.1 x 10 ⁻² (25) | 6.0 x 10 ⁻³ (35) | 1.5 x 10 ⁻² (25) |
| | Closed room (500 s) | | | | | 1.13 (25) 0.92 (25) (10) | 3.6 x 10 ⁻² (2) | 4.6 x 10 ⁻⁴ (8) | 1.9 x 10 ⁻³ (4) |
| Radiant | O ₂ initial | Specimen | | | | (23) | | | |
| furnace | 0.21 | intact | | | | 1.68 (10) | 2.8 x 10 ⁻² (32) | < 1 x 10 ⁻³ | < 3 x 10 ⁻³ |
| | 0.21 | diced | | | | 1.66 (7) | 3.4 x 10 ⁻² (15) | 1 x 10 ⁻³ (25) | 3.4 x 10 ⁻³ (45) |
| | 0.17 | Intact | | | | 1.64 (8) | 3.6 x 10 ⁻² (14) | < 7 x 10 ⁻⁴ | 1.0 x 10 ⁻³ (70) |
| | 0.17 | diced | | | | 1.59 (8) | 4.9 x 10 ⁻² (26) | < 5 x 10 ⁻⁴ | 3.4 x 10 ⁻³ (65) |
| Smoke | Irradiance (kW/m²) | Pilot | | | | (8) | | | |
| density | 50 | unpiloted | | | | 1.65 | 1.9 x 10 ⁻² (12) | < 3 x 10 ⁻³ | $< 4 \times 10^{-3}$ |
| chamber | 50 | piloted | | | | 1.65 (2) 1.33 (53) | 6.6 x 10 ⁻³ (x2) | < 3 x 10 ⁻³ | < 4 x 10 ⁻³ |
| | 25 | piloted | | | | 1.76 (60) | 4.3 x 10 ⁻³ (34) | $< 4 \times 10^{-3}$ | $< 6 \times 10^{-3}$ |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | |
| | 650 °C | intact | 1 | 1 | 1 | 1.87 | 2.6 x 10 ⁻² (10) | < 1 x 10 ⁻³ | $< 3 \times 10^{-3}$ |
| | (well ventilated) | diced | 1 | 1 | 1 | (9) | | | |
| | | intact | x 1.3 | 1 | 1 | 0.91 | 2.3 x 10 ⁻² (38) | < 2 x 10 ⁻³ | 3.2 x 10 ⁻³ (30) |
| | | intact | x2 | x 2 | 1 | 0.91 (5) | 1.0 x 10 ⁻² (31) | < 2 x 10 ⁻³ | $< 4 \times 10^{-3}$ |
| | | intact | x1.5 | 1 | x 1.5 | 0.79 (14) | 0.3 x 10 ⁻² (88) | < 3 x 10 ⁻³ | < 2 x 10 ⁻³ |
| | 825 °C | intact | 1 | 1 | 1 | 0.56 (7) | 1.43 x 10 ⁻¹ (1) | < 2 x 10 ⁻³ | 8.1 x 10 ⁻³ (33) |
| | (underventilated) | diced | 1 | 1 | 1 | (') | | | |
| | | intact | x 0.7 | 1 | 1 | 0.35 (10) | 1.66 x 10 ⁻¹ (4) | < 2 x 10 ⁻³ | 8.8 x 10 ⁻³ (19) |
| | | intact | x2 | x 2 | 1 | 0.23 (18) | | < 3 x 10 ⁻³ | 5.8 x 10 ⁻³ (19) |
| | | intact | x1.5 | 1 | x 1.5 | 0.28 (7) | 1.43 x 10 ⁻¹ (10) | < 2 x 10 ⁻³ | 9.8 x 10 ⁻³ (12) |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | (') | | | |
| calorimeter | 50 | 25 | 21 | | | 1.41 | 2.7 x 10 ⁻² (2) | < 5 x 10 ⁻³ | 3.7 x 10 ⁻³ (29) |
| | | | 18 | | | 1.41 (2) | 3.5 x 10 ⁻² (4) | < 6 x 10 ⁻³ | 7.7 x 10 ⁻³ (23) |
| | | | 16 | | | 1.46 (2) | 4.4 x 10 ⁻² (2) | < 6 x 10 ⁻³ | 1.25 x 10 ⁻² (15) |
| | 50 | 12.5 | 21 | | | 1.36 (3) | 2.4 x 10 ⁻² (1) | $< 3 \times 10^{-3}$ | 3.6 x 10 ⁻³ (15) |
| | | | 16 | | | 1.38 (4) | 3.5 x 10 ⁻² (7) | < 3 x 10 ⁻³ | 9.6 x 10 ⁻³ (43) |
| | | | 14 | | | 1.39 (1) | 3.3 x 10 ⁻² (4) | $< 3 \times 10^{-3}$ | 3.9 x 10 ⁻³ (50) |
| | 25 | 25 | 21 | | | 1.55 (6) | 2.4 x 10 ⁻² (1) | | |
| | | | 18 | | | 1.33 (30) | 2.9 x 10 ⁻² (16) | | |
| | | | 16 | | | 1.36 (51) | 2.0 -: 10-2 | | |

Table 4. Yields of Combustion Products from Cable Specimens

| | | | | | | Yields | | | | | | | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|---------|-----------------|------------------------------|-----------------------------|-----------------------------|--|--|--|
| Test Type | | Tes | t Variables | | | (| CO ₂ | CO | HCl | HCN | | | |
| Room | Ventilation | | | | | | | | | | | | |
| | Preflashover | | | | | 0.12 | | 5.5 x 10 ⁻³ (50) | 6.6 x 10 ⁻³ (35) | 6.3 x 10 ⁻⁴ (50) | | | |
| | Postflashover | | | | | 1.38 (4 | 5) | 1.48 x 10 ⁻¹ (15) | 2.1 x 10 ⁻¹ (15) | $4.0 \times 10^{-3} (30)$ | | | |
| | Closed room | | | | | (1 | 5 5 | | | | | | |
| Radiant | O ₂ initial | Specimen | | | | (1 | <i>J</i>) | | | | | | |
| furnace | 0.21 | intact | | | | 1.16 | (10) | 5.8 x 10 ⁻² (7) | 0.20 (35) | 9 x 10 ⁻³ (65) | | | |
| | 0.21 | diced | | | | 1.13 | (7) | $6.7 \times 10^{-2} (15)$ | 0.35 (40) | < 6 x 10 ⁻⁴ | | | |
| | 0.17 | Intact | | | | 1.05 | (8) | $6.2 \times 10^{-2} (30)$ | 0.25 (40) | 5 x 10 ⁻⁴ (50) | | | |
| | 0.17 | diced | | | | 1.24 | (8) | 7.3x 10 ⁻² (20) | 0.32 (18) | $< 7 \times 10^{-3}$ | | | |
| Smoke | Irradiance (kW/m²) | Pilot | | | | | (0) | | | | | | |
| density | 50 | unpiloted | | | | 1.12 | (5) | 3.0x 10 ⁻² (8) | 0.18 (50) | $< 2 \times 10^{-3}$ | | | |
| chamber | 50 | piloted | | | | 1.18 | (5) | 2.8x 10 ⁻² (7) | 0.05 (x^2) | $< 2 \times 10^{-3}$ | | | |
| | 25 | piloted | | | | 0.77 | (12) | 1.2x 10 ⁻² (17) | 0.10 (13) | $< 3 \times 10^{-3}$ | | | |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | (13) | | | | |
| | 650 °C | intact | 1 | 1 | 1 | 1.43 | (27) | 8.8 x 10 ⁻² (16) | 0.30 (34) | $< 3 \times 10^{-3}$ | | | |
| | (well ventilated) | diced | 1 | 1 | 1 | 1.33 | (6) | 9.1 x 10 ⁻² (9) | 0.30 (18) | $< 3 \times 10^{-3}$ | | | |
| | | intact | x 1.3 | 1 | 1 | 1.27 | (5) | $7.0 \times 10^{-2} (10)$ | 0.25 (14) | $< 3 \times 10^{-3}$ | | | |
| | | intact | x2 | x 2 | 1 | 1.15 | (6) | 7.1 x 10 ⁻² (9) | 0.19 (19) | $< 1 \times 10^{-3}$ | | | |
| | | intact | x1.5 | 1 | x 1.5 | 1.20 | | 6.5×10^{-2} (2) | 0.24 (14) | $< 2 \times 10^{-3}$ | | | |
| | 825 °C | intact | 1 | 1 | 1 | 0.33 | (2) (12) | $4.3 \times 10^{-2} (14)$ | 0.14 (29) | $< 3 \times 10^{-3}$ | | | |
| | (underventilated) | diced | 1 | 1 | 1 | 0.31 | (11) | 3.7 x 10 ⁻² (10) | 0.14 (19) | $< 3 \times 10^{-3}$ | | | |
| | | intact | x 0.7 | 1 | 1 | 0.22 | (1) | 9.8 x 10 ⁻² (20) | 0.14 (14) | $< 3 \times 10^{-3}$ | | | |
| | | intact | x2 | x 2 | 1 | 0.41 | (8) | 5.2 x 10 ⁻² (11) | 0.14 (16) | < 1 x 10 ⁻³ | | | |
| | | intact | x1.5 | 1 | x 1.5 | 0.49 | (2) | 9.0×10^{-2} (2) | 0.23 (12) | < 2 x 10 ⁻³ | | | |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | | (-) | | | | | | |
| calorimeter | 50 | 25 | 21 | | | 1.04 | (9) | 5.4 x 10 ⁻² (5) | 0.23 (14) | < 1.4 x 10 ⁻² | | | |
| | | | 18 | | | 1.17 | (3) | 6.7 x 10 ⁻² (4) | 0.26 (12) | $< 1.6 \times 10^{-2}$ | | | |
| | | | 16 | | | 1.11 | (7) | 7.1 x 10 ⁻² (11) | 0.30 (15) | < 1.7 x 10 ⁻² | | | |
| | 50 | 12.5 | 21 | | | 1.02 | (3) | 5.0×10^{-2} (3) | 0.22 (15) | < 0.7 x 10 ⁻² | | | |
| | | | 16 | | | 1.02 | (3) | 6.1 x 10 ⁻² (3) | 0.23 (14) | < 0.8 x 10 ⁻² | | | |
| | | | 14 | | | 0.88 | (6) | $5.4 \times 10^{-2} (10)$ | 0.28 (12) | < 0.9 x 10 ⁻² | | | |
| | 25 | 25 | 21 | | | 1.13 | (6) (6) | 5.1 x 10 ⁻² (1) | | | | | |
| | | | 18 | | | 1.28 | () | 6.3×10^{-2} (7) | | | | | |
| | | | 16 | | | 0.68 | (4) | 4.2×10^{-2} (6) | | | | | |
| | | | 1 | | ļ | | (6) | (0) | ļ | 12 | | | |

Table 5. Fractions of Notional Yields of Combustion Products from Bookcase Specimens

| | | | | | | | | | Yields | | | | | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|---------|--------------|-----------------------------|-----------------------------|-----------------------------|--|--|--|--|
| Test Type | | Tes | t Variables | | | | CO_2 | CO | HCl | HCN | | | | |
| Room | Ventilation | | | | | | | | | | | | | |
| | Preflashover | | | | | 0.29 | | 2.2 x 10 ⁻² (55) | 0.85 (75) | 8.1 x 10 ⁻³ (10) | | | | |
| | Postflashover | | | | | 1.10 (5 | :0) | 4.2 x 10 ⁻² (30) | 0.85 (65) | 4.4 x 10 ⁻² (45) | | | | |
| | Closed room | | | | | (3 | <u>(5)</u> | | | | | | | |
| Radiant | O ₂ initial | Specimen | | | | (, | 3) | | | | | | | |
| furnace | 0.21 | intact | | | | 0.51 | (9) | 1.7 x 10 ⁻² (40) | 0.12 (x3) | $< 4 \times 10^{-3}$ | | | | |
| | 0.21 | diced | | | | 0.53 | (9) | 1.6 x 10 ⁻² (15) | 2.3 x 10 ⁻¹ (60) | $< 2 \times 10^{-3}$ | | | | |
| | 0.17 | Intact | | | | 0.49 | (9) | 1.7 x 10 ⁻² (9) | < 8 x 10 ⁻² | $< 4 \times 10^{-3}$ | | | | |
| | 0.17 | diced | | | | 0.44 | (9) | 1.9 x 10 ⁻² (15) | < 3 x 10 ⁻¹ | < 2 x 10 ⁻³ | | | | |
| Smoke | Irradiance (kW/m²) | Pilot | | | | | | | | | | | | |
| density | 50 | unpiloted | | | | 0.12 | (50) | 7.0 x 10 ⁻² (40) | < 2 x 10 ⁻¹ | < 1 x 10 ⁻² | | | | |
| chamber | 50 | piloted | | | | 0.62 | (13) | < 4 x 10 ⁻⁴ | < 2 x 10 ⁻¹ | < 1 x 10 ⁻² | | | | |
| | 25 | piloted | | | | | | | | | | | | |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | | | | | | |
| | 650 °C | intact | 1 | 1 | 1 | 0.83 | (4) | < 1 x 10 ⁻³ | < 0.4 | < 0.04 | | | | |
| | (well ventilated) | diced | 1 | 1 | 1 | 0.87 | (6) | $< 1 \times 10^{-3}$ | < 0.8 | < 0.04 | | | | |
| | | intact | x 1.3 | 1 | 1 | 0.97 | (2) | < 1 x 10 ⁻³ | < 0.8 | < 0.04 | | | | |
| | | intact | x2 | x 2 | 1 | 0.92 | (8) | < 6 x 10 ⁻⁴ | < 0.4 | < 0.02 | | | | |
| | | intact | x1.5 | 1 | x 1.5 | 0.48 | (12) | < 7 x 10 ⁻⁴ | < 0.4 | < 0.02 | | | | |
| | 825 °C | intact | 1 | 1 | 1 | 0.21 | (40) | 5.7 x 10 ⁻² (45) | < 0.8 | < 0.04 | | | | |
| | (underventilated) | diced | 1 | 1 | 1 | 0.17 | (3) | 3.7 x 10 ⁻² (22) | < 0.8 | < 0.04 | | | | |
| | | intact | x 0.7 | 1 | 1 | 0.12 | (10) | 5.7 x 10 ⁻² (22) | < 0.8 | < 0.04 | | | | |
| | | intact | x2 | x 2 | 1 | 0.18 | (11) | 5.1 x 10 ⁻² (17) | < 0.4 | < 0.02 | | | | |
| | | intact | x1.5 | 1 | x 1.5 | 0.16 | (9) | 4.5 x 10 ⁻² (10) | < 0.4 | < 0.02 | | | | |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | | (2) | | | | | | | |
| calorimeter | 50 | 25 | 21 | | | 0.65 | (3) | $0.9 \times 10^{-2} $ (9) | < 3 | < 0.2 | | | | |
| | | | 18 | | | 0.64 | (1) | 1.2 x 10 ⁻² (4) | < 3 | < 0.2 | | | | |
| | | | 16 | | | 0.62 | (5) | 1.8 x 10 ⁻² (8) | < 3 | < 0.1 | | | | |
| | 50 | 12.5 | 21 | | | 0.59 | (2) | 0.6×10^{-2} (4) | < 2 | < 0.1 | | | | |
| | | | 16 | | | 0.60 | (<u>2</u>) | $0.8 \times 10^{-2} (10)$ | < 2 | < 0.09 | | | | |
| | | | 14 | | | 0.54 | (1) | 2.9 x 10 ⁻² (2) | < 2 | < 0.09 | | | | |
| | 25 | 25 | 21 | | | 0.66 | (2) | 1.7 x 10 ⁻² (21) | | | | | | |
| | | | 18 | | | 0.52 | (5) | 2.1 x 10 ⁻² (18) | | | | | | |
| | | | 16 | | | 0.49 | (2) | 2.5 x 10 ⁻² (2) | | | | | | |

Table 6. Fractions of Notional Yields of Combustion Products from Sofa Specimens

| | | | | | | | | | elds | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|------|----------------|-----------------------------------|-----------------------------|-----------------------------|
| Test Type | | Tes | t Variables | | | C | \mathbf{O}_2 | CO | HCl | HCN |
| Room | Ventilation | | | | | | | | | |
| | Preflashover | | | | | 0.80 | | 1.13 x 10 ⁻² (35) | 2.6 (30) | 1.8 x 10 ⁻³ (50) |
| | Postflashover | | | | | 0.57 | 5) | 4.0 x 10 ⁻² (25) | 0.86 (35) | 7.8 x 10 ⁻² (25) |
| | Closed room (500 s) | | | | | 0.46 | 5) (11) | 1.8 x 10 ⁻² (3) | 6.6 x 10 ⁻² (12) | 9.8 x 10 ⁻³ (5) |
| Radiant | O ₂ initial | Specimen | | | | (2. |)) | | | |
| furnace | 0.21 | intact | | | | 0.86 | (14) | 2.3 x 10 ⁻² (36) | < 0.2 | 5 x 10 ⁻² (70) |
| | 0.21 | diced | | | | 0.85 | (11) | 2.7 x 10 ⁻² (19) | 0.14 (45) | $< 3 \times 10^{-3}$ |
| | 0.17 | Intact | | | | 0.84 | (12) | 2.9 x 10 ⁻² (18) | < 0.1 | 3 x 10 ⁻³ (55) |
| | 0.17 | diced | | | | 0.82 | (12) | 4.09 x 10 ⁻² (30) | < 0.07 | < 4 x 10 ⁻² |
| Smoke | Irradiance (kW/m²) | Pilot | | | | | | | | |
| density | 50 | unpiloted | | | | 0.85 | (6) | 1.5 x 10 ⁻² (16) | < 0.4 | < 0.02 |
| chamber | 50 | piloted | | | | 0.68 | (60) | $5.3 \times 10^{-3} \text{ (x2)}$ | < 0.4 | < 0.02 |
| | 25 | piloted | | | | 0.90 | (65) | $3.5 \times 10^{-3} (40)$ | < 0.6 | < 0.03 |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | | |
| | 650 °C | intact | 1 | 1 | 1 | 0.96 | (13) | 2.6 x 10 ⁻² (10) | < 1 x 10 ⁻³ | < 0.02 |
| | (well ventilated) | diced | 1 | 1 | 1 | - | | | | |
| | | intact | x 1.3 | 1 | 1 | 0.47 | (9) | 1.9 x 10 ⁻² (40) | < 0.3 | 1.7 x 10 ⁻² (35) |
| | | intact | x2 | x 2 | 1 | 0.34 | (9) | 8.1 x 10 ⁻³ (35) | < 0.3 | < 0.02 |
| | | intact | x1.5 | 1 | x 1.5 | 0.41 | (18) | 0.2 x 10 ⁻³ (90) | < 0.4 | < 0.01 |
| | 825 °C | intact | 1 | 1 | 1 | 0.29 | (11) | 1.15 x 10 ⁻¹ (5) | < 0.3 | 4.2 x 10 ⁻² (37) |
| | (underventilated) | diced | 1 | 1 | 1 | | | | | |
| | | intact | x 0.7 | 1 | 1 | 0.18 | (14) | 1.3 x 10 ⁻¹ (8) | < 0.3 | 4.6 x 10 ⁻² (23) |
| | | intact | x2 | x 2 | 1 | 0.12 | (22) | 4.2 x 10 ⁻² (70) | < 0.4 | 3.0 x 10 ⁻² (23) |
| | | intact | x1.5 | 1 | x 1.5 | 0.14 | (11) | 1.12 x 10 ⁻¹ (14) | < 0.3 | 5.1 x 10 ⁻³ (16) |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | | | | | |
| calorimeter | 50 | 25 | 21 | | | 0.72 | (6) | 2.2 x 10 ⁻² (6) | < 0.7 | 1.9 x 10 ⁻² (33) |
| | | | 18 | | | 0.75 | (6) | 2.8 x 10 ⁻² (8) | < 0.9 | 4.0 x 10 ⁻² (27) |
| | | | 16 | | | 0.72 | (6) | 3.6 x 10 ⁻² (6) | < 0.9 | 6.5 x 10 ⁻² (19) |
| | 50 | 12.5 | 21 | | | 0.70 | (7) | 1.9 x 10 ⁻² (5) | < 0.4 | 1.9 x 10 ⁻² (19) |
| | | | 16 | | | 0.71 | (8) | 2.8 x 10 ⁻² (11) | < 0.4 | 5.0 x 10 ⁻² (47) |
| | | | 14 | | | 0.71 | (5) | 2.7 x 10 ⁻² (8) | < 0.4 | 2.0 x 10 ⁻² (55) |
| | 25 | 25 | 21 | | | 0.79 | (10) | 1.9×10^{-2} (5) | | |
| | | | 18 | | | 0.68 | (35) | 2.3 x 10 ⁻² (20) | | |
| | | | 16 | | | 0.70 | (55) | 2.3 x 10 ⁻² (20) | | |

Table 7. Fractions of Notional Yields of Combustion Products from Cable Specimens

| | Yields | | | | | | | | | |
|--------------|------------------------|----------------|------------------------|--------------|----------------|---------|---------------|------------------------------|-----------------------------|-----------------------------|
| Test Type | | Tes | t Variables | | | | CO_2 | СО | HCl | HCN |
| Room | Ventilation | | | | | | | | | |
| | Preflashover | | | | | 5.7 x 1 | 0^{-2} (45) | $4.1 \times 10^{-3} (50)$ | 2.0 x 10 ⁻² (35) | 1.6 x 10 ⁻² (55) |
| | Postflashover | | | | | 0.65 | | 1.11 x 10 ⁻¹ (15) | 0.63 (15) | 1.0 x 10 ⁻¹ (35) |
| | Closed room | | | | | (1 | 5) | | | |
| Radiant | O ₂ initial | Specimen | | | | (. | , | | | |
| furnace | 0.21 | intact | | | | 0.55 | (12) | 4.4 x 10 ⁻² (8) | 0.60 (35) | 0.22 (70) |
| | 0.21 | diced | | | | 0.54 | (12) | 5.0 x 10 ⁻² (16) | 0.94 (40) | < 8 x 10 ⁻² |
| | 0.17 | Intact | | | | 0.50 | (18) | 4.7 x 10 ⁻² (30) | 0.75 (40) | 1.2 x 10 ⁻² (55) |
| | 0.17 | diced | | | | 0.59 | (12) | 5.5 x 10 ⁻² (20) | 0.96 (20) | < 0.2 |
| Smoke | Irradiance (kW/m²) | Pilot | | | | | | | | |
| density | 50 | unpiloted | | | | 0.53 | (5) | 2.3 x 10 ⁻² (9) | 0.55 (50) | < 6 x 10 ⁻² |
| chamber | 50 | piloted | | | | 0.56 | | 2.1 x 10 ⁻² (8) | 0.15 (x 2) | $< 6 \times 10^{-2}$ |
| | 25 | piloted | | | | 0.36 | (5) (13) | 0.9 x 10 ⁻² (19) | 0.29 (14) | $< 6 \times 10^{-2}$ |
| Tube furnace | Temperature | Specimen | Air flow | Mass loading | Mass feed rate | | | | (14) | |
| | 650 °C | intact | 1 | 1 | 1 | 0.66 | (28) | 6.6 x 10 ⁻² (17) | 0.90 (36) | < 7 x 10 ⁻² |
| | (well ventilated) | diced | 1 | 1 | 1 | 0.63 | (7) | 6.8 x 10 ⁻² (10) | 0.90 (18) | $< 6 \times 10^{-2}$ |
| | | intact | x 1.3 | 1 | 1 | 0.56 | (6) | 5.3 x 10 ⁻² (11) | 0.75 (14) | < 6 x 10 ⁻² |
| | | intact | x2 | x 2 | 1 | 0.55 | (7) | 5.3 x 10 ⁻² (10) | 0.58 (19) | < 3 x 10 ⁻² |
| | | intact | x1.5 | 1 | x 1.5 | 0.57 | (3) | 4.9×10^{-2} (3) | 0.73 (13) | $< 4 \times 10^{-2}$ |
| | 825 °C | intact | 1 | 1 | 1 | 0.16 | (13) | 3.2 x 10 ⁻² (15) | 0.41 (29) | $< 6 \times 10^{-2}$ |
| | (underventilated) | diced | 1 | 1 | 1 | 0.15 | (12) | 2.8 x 10 ⁻² (11) | 0.43 (19) | $< 6 \times 10^{-2}$ |
| | | intact | x 0.7 | 1 | 1 | 0.10 | (1) | 7.4 x 10 ⁻² (21) | 0.43 (14) | $< 6 \times 10^{-2}$ |
| | | intact | x2 | x 2 | 1 | 0.19 | (9) | $3.9 \times 10^{-2} (12)$ | 0.42 (16) | < 3 x 10 ⁻² |
| | | intact | x1.5 | 1 | x 1.5 | 0.23 | (3) | 6.7×10^{-2} (3) | 0.70 (12) | $< 5 \times 10^{-2}$ |
| Cone | Irradiance (kW/m²) | Air Flow (L/s) | O ₂ initial | | | | | | | |
| calorimeter | 50 | 25 | 21 | | | 0.49 | (10) | 4.1 x 10 ⁻² (6) | 0.69 (15) | < 0.3 |
| | | | 18 | | | 0.55 | (4) | 5.1 x 10 ⁻² (5) | 0.78 (13) | < 0.4 |
| | | | 16 | | | 0.53 | (8) | 5.4×10^{-2} (12) | 0.91 (16) | < 0.4 |
| | 50 | 12.5 | 21 | | | 0.48 | (4) | 3.7×10^{-2} (4) | 0.67 (16) | < 0.2 |
| | | | 16 | | | 0.48 | (4) | 4.6 x 10 ⁻² (4) | 0.71 (15) | < 0.2 |
| | | | 14 | | | 0.42 | (7) | 4.0×10^{-2} (11) | 0.86 (13) | < 0.2 |
| | 25 | 25 | 21 | | | 0.53 | (7) | 3.8×10^{-2} (2) | | |
| | | | 18 | | | 0.61 | (5) | 4.7 x 10 ⁻² (8) | | |
| | | | 16 | | | 0.32 | (7) | 3.1×10^{-2} (7) | | |

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IV. ANALYSIS

The test methods are evaluated following the criteria in ISO 29903¹² and ISO 16312.²⁸ There are additional considerations that reflect the use of the output data in fire hazard and risk analyses.

A. FIRE STAGES

Fires are generally turbulent diffusion flames. The fires that pose a threat to life safety involve flames that extend over large areas of the combustible item(s). For a single value of the global equivalence ratio, local equivalence ratios can vary considerably, i.e., the oxygen availability is different at various locations along the fuel surface. The combustion products measured downstream from a fire, whether well ventilated, or ventilation limited, are integrated over a range of equivalence ratios.

Ideally, the combustion and/or pyrolysis conditions in the combustor section of a bench-scale apparatus reproduce the conditions in one or more stages of actual fires. The specimens should thus be burned under relatively constant, pre-selected conditions of thermal insult and oxygen availability (ventilation).

This work focused on the three flaming stages that were identifiable from the room tests: well ventilated, vitiated preflashover (sofa material only), and postflashover. A pre-appraisal of how the four bench-scale apparatus related to these is as follows.

- At the beginning of a test in either of the two closed-chamber tests (radiant furnace and smoke density chamber), the oxygen volume percent is that of fresh air, and the test specimen is exposed to an external radiative flux of 50 kW/m². These conditions are similar to the well ventilated fire stage in the room tests, although the irradiance might be somewhat higher in the bench-scale test. The flames were laminar. During a test, the radiant flux was constant, but the oxygen volume percent declined to approximately 17 percent to 18 percent. Accordingly, tests were performed at an initial oxygen level of 17 volume percent (or lower) and an irradiance of 25 kW/m² (smoke density chamber only) to determine sensitivity to these parameters.
- The tube furnace standard explicitly defines operating conditions for two fire stages, simulating well ventilated combustion with a peak furnace temperature of 650 °C and an equivalence ratio below 0.75, and underventilated combustion with a furnace temperature of 825 °C and an equivalence ratio of 2.0. These correspond to radiation temperatures of 40 kW/m² and 80 kW/m². The lower irradiance only is a little high for well ventilated burning, and the higher irradiance is not unreasonable for postflashover burning. 80 kW/m² is very high for the irradiance in the vitiated preflashover (closed room) scenario.
- The cone calorimeter can normally only simulate well ventilated combustion. However, we added an enclosure and gas delivery system to allow oxygen levels as low as 14 volume percent to attempt to simulate postflashover combustion.

The effects of these measures will be discussed in the analysis of gas yields below.

B. APPLICABILITY

All three of the finished products are layered and thus non-homogeneous. The radiant apparatus, the smoke density chamber, and the cone calorimeter are all designed to accommodate this

complexity of test specimen. In all three apparatus, the heat is applied radiatively to the top surface, as would be the case in a flaming environment.

The tube furnace standard is limited to testing of homogenous materials. Thus, the inclusion of this apparatus in this project is an exploration. The heat to the specimen is applied to all surfaces, unlike the other three methods and unlike most fire environments.

The outer layer in each of the three types of test specimens is not designed to protect the interior layer from thermal stress. If the outer layer had such a purpose, some additional consideration would be needed for the specimen design in the tube furnace, since the specimen is heated on all sides, and the sample boat is not very deep.

As an initial step in assessing the importance of preserving the (nonprotective) layered structure of products, specimens were constructed to the dimensions prescribed by the standards. The same mass of specimen was then cut into small pieces and combusted.

The specimens in the small-scale apparatus were cut from the same products tested in the room tests. Thus, any differences in yields can be attributed to the differences in the specimen preparation and the combustion environments. The specimens in the radiant apparatus, smoke density chamber, and cone calorimeter are similar to each other and to a portion of the combustibles in the room tests. Thus, good agreement among the yields can be attributed to similarity, or offsetting dissimilarities, in simulating any of the three fire stages. The bookcase and sofa material test specimens in the tube furnace are quite different; good agreement among the yields can be attributed to independence of the test specimen conformation and similarity of the combustion conditions, as well as any offsetting dissimilarities.

C. APPARATUS INDEPENDENCE

Each of the four apparatus designs might have some effect on the nature and concentrations of the gases reaching the analyzers.

For all the bench-scale tests, the flame shapes and/or the flow fields differ significantly from those in the room tests. In none of the four apparatus does the flame from the specimen rise unperturbed to a height where all chemical reaction has ceased.

- In the smoke density chamber and the cone calorimeter, the upward flow is channeled through the conical heater. Some of the buoyant flow is close to the heater surface which, at an irradiance of 50 kW/m², is at approximately 700 °C.
- In the radiant apparatus, the buoyant plume rises through a chimney, which is narrower than the opening in the conical heaters but is not as hot.
- The flame in the tube furnace extends horizontally and immediately impinges on the top surface of the tube, the temperature of which varies with the location along the tube and the intensity of the burning of the test specimen. The inlet air flow is uniform through a test, but the oxygen volume fraction in the downstream flame zone is determined by the oxygen that is unconsumed as it flows over the burning specimen and also the degree of mixing downstream of the specimen boat.

In three of the apparatus (excluding the cone calorimeter), the product gases are sampled from a collection chamber. There is thus time for the gases, especially HCl, to adsorb on soot or walls.

In all four apparatus, the gases are sampled through heated lines. We did not insert a filter in the sampling lines in order to eliminate this possible source of perturbation.

For the two closed chamber apparatus, the test duration is longer than the flaming portion of a test. For the radiant furnace, to abate the inclusion of post-flaming (oxidative pyrolysis) gas generation, we modified the procedure to cease irradiation and isolate the specimen from the sampling chamber once flaming ended. For the smoke density chamber apparatus, this isolation is not possible, and significant CO was generated postflaming. Also in these two apparatus, the recirculation of gas that had been passed through cold traps (necessary to protect the fixed-gas analyzers) as well as wall loses could potentially lead to a measurable decline in HCl as the test progresses. This is also true for the tube furnace, since the gas sampling is from a relatively small collection chamber.

Given these dissimilarities, it was not assured that any of the bench-scale apparatus would demonstrate a high degree of replication of the yields of combustion products from the room tests.

D. OPERATIONAL EFFICIENCY

All of the apparatus were simple and capable of safe operation.

E. DATA GENERATED

All four methods allow for recording gas volume fractions using NDIR for CO₂ and CO, paramagnetic oxygen analysis, and FTIR for CO₂, CO, HCN, HCl, NO, NO₂, acrolein, and formaldehyde. For the cone calorimeter, the time delay between gas generation and gas measurement is essentially the travel time through the sampling line. For the other three apparatus, the sampling of the gases from the respective collection chambers imposes a time averaging function on the measured results. The procedure for the tube furnace directs that gas sampling begin when steady state burning has been achieved. With all four apparatus, we began sampling before the test specimen was ignited or exposed to a heat source.

The volume fractions of the gases were used to calculate yields using chamber volumes or gas flows and the mass lost by the specimen. The radiant furnace, smoke density chamber, and cone calorimeter included real time mass measurement, whereas the mass loss of a specimen in the tube furnace was measured by weighing before and after the test. Although none of our recent tests included bioassays, all four apparatus are adaptable for either direct exposure or extractive sampling.

F. ACCURACY OF THE PHYSICAL FIRE MODELS

When comparing the room-scale and bench-scale test results, it must be remembered that the current status of computational fire modeling does not include reliable prediction of the yields of the product gases. Prediction of the solid fuel gasification rate, the composition of the pyrolyzate, the potentially changing chemistry of the fuel (and thus the pyrolyzate) during a fire, and the conversion of the pyrolyzate to toxic combustion products are all the subjects of current research. Thus, the yields of the product gases are *inputs* to the models. As a result, predicting whether a fire environment is tenable or the time at which occupants become incapacitated

depends on the accuracy of the input yields. This, in turn, depends on the accuracy of the physical fire model used to generate those yields.

In the following sections, unless otherwise noted, each yield comparison is between the room test value and the value from a standard operating condition for a bench-scale test.

1. CO₂

a. Room Tests

The CO₂ yield is the link between the mass burning rate and the overall formation of combustion products. In a computational fire model, the concentrations of all of the other toxic species depend on the mass burning rate. It is therefore of prime importance to examine CO₂ generation in the room fire tests.

If a heated test specimen pyrolyzes without changing the elemental composition of the condensed residue, and if the carbon in the pyrolyzate is subsequently fully oxidized, the calculated yield of CO₂ should equal the notional yield. This was generally not the case for the products examined here.

For the room-scale cable tests, the preflashover CO_2 yields were well below 10 percent of the notional yield. There were clearly some regions of the post-fire residue that were no more than copper wire and a tarry black residue, indicating a substantial change in the organic composition. Other regions were unburned. During the early burning, it is likely that the plasticizer was volatilized without efficient burning. (The smoke yield was approximately 0.2.) In addition, it is likely that HCl was emitted during pyrolysis of the PVC. These two processes would have substantially decreased the mass of the residue while generating no CO_2 and may well account for the very low preflashover CO_2 yield.

Following flashover, the more vigorous burning increased the CO₂ yield, and the measured postflashover CO₂ yield was approximately two-thirds of the notional value. The smoke and CO yields were each a little over 0.1, so the carbon is accounted for, within experimental uncertainty.

The CO₂ yield from the postflashover portion of the bookcase tests was close to the notional yield. The soot yield was low, and the flaming was very vigorous. For the preflashover portion of the tests, the CO₂ yield was approximately one-third of the notional yield. The flames were not particularly vigorous or spatially extensive, so it is reasonable that much of the pyrolyzate was not oxidized.

The preflashover CO_2 yields from the sofa tests were just below the notional yield, and the smoke yields were approximately 0.2. Postflashover, the CO_2 yields were approximately one-half of the notional value. The yields from the closed room tests were similar to the postflashover results, suggesting that vitiation reduced the completeness of combustion.

b. Radiant Apparatus

The CO₂ yields for the bookcase material from the radiant apparatus were not very sensitive to the variation in initial oxygen volume fraction and whether the specimens were diced or intact. All the yield values were close to one-half the notional value. All the yields were high for the

preflashover phase of the room fire tests and somewhat low (but within the large variability of the room tests) for the postflashover case.

For the sofa material specimens, the CO₂ yields were about 15 percent lower than the notional yield, regardless of the variation in initial oxygen mole fraction and specimen conformation. The agreement with the preflashover room fire CO₂ yield was excellent. The bench-scale yields were almost 50 % higher than the postflashover or closed room values.

The CO₂ yields from the cable material specimens also did not vary with initial oxygen mole fraction and specimen conformation. The values were in agreement with the postflashover room fire value. The forced combustion in the bench-scale tests did not reflect the lightly burning conditions in the preflashover room tests, with the bench-scale value overpredicting the room fire yield by an order of magnitude.

c. Smoke Density Chamber

For the smoke density chamber, the piloted, 50 kW/m² exposure generated CO₂ yields that agreed within the experimental uncertainty with the postflashover yields for all three types of specimens and the closed room yields for the sofa specimens. The unpiloted 50 kW/m² values for the bookcase and sofa materials captured the essence of the preflashover results within the experimental variability. None of the bench-scale operating conditions led to agreement with the preflashover CO₂ yields from the cable materials. Under three of the nine combinations of apparatus conditions and test specimen, the repeatability of the CO₂ yields was distinctively poor, relative to measurements made with the other three physical fire models.

d. Tube Furnace

Under the standard 650 °C exposure corresponding to well ventilated combustion, the tube furnace greatly overpredicted the preflashover CO₂ yield from the bookcase (x 3) and cable (x 10) materials, while properly predicting the preflashover CO₂ yield from the sofa materials. Changing the mass and air flow conditions, but maintaining the same global equivalence ratio, led to severe underprediction of the preflashover yield for the sofa specimens and no improvement for the cable or bookcase materials.

Under the intact specimen and standard 825 °C exposure corresponding to underventilated combustion, the CO₂ yield was within experimental uncertainty of the postflashover room yield for the bookcase specimens, although the repeatability for both data sets was quite poor. (The mean values were a factor of 5 apart.) The yield was approximately a factor of two lower than the yields from the postflashover and closed room tests for the sofa materials, and was a factor of 4 lower than the postflashover cable yield. Varying the test conditions did not substantially improve the agreement with the room test yields.

e. Cone Calorimeter

The examined variations in the radiant flux, air flow, and oxygen volume fraction (down to 0.14) did not alter the general consistency with the room fire test yields. For the bookcase materials, the bench-scale yields overpredicted the preflashover yield and underpredicted the postflashover yield. The prediction of the preflashover and postflashover yields from the room sofa tests was within experimental repeatability. The underprediction of the postflashover cable tests was just outside experimental repeatability. The preflashover CO_2 yield from the room cable tests was greatly overpredicted.

f. Summary

Table 8 summarizes the findings for the comparison of CO_2 yields (in Tables 2 through 4) from the various bench-scale tests under their standard operating conditions relative to the room test results. "Good" means that the agreement is within the repeatability of the tests. "Low" and "high" indicate disagreement up to approximately \pm 50 %. "Very high" and very low" indicate disagreement larger than approximately a factor of two. An asterisk (*) indicates that the basis for the rating is that the repeatability of the room data is \pm 50 % or worse.

The rows marked "Better" are for identifying varied apparatus conditions where the agreement for *all three types of specimens* is improved. For the CO₂ yields, none of our variations resulted in improvements that allowed movement from one agreement designation to a superior one.

Table 8. CO₂ Yields from Bench-scale Tests Relative to Yields from Room Tests.

| Bench-scale Test and | | | Room T | est Result | | | |
|--------------------------------|-----------|-----------|-----------|------------|-------------|-------|--|
| Conditions | Prefla | shover | Postfla | ashover | Closed Room | | |
| Radiant apparatus | | | | | | | |
| Standard | Bookcase: | good* | Bookcase: | good* | Bookcase: | | |
| | Sofa: | good | Sofa: | high | Sofa: | high | |
| | Cable: | very high | Cable: | good | Cable: | | |
| Better | None | | None | | None | | |
| Smoke Density Chamber | | | | | | | |
| 50 kW/m ² , piloted | Bookcase: | high* | Bookcase: | good* | Bookcase: | | |
| | Sofa: | good | Sofa: | good | Sofa: | good* | |
| | Cable: | very high | Cable: | good | Cable: | | |
| Better | None | | None | | None | | |
| Tube Furnace | | | | | | | |
| 650 °C, standard | Bookcase: | very high | | | | | |
| | Sofa: | good | | | | | |
| | Cable: | very high | | | | | |
| 650 °C, better | None | | | | | | |
| 825 °C, standard | | | Bookcase: | very low* | Bookcase: | | |
| | | | Sofa: | low | Sofa: | low | |
| | | | Cable: | very low | Cable: | | |
| 825 °C, better | | | None | | None | | |
| Cone Calorimeter | | | | | | | |
| 50 kW/m ² , 25 L/s | Bookcase: | high* | Bookcase: | good* | Bookcase: | | |
| | Sofa: | good | Sofa: | good | Sofa: | high | |
| | Cable: | very high | Cable: | good | Cable: | | |
| Better | None | | None | | None | | |

2. CO

Pitts' analysis of well ventilated compartment fires indicates that CO yields should be very low and rise sharply as the fuel/air equivalence ratio approaches unity. Near a ratio of 1.5, the CO yield reaches a plateau.²⁹ A compilation of postflashover CO yields¹⁴ shows that the yield of CO

from postflashover room fire tests of a variety of combustibles is 0.2 ± 0.09 . This results from vitiation (and thus truncation of the fuel oxidation process) in the upper layer of the burn room. In our room-scale tests, the CO yields were somewhat lower than this. Our hypothesis is that since the postflashover portion of those tests had visible flames coming out the door, that hot effluent was reigniting on contact with fresh air, and that this was causing some of the CO to oxidize, reducing its yield as measured further downstream. The recommendation was that a CO yield of 0.2 be used in fire hazard calculations, being indicative of the established conservative value. In the following, all bench-scale values are compared with this postflashover value of 0.2.

None of the test methods consistently found postflashover CO yields near 0.2. The tube furnace generated the nearest yield for the sofa materials with the standard underventilated operating condition (825 °C). However, these results greatly overpredicted the CO yield from the closed room, which is also an underventilated fire test.

The CO yields from the radiant apparatus predicted the preflashover yields from the bookcases and sofa materials within experimental repeatability, but severely overpredicted the yield from the cable arrays. None of the variations in operating conditions improved the agreement substantially.

The CO yields from the smoke density chamber, operated at 50 kW/m² with a pilot flame, greatly overpredicted the preflashover yields from the cable arrays, but severely underpredicted the yields from bookcase materials and was consistent with the sofa fires due to very poor repeatability in the bench-scale data. At the same irradiance but unpiloted, this apparatus overpredicted the preflashover bookcase and cable yields and agreed with the sofa yield. Both the piloted and unpiloted results substantially underpredicted the closed room CO yield from the sofas.

The tube furnace, operated under the standard well ventilated operating condition (650 °C), severely underpredicted the preflashover bookcase yield, predicted the yield from the preflashover cable fires (with help from a large variability in the room data), and overpredicted the preflashover yield from the sofa fires. Increasing the air flow (decreasing the global equivalence ratio), or increasing the mass loading while keeping the global equivalence ratio unchanged, led to improved agreement with the sofa and cable yields. Increasing the mass feed rate, which should be equivalent to increasing the mass loading, deteriorated the agreement with the sofa yield.

The cone calorimeter, which is generally regarded as overventilated when operated at 50 kW/m² and 25 L/s, generated low CO yields for the bookcase materials, while generating high CO yields for the sofa and cable materials. Reducing the radiant flux to 25 kW/m² improved the agreement for the bookcase specimens, but not the cable and sofa materials. This brought all the yields to within about a factor of two agreement with the preflashover CO yield. However, at this heat flux, a number of materials do not ignite repeatably (or at all), making this an unsuitable operating condition for standard testing.

Table 9 summarizes the findings for the comparison of CO yields from the various bench-scale tests under their standard, or chosen (by us), operating conditions relative to the room test results (preflashover or closed room) or a postflashover yield of 0.2. "Good" means that the agreement is within the repeatability of the tests. "Low" and "high" indicate disagreement up to approximately \pm 50 %. "Very high" and very low" indicate disagreement larger than approximately a factor of two. An asterisk (*) indicates that the basis for the rating is that the

repeatability of the room data is \pm 50 % or worse. A double asterisk (**) indicates that the basis for the rating is that the repeatability of the small-scale data is \pm 50 % or worse.

The rows marked "Better" are for identifying varied apparatus conditions where the agreement for *all three types of specimens* is improved. For the CO yields, none of our variations resulted in improvements that allowed movement from one agreement designation to a superior one.

Table 9. CO Yields from Bench-scale Tests Relative to Yields from Room Tests.

| Bench-scale Test and | | | Room T | est Result | | | |
|--------------------------------|-----------|-----------|-----------|------------|-------------|-----------|--|
| Conditions | Prefla | shover | Postfl | ashover | Closed Room | | |
| Radiant apparatus | | | | | | | |
| Standard | Bookcase: | good | Bookcase: | very low | Bookcase: | | |
| | Sofa: | good | Sofa: | low | Sofa: | good | |
| | Cable: | very high | Cable: | very low | Cable: | | |
| Better | None | | None | | None | | |
| Smoke Density Chamber | | | | | | | |
| 50 kW/m ² , piloted | Bookcase: | very low | Bookcase: | very low | Bookcase: | | |
| _ | Sofa: | good* | Sofa: | very low | Sofa: | very low | |
| | Cable: | very high | Cable: | very low | Cable: | | |
| Better | None | | None | | None | | |
| Tube Furnace | | | | | | | |
| 650 °C, standard | Bookcase: | very low | | | | | |
| | Sofa: | good | | | | | |
| | Cable: | very high | | | | | |
| 650 °C, better | None | | | | | | |
| 825 °C, standard | | | Bookcase: | good | Bookcase: | | |
| | | | Sofa: | very high | Sofa: | very high | |
| | | | Cable: | very low | Cable: | | |
| 825 °C, better | | | None | | None | | |
| Cone Calorimeter | | | | | | | |
| 50 kW/m ² , 25 L/s | Bookcase: | low | Bookcase: | very low | Bookcase: | | |
| | Sofa: | high | Sofa: | low | Sofa: | low | |
| | Cable: | very high | Cable: | very low | Cable: | | |
| Better | None | | None | | None | | |

3. HCI

If a test specimen burned completely and at steady state and if there were no wall losses, the HCl yield would equal the notional yield for the tests of the bookcase and sofa materials. For the cables, there is sufficient calcium in the jacket and insulation to bind only approximately one-fourth of the chlorine. Thus, calculated yields of HCl that are substantially different from the notional yields reflect deviation from one or more of these conditions.

The mass fractions of chlorine in the bookcases and sofas were very small, 0.3% and 0.7%, respectively. For nearly all of the bench-scale tests, the concentrations were below the detection

limits. Otherwise, the low concentrations of HCl resulted, in most cases, in high variability in the calculated yields.

None of the calculated HCl yields or upper limits to the HCl yields from the radiant apparatus or the smoke density chamber was as large as the HCl yields measured in either the preflashover or postflashover stages of the room fire tests or these two products. For the bookcase specimens tested in the tube furnace and the cone calorimeter, the upper limits to the HCl yields approached the preflashover and postflashover values from the room fire tests. However, this is not sufficient to constitute agreement. For the sofa specimens, the HCl yields from these two apparatus were far smaller than the preflashover yield from the room tests. The upper limits to the HCl yields from the cone calorimeter approached the measured postflashover yield.

The upper limits of the HCl yields measured in the tube furnace, smoke density chamber, and cone calorimeter were generally higher than the calculated yields from the closed room sofa tests, disabling any basis for comparison. The yields from the radiant apparatus, whether calculated or upper limits, were not inconsistent with the closed room value, but did not enable a clear comparison.

The chlorine content of the cable materials was considerably higher than in the other materials. Nonetheless, the preflashover HCl yield from the room fire testing was quite low, approximately one-fiftieth of the notional yield. The yields from all four apparatus were all substantially higher than this. The radiant apparatus and cone calorimeter yields agreed with the postflashover yields from the room tests. The smoke density chamber and the tube furnace simulating underventilated conditions, underpredicted the postflashover yields. The tube furnace showed good agreement with the postflashover room fires when operated at the well ventilated conditions.

Table 10 summarizes the findings for the comparison of HCl yields from the various bench-scale tests under their standard operating conditions relative to the room test results. "Good" means that the agreement is within the repeatability of the tests. "Low" and "high" indicate disagreement up to approximately \pm 50 %. "Very high" and very low" indicate disagreement larger than approximately a factor of two. "Ind" indicates that the result of the comparison is indeterminate, generally because the yield from the room tests is lower than or comparable to the upper limit for the bench-scale tests. An asterisk (*) indicates that the basis for the rating is that the repeatability of the room data is \pm 50 % or worse.

The rows marked "Better" are for identifying varied apparatus conditions where the agreement for *all three types of specimens* is improved. For the HCl yields, none of our variations resulted in improvements that allowed movement from one agreement designation to a superior one.

Table 10. HCI Yields from Bench-scale Tests Relative to Yields from Room Tests.

| Bench-scale Test and | | | Room To | est Result | | | |
|--------------------------------|-----------|-----------|-----------|------------|-------------|-----|--|
| Conditions | Prefla | shover | Postfla | ashover | Closed Room | | |
| Radiant apparatus | | | | | | | |
| Standard | Bookcase: | very low | Bookcase: | very low | Bookcase: | | |
| | Sofa: | very low | Sofa: | very low | Sofa: | ind | |
| | Cable: | very high | Cable: | good | Cable: | | |
| Better | None | | None | | None | | |
| Smoke Density Chamber | | | | | | | |
| 50 kW/m ² , piloted | Bookcase: | very low | Bookcase: | very low | Bookcase: | | |
| | Sofa: | very low | Sofa: | low | Sofa: | ind | |
| | Cable: | very high | Cable: | low | Cable: | | |
| Better | None | | None | | None | | |
| Tube Furnace | | | | | | | |
| 650 °C, standard | Bookcase: | good | | | | | |
| | Sofa: | very low | | | | | |
| | Cable: | very high | | | | | |
| 650 °C, better | None | | | | | | |
| 825 °C, standard | | | Bookcase: | ind | Bookcase: | | |
| | | | Sofa: | very low | Sofa: | ind | |
| | | | Cable: | low | Cable: | | |
| 825 °C, better | | | None | | None | | |
| Cone Calorimeter | | | | | | | |
| 50 kW/m ² , 25 L/s | Bookcase: | ind | Bookcase: | ind | Bookcase: | | |
| | Sofa: | very low | Sofa: | ind | Sofa: | ind | |
| | Cable: | very high | Cable: | good | Cable: | | |
| Better | None | | None | | None | | |

4. HCN

In general, concentrations of HCN were challenging to quantify, as it has relatively weak IR absorption and is a contributor to incapacitation within 5 minutes of exposure at concentrations that are only a few times its limit of detection with this FTIR spectrometer.

HCN was quantified from all of the specimens at the room scale. HCN was not detected in any of the bench-scale tests of the bookcase materials, was only detected in the radiant apparatus for the cable specimens, and was detected in all bench-scale apparatus for the sofa materials.

For the sofa materials, the yields from the radiant apparatus were in good agreement with the preflashover and closed room yields, but lower than the postflashover yield. Reducing the initial oxygen concentration had no discernible effect on the HCN yield. The upper limits of the yields from the smoke density chamber tests indicated that far less HCN was formed than in the room tests.

In the tube furnace, operation under the standard well ventilated operating condition (650 °C) but with a 30 percent reduction in equivalence ratio led to good agreement with the preflashover HCN yield. The standard underventilated operating conditions led to an HCN yield smaller than the postflashover yield, but substantially higher than the closed room yield. Variation in the operating conditions did not add additional information. The standard cone calorimeter values were in good agreement with the preflashover yields and higher than the closed room yields. They were lower than the postflashover yield, although reducing the oxygen volume fraction at full air flow and radiant flux increased the yield to a value approaching the postflashover yield.

For the bookcase materials, the upper limits to the yields from the radiant apparatus were all smaller than the preflashover and postflashover yields. The upper limits from the smoke density chamber were substantially lower than the postflashover yields from the room tests. The upper limits to the tube furnace and cone calorimeter HCN yields did not allow for comparison with room test yields.

For the cable materials, the yield from the radiant apparatus was much higher than the preflashover yield from the room tests and comparable to the postflashover yield (due in part to the poor repeatability of the bench-scale data. Reducing the initial oxygen volume fraction to 0.17 reduced the HCN yield by an order of magnitude, making it far lower than the room fire yields. The yields from the smoke density chamber and the tube furnace were much lower than the postflashover room fire yields. The upper limits of the HCN yields from the cone calorimeter were far higher than the postflashover room fire yields.

Table 11 summarizes the findings for the comparison of HCN yields from the various bench-scale tests under their standard operating conditions relative to the room test results. "Good" means that the agreement is within the repeatability of the tests. "Low" and "high" indicate disagreement up to approximately \pm 50 %. "Very high" and very low" indicate disagreement larger than approximately a factor of two. "Ind" indicates that the result of the comparison is indeterminate, generally because the yield from the room tests is lower than or comparable to the upper limit for the bench-scale tests. An asterisk (*) indicates that the basis for the rating is that the repeatability of the room data is \pm 50 % or worse. A double asterisk (**) indicates that the basis for the rating is that the repeatability of the small-scale data is \pm 50 % or worse.

The rows marked "Better" are for identifying varied apparatus conditions where the agreement for *all three types of specimens* is improved. For the CO₂ yields, none of our variations resulted in improvements that allowed movement from one agreement designation to a superior one.

5. HBr and HF

None of the combustibles contained Br or F, and therefore we have no data on their corresponding irritant gases.

6. NO₂, Acrolein and Formaldehyde

None of these gases were detected in either the room-scale or bench-scale tests.

In the room tests, the low preflashover concentrations of all the toxicants just outside the doorway indicate that effluent concentrations would not reach incapacitating levels outside the fire room. The maximum postflashover concentrations of NO₂, acrolein, and formaldehyde that

could have been present would have made secondary contributions to incapacitation relative to the concentrations of HCl in the sofa and cable effluents. In the bookcase tests, where the HCl levels were low, the high postflashover levels of CO and HCN suggest incapacitation due to narcotic gases might occur for many occupants at exposure times of the order of a few minutes. This reduces the importance of these three gases (NO₂, acrolein, and formaldehyde) in particular and irritant gases in general in causing incapacitation for these combustibles.

In the cable effluent in all of the physical fire models, the contributions of these three gases to the total irritant FED was secondary to the HCl contribution. ^{22,24,25} In the effluent from the bookcase and sofa tests in all of the physical fire models (except the preflashover tests with the tube furnace), the high levels of CO lead to estimated incapacitation times of the order of 2 min. This suggests a secondary role for the irritant gases in causing incapacitation for these combustibles, as in the room-scale tests.

Table 11. HCN Yields from Bench-scale Tests Relative to Yields from Room Tests.

| Bench-scale Test and | Room Test Result | | | | | | | | | | | | |
|--------------------------------|------------------------------|-------------------------------|------------------------------|----------------------------------|------------------------------|--------------|--|--|--|--|--|--|--|
| Conditions | Prefla | shover | Postfl | ashover | Closed Room | | | | | | | | |
| Radiant apparatus | | | | | | | | | | | | | |
| Standard | Bookcase: Sofa: Cable: | very low good very high | Bookcase: Sofa: Cable: | very low very low good** | Bookcase: Sofa: Cable: | good | | | | | | | |
| Better | None | | None | | None | | | | | | | | |
| Smoke Density Chamber | | | | | | | | | | | | | |
| 50 kW/m ² , piloted | Bookcase: Sofa: Cable: | ind ind ind | Bookcase: Sofa: Cable: | very low very low very low | Bookcase: Sofa: Cable: | ind | | | | | | | |
| Better | None | | None | | None | | | | | | | | |
| Tube Furnace | | | | | | | | | | | | | |
| 650 °C, standard | Bookcase: Sofa: Cable: | ind good ind | | | | | | | | | | | |
| 650 °C, better | None | | | | | | | | | | | | |
| 825 °C, standard | | | Bookcase: Sofa: Cable: | ind low ind | Bookcase: Sofa: Cable: | very high | | | | | | | |
| 825 °C, better | | | None | | None | | | | | | | | |
| Cone Calorimeter | | | | | | | | | | | | | |
| 50 kW/m ² , 25 L/s | Bookcase: Sofa: Cable: | ind good ind | Bookcase: Sofa: Cable: | ind very low ind | Bookcase: Sofa: Cable: | high | | | | | | | |
| Better | None | | None | | None | | | | | | | | |

V. RECOMMENDATIONS ON THE USE OF BENCH-SCALE APPARATUS FOR OBTAINING TOXIC GAS YIELDS FOR USE IN FIRE HAZARD AND RISK ANALYSES

A. EFFECT ON HEAT RELEASE

In fire hazard modeling, the composition of the fire effluent feeds into two types of calculations. Of initial importance is the heat release rate of the burning items, which determines both fire growth and the temperature of the fire environment. The heat release is the mass loss rate multiplied by an effective heat of combustion, ΔH_{eff} . The total carbon in the effluent is a marker for the mass loss rate. The degree of accuracy of the total carbon yield is a determinant of the accuracy of the model's calculation of both heat release and effluent. In flaming combustion, most of the carbon appears as CO_2 , so modeling calculations of heat release are most sensitive to the yield of this gas.

Table 12, compiled from Tables 5 through Table 7, summarizes the fractions of notional yields of CO₂ from the room tests and from the bench-scale tests operated at their standard conditions.

Table 12. Fractions of Notional Yields of CO₂ in the Effluent from Fire Tests.

| Apparatus | Test Condition ^a | Bookcase | Sofa | Cable |
|------------------|---------------------------------|-------------------|-----------|-----------|
| Room | Preflashover | $0.29 	 (50)^{b}$ | 0.80 (25) | 0.06 (45) |
| | Postflashover | 1.10 (75) | 0.57 (25) | 0.65 (15) |
| | Closed room | | 0.46 (11) | |
| Radiant furnace | O_2 volume fraction = 0.21 | 0.51 (9) | 0.86 (14) | 0.55 (12) |
| Smoke density | 50 kW/m ² ; piloted; | 0.62 (13) | 0.68 (60) | 0.56 (5) |
| chamber | O_2 volume fraction = 0.21 | | | |
| Tube furnace | 650 °C | 0.83 (4) | 0.96 (13) | 0.66 (28) |
| | 825 °C | 0.21 (40) | 0.29 (11) | 0.16 (13) |
| Cone calorimeter | 50 kW/m2; air flow = 25 L/s | 0.65 (3) | 0.72 (6) | 0.49 (10) |

^a The conditions in the physical fire models are those in their respective standards, with delineation provided if a standard includes more than one operating condition.

All four bench-scale apparatus, when operated under conditions that are expected to be reflective of well ventilated burning, generated similar fractional CO₂ yields for the three types of test specimens. The values are consistent with (a) specimens that are being forced to burn and (b) allowances for CO and soot yields, some evaporated water, and enrichment of the carbon fraction in the residue (principally for the bookcase and cable materials). In the room tests, the combustible portion of the sofas burned efficiently before flashover, and as a result, the fraction of the notional CO₂ yield is similar to the results from the bench-scale tests. For the other two combustibles, the mass loss was large compared to the mass of carbon that was oxidized. The early mass loss from the cable arrays was disproportionately from gasified HCl and plasticizer –

^b The numbers in parentheses are the uncertainty percentages in the values.

the flames were not steady and strong, and there was substantial tarry residue. The early burning of the bookcases was characterized by white smoke, indicative of gasified water and unburned organic molecules. Consistent with this, the shelves were significantly charred. After room flashover, all three combustibles burned vigorously. The fractions of notional CO_2 yields for the three types of test specimens are reasonable, given soot and CO yields that approached 0.3 of the notional carbon consumption.

What was surprising was the low CO₂ yields for all three types of test specimens burned in the tube furnace operating at the underventilated burning condition. We were unable to account for approximately two-thirds of the carbon. Qualitatively, there was no evidence in the FTIR spectra of large concentrations of gasified organic material, nor was there unusual residue in the downstream portion of the tube or in the collection chamber. The mass losses from the test specimens were close to the mass losses in the other three bench-scale apparatus. This an issue that merits further research.

Nearly all the heat release results from oxidation of the carbon in the fuel to CO_2 and the hydrogen in the fuel to H_2O . With this large a discrepancy in the carbon balance, the calculated heat release from the fire would be in error, as will the resulting compartment temperatures.

B. EFFECT ON TENABILITY CALCULATIONS

There are two prime considerations in delineating a methodology for obtaining input data for toxic hazard modeling. The first consideration is the degree of accuracy that is sufficient for the purpose of the model. The needed accuracy is appropriately defined in terms of the acceptable uncertainty in the calculated times at which survival in a burning building is compromised. The consequences of assessments that err substantially in either direction were presented in the introduction to this report.

There are many factors with large uncertainties that are encompassed in such a calculation, and it is both unfair and unrealistic to expect that the burden of precision should fall entirely on the assessment of toxic potency of the fire effluent. A more measured approach is as follows.

A compilation of published animal exposure data³⁰ found that the mean value of the LC_{50} of the smoke from a diverse group of materials and products was approximately 30 g/m³ from well ventilated flaming combustion, about three-fourths of that for underventilated combustion, and a value in between for oxidative pyrolysis. The mean IC_{50} value was about 40 % of that range. In a building fire, all three processes are occurring simultaneously, so let us presume that the overall IC_{50} is approximately 10 g/m³.

If the effluent from all burning items generated effluent with the same toxic potency, then it would be quite accurate to use this single value in a fire hazard or risk assessment. However, this compilation found common materials whose smoke toxic potency was up to five times the mean. There were also materials whose smoke toxic potency was as low as one-third the mean.

The need in a fire hazard or risk analysis is to account for a combustible item whose smoke is of high toxic potency. This is significant if:

• the product of the combustible mass of the item and the toxic potency of the smoke is a sizable fraction of the summed (mass • potency) products for all the combustible items accessible to the fire, and especially

• this product is unusually large for the first item ignited, such that it alone can result in a fire that threatens life safety.

It follows that the calculation of the two components of toxic potency, the fractional effective dose (FED) due to inhalation of narcotic gases and the fractional effective concentration (FEC) due to exposure to sensory irritants, each be sufficiently accurate to identify significant deviations from "ordinary" toxic hazard. Given the current state of the art in fire modeling and the limits of precision of the IC_{50} data, it seems reasonable to ask that the accuracy be within a factor of two

The second consideration is the identification of a procedure for obtaining smoke toxic potency of that accuracy. In evaluation apparatus for this purpose, the accuracies of the yields of the toxic gases are not equally important. Due to the prevalence of fire deaths due to smoke being from postflashover fires¹¹, a greater importance was attached to the postflashover gas yields. The yield of CO₂ affects the carbon balance, and thus the relationship between the gas yields and the heat release. This, in turn, affects the calculated room temperatures and the burning rates of combustibles. It also exponentially increases a person's breathing rate and thus the volume of inhaled smoke. CO is an important toxicant in virtually all fires. When nitrogen is present in the fuel, it can also be a significant contributor to the FED. All three fuels in this study were nitrogen-containing, but HCN was only a contributor to the FED from the sofa materials. The cable was the only fuel that contained a high mass fraction of Cl, and HCl dominated the FEC. For the other two fuels, all the irritant concentrations were low, and tenability was dominated by the narcotic gases.

The findings regarding the comparison between the gas yields from the room-scale tests and the bench-scale apparatus were as follows.

- CO₂: The yields from apparatus A, B, and D were within experimental uncertainty of the postflashover room test yield and within a factor of 2 of the preflashover yield.
 - The underventilated yield from apparatus D was low compared to the postflashover room value, and the well ventilated value was high relative to the preflashover room value. This may be indicative of the room yields being an average over a range of local equivalence ratios.
 - The CO₂ yields from all four apparatus agreed with the sofa material yield from the closed room tests to within a factor of 2.
- CO: None of the apparatus generated CO volume fractions comparable to the 0.2 value compiled from multiple series of postflashover room tests. ¹⁴ This is because the postflashover CO yields result from room conditions that are not readily replicated in a simple bench-scale device. The yield value of 0.2 should be used in hazard calculations. (This corrected value is contained in the standards for the radiant furnace. ^{13,14}) The yields from Apparatus A and D agreed with the preflashover room yield within a factor of 2. Decreasing the oxygen volume fraction to 0.16 in Apparatus D appears to have improved the agreement. A decrease in the oxygen volume fraction to 0.18 in Apparatus D led to agreement with the closed room yield.
- HCl: For the cable, the postflashover yields from Apparatus A and D were within experimental uncertainty. Decreasing the oxygen volume fraction in Apparatus D

degraded the agreement, but it was still well within a factor of 2. The yields from Apparatus B and C were not as good, but were still within a factor of 2 of the room test yield.

The yields from all four apparatus were very high compared to the preflashover room test yield, which was a very low value.

The upper limits of the HCl yields from the bench-scale tests of the sofa materials were too high for quantitative comparison with the very low yield from the closed room tests.

• HCN: The underventilated yield from Apparatus C tests of the sofa materials was within a factor of 2 of the postflashover room yield. The value from Apparatus D at an oxygen volume fraction of 0.21 was very low, but at a volume fraction of 0.16, the yield agreement was within experimental error. The values from the other apparatus were very low. The values for the sofa materials from Apparatus A, C, and D agreed with the preflashover room value within experimental uncertainty.

The yields from the bench-scale tests of the sofa materials were within a factor of 2 of the closed room values for Apparatus A and D. The yield from Apparatus C operated at underventilated conditions was very high.

As noted earlier, CO_2 affects the narcotic gas potency by increasing respiration rate. It multiplies the contribution of CO and HCN by a factor of exp (volume % $CO_2/5$). For the preflashover room fire tests, this factor is negligibly different from unity. Therefore, the effect of poor prediction of the CO_2 by a physical fire model manifests only on the postflashover heat release rate (Section V.A.).

For the postflashover fires, this respiration rate enhancement factor was as high as ten in the room fire test effluent. The CO_2 yields from the radiant furnace, smoke density chamber, and cone calorimeter predicted the room fire yields almost to within experimental uncertainty. Using the tube furnace yields would introduce significant error into the exponential factor.

C. RECOMMENDATIONS

It should not be surprising that physical fire models, being imperfect approximations of some stage of real-scale burning, did not precisely predict the yields of multiple toxic gases from a set of diverse, non-homogeneous products that burned quite differently from each other. It should also not be surprising that under certain test conditions, the yields from both the room tests and the physical fire models showed large uncertainties. Nonetheless, one of the purposes of this project was to identify the more promising physical fire models to use for obtaining input data for fire hazard and risk analysis. The data indicate the following choices:

Underventilated fires:

• The cone calorimeter operated at 50 kW/m^2 and a reduced oxygen volume fraction in the range of 0.16 to 0.18.

Well ventilated fires:

• The cone calorimeter operated at 50 kW/m² and an oxygen volume fraction of 0.21. None of the apparatus predict the HCl yield within a factor of two.

There are some recommendations regarding modifications to the standard operating conditions for these physical fire models.

- In all cases, the CO yields from the physical fire model should be adjusted to 0.2.
- In the radiant furnace, the shutter isolating the combustion chamber from the collection chamber should be closed immediately following the cessation of flaming.
- For the products examined, there was no sizable effect of cutting the specimens into small pieces. However, it is likely that the effect would be significant if some or all of the combustible mass were intentionally being protected by a fire barrier.
- The extensive ongoing research using various designs of the cone calorimeter with variable oxygen volume fraction and total inflow should include measurement of toxic species. This would further refine the operating conditions that provide the broadest agreement with the gas yields from room fire tests.

Further investigation of the tube furnace is warranted. It is important to understand why the CO₂ yields for the underventilated condition are low and why the yields from the well ventilated condition are in agreement with the postflashover fire stages of the room fires for all three combustibles. It would also be helpful to understand the observed changes in some yields when the same equivalence ratio was achieved with different combinations of mass and air flow.

The results of this study provide a better basis for obtaining toxic potency input data for fire modeling than currently exists. A more robust basis for future engineering assessments of fire safety designs would result from the performance of

- Additional room-scale tests with more combustibles and room placements.
- A series of parametric runs of a zone or field fire model in order to define better the effect
 of input data accuracy and variability on the times to threats to building occupant life
 safety.

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APPENDIX A. CHEMISTRY OF THE TEST COMBUSTIBLES

Table 1. Elemental Analysis of Fuels.

| | Mass % | | | | | | | | | | | | | | |
|-------------------------------|--------|------|-------|------|----|----|----|----|------|----|----|-------|-------|------|-----------|
| Sample | С | Н | N | CI | Ca | Pb | Al | Sb | Р | Sn | Ti | Total | Δ* | 0 | Remainder |
| Particle Board, with laminate | 46.89 | 6.70 | 2.68 | 0.26 | n | n | n | n | n | n | n | 56.53 | 43.47 | | |
| | 46.56 | 6.68 | 3.35 | 0.24 | n | n | n | n | n | n | n | 56.83 | 43.17 | | |
| | 47.12 | 6.60 | 2.76 | 0.26 | n | n | n | n | n | n | n | 56.74 | 43.26 | | |
| Mean value | 46.86 | 6.66 | 2.93 | 0.25 | | | | | | | | 56.70 | 43.30 | 42.6 | 0.7 |
| Standard deviation | 0.28 | 0.05 | 0.37 | 0.01 | | | | | | | | 0.15 | 0.15 | | |
| Pressboard, with laminate | 43.04 | 6.12 | 0.21 | 0.14 | n | n | n | n | n | n | n | 49.51 | 50.49 | | |
| | 43.12 | 6.08 | 0.21 | 0.15 | n | n | n | n | n | n | n | 49.56 | 50.44 | | |
| | 42.73 | 6.20 | 0.18 | 0.14 | n | n | n | n | n | n | n | 49.25 | 50.75 | | |
| Mean value | 42.96 | 6.13 | 0.20 | 0.14 | | | | | | | | 49.44 | 50.56 | | |
| Standard deviation | 0.21 | 0.06 | 0.02 | 0.01 | | | | | | | | 0.17 | 0.17 | | |
| Cushion fabric | 47.23 | 6.23 | 0.18 | n | n | n | n | n | n | n | n | 53.64 | 46.36 | | |
| | 48.12 | 6.10 | 0.19 | n | n | n | n | n | n | n | n | 54.41 | 45.59 | | |
| | 47.38 | 5.99 | 0.20 | n | n | n | n | n | n | n | n | 53.57 | 46.43 | | |
| Mean value | 47.58 | 6.11 | 0.19 | | | | | | | | | 53.87 | 46.13 | 46.5 | 0.4 |
| Standard deviation | 0.48 | 0.12 | 0.01 | | | | | | | | | 0.47 | 0.47 | | |
| Cushion padding | 56.38 | 8.48 | 12.58 | 0.95 | n | n | n | n | 0.20 | n | n | 78.59 | 21.41 | | |
| y | 56.33 | 8.58 | 12.50 | 0.90 | n | n | n | n | 0.15 | n | n | 78.46 | 21.54 | | |
| | 56.36 | 8.53 | 12.46 | 0.71 | n | n | n | n | 0.21 | n | n | 78.27 | 21.73 | | |
| Manazakia | 56.36 | 8.53 | 12.51 | 0.85 | | | | | 0.19 | | | 78.44 | 21.56 | 25 | -3.5 |
| Mean value Standard deviation | 0.03 | 0.05 | 0.06 | 0.13 | | | | | 0.03 | | | 0.16 | 0.16 | | |

| | | | | | | | | M | ass % | | | | | | |
|--------------------|-------|------|-------|-------|-------|--------|------|------|-------|----|----|-------|-------|----------------------|-----------|
| Sample | С | Н | N | CI | Ca | Pb | Al | Sb | Р | Sn | Ti | Total | Δ* | 0 | Remainder |
| Cable jacket | 40.83 | 5.07 | <0.10 | 26.77 | 10.42 | < 0.05 | | | | | | 72.67 | 27.33 | | |
| | 40.94 | 5.20 | <0.10 | 26.53 | 10.18 | < 0.05 | | | | | | 72.67 | 27.33 | | |
| | 40.87 | 5.15 | <0.10 | 26.68 | 10.24 | < 0.05 | | | | | | 72.70 | 27.30 | | |
| Mean value | 40.88 | 5.14 | | 26.66 | 10.28 | < 0.05 | | | | | | 72.68 | 27.32 | 16.7 | 10.6 |
| Standard deviation | 0.06 | 0.07 | | 0.12 | 0.10 | | | | | | | 0.02 | 0.02 | | |
| Wire insulation | 48.25 | 6.73 | 2.39 | 26.04 | | | 0.80 | 0.62 | | | | 83.41 | 16.59 | | |
| | 48.20 | 6.98 | 2.65 | 26.08 | | | 0.81 | 0.62 | | | | 83.91 | 16.09 | | |
| | 48.57 | 6.82 | 2.40 | 26.22 | | | 0.72 | 0.63 | | | | 84.01 | 15.99 | | |
| Mean value | 48.34 | 6.84 | 2.48 | 26.11 | | | 0.78 | 0.62 | | | | 83.78 | 16.22 | 9.2 | 7.0 |
| Standard deviation | 0.20 | 0.13 | 0.15 | 0.09 | | | 0.04 | 0.00 | | | | 0.32 | 0.32 | | |
| Cable filler | 42.58 | 6.65 | <0.10 | n | | | | | | | | 49.23 | 50.77 | | |
| | 42.42 | 6.84 | <0.10 | n | | | | | | | | 49.26 | 50.74 | | |
| | 42.72 | 6.80 | <0.10 | n | | | | | | | | 49.52 | 50.48 | | |
| Mean value | 42.57 | 6.76 | | | | | | | | | | 49.34 | 50.66 | 38.4 (C) 49.0 (H) | |
| Standard deviation | 0.15 | 0.10 | | | | | | | | | | 0.16 | 0.16 | | |
| Cable residue | 18.39 | 2.30 | 0.20 | 22.99 | | | | | | | | 43.88 | 56.12 | | |
| | | | | 25.42 | | | | | | | | | | | |
| | 19.03 | 2.45 | 0.21 | 27.76 | | | | | | | | 49.45 | 50.55 | | |
| | | | | 28.62 | | | | | | | | | | | |
| | 17.91 | 2.47 | 0.14 | 30.00 | | | | | | | | 50.52 | 49.48 | | |
| | | | | 27.87 | | | | | | | | | | | |
| Mean value | 18.44 | 2.41 | 0.18 | 26.96 | | | | | | | | 47.95 | 52.05 | | |
| Standard deviation | 0.56 | 0.09 | 0.04 | 2.51 | | | | | | | | 3.57 | 3.57 | | |

^{* [1 -} Σ (mass %) of listed elements]

Table 2. Elemental Analysis of Fuel Components.

| | | Mass % | | | | | | | | | | | |
|----------------------------|------|--------|------|------|----|----|----|----|---|----|----|-----|------|
| Sample | С | Н | N | CI | Ca | Pb | Al | Sb | Р | Sn | Ti | Ash | 0 |
| Wood | 49.0 | 6.1 | 0.2 | | | | | | | | | 0.5 | 44 |
| Paper | 49.0 | 6.1 | 0.2 | | | | | | | | | 0.5 | 44 |
| Urea formaldehyde | 33.3 | 5.6 | 38.9 | | | | | | | | | | 22.2 |
| PVC | 38.4 | 4.8 | | 56.7 | | | | | | | | | 0 |
| Dioctyl phthalate | 73.8 | 9.8 | | | | | | | | | | | 16.4 |
| Melamine | 28.6 | 4.8 | 66.7 | | | | | | | | | | 0 |
| Cotton (= cellulose) | 44.5 | 6.2 | | | | | | | | | | | 49.3 |
| Polyethylene terephthalate | 62.5 | 4.2 | | | | | | | | | | | 33.3 |
| Nylon 6,6 | 64 | 9.3 | 12 | | | | | | | | | | 14 |
| Nylon 6 | 66 | 10.2 | 11 | | | · | | | | | | | 13 |
| FPU foam | 57.6 | 5.6 | 11.2 | | | | | | | | | | 25.6 |

Table 3. Heats of Combustion of Fuels.

| Sample | | ΔH _c (MJ/kg) | Mean | σ | | | | |
|-------------------------------|----------------|-------------------------|-------|-------|------|--|--|--|
| Particle Board, with laminate | 18.24 | 18.17 | 18.07 | 18.16 | 0.07 | | | |
| Pressboard, with laminate | 16.48 | 16.18 | 16.26 | 16.31 | 0.03 | | | |
| Cushion fabric | 18.17 | 17.96 | 17.94 | 18.02 | 0.10 | | | |
| Cushion padding | 26.09 | 26.02 | 26.12 | 26.08 | 0.04 | | | |
| Cable jacket | 18.30 | 18.41 | 18.36 | 18.36 | 0.04 | | | |
| Wire insulation | 23.39 | 23.33 | 23.45 | 23.39 | 0.06 | | | |
| Cable filler | 17.01 | 17.00 | 17.00 | 17.00 | 0.00 | | | |
| Cable residue | Did not ignite | | | | | | | |

The mass fractions of cover fabric and padding in the sofa cushions were determined to be 0.205 ± 0.004 and 0.795 ± 0.004 , respectively. Since the cushions appeared to burn evenly (*i.e.*, the fabric was generally not burned away well before the foam was) and since they were virtually consumed in the tests, we presumed that the elemental composition of the fuel was steady during the tests. We then estimated the cushion composition (mass fraction) to be:

C:
$$0.545 \pm 1 \%$$

H:
$$0.080 \pm 1 \%$$

N:
$$0.100 \pm 1 \%$$

C1:
$$0.0068 \pm 16\%$$

P:
$$0.0015 \pm 17 \%$$

O:
$$0.267 \pm 4 \%$$

The derived value for the heat of combustion for the cushions is 24.4 MJ/kg \pm 3

For the bookcases, we estimated the fuel composition to be:

C:
$$0.481 \pm 0.6 \%$$

H:
$$0.062 \pm 0.8 \%$$

N:
$$0.029 \pm 13 \%$$

C1:
$$0.0030 \pm 4 \%$$

O:
$$0.426 \pm 1 \%$$

The heat of combustion for the bookcase is 18.2 MJ/kg \pm 0.4 %.

For the electric power cable, we measured the mass fractions of the insulation, filler paper, and jacket to be 0.516 ± 0.007 , 0.033 ± 0.0007 , and 0.239 ± 0.007 , respectively. The remainder of the mass was the copper wire. For the combustible material, the elemental composition was:

C:
$$0.576 \pm 0.5 \%$$

H:
$$0.080 \pm 1.5 \%$$

C1:
$$0.323 \pm 0.4 \%$$

N:
$$0.021 \pm 6 \%$$

The heat of combustion for the combustible fraction of the cable is $21.60 \text{ MJ/kg} \pm 0.6 \%$.