Large-Scale Toxicity Correlations

VYTENIS BABRAUSKAS
Center for Fire Research
National Institute of Standards and Technology
Gaithersburg, MD 20899, U.S.A.

ABSTRACT

Some of the recent work done at NIST in the area of validating reduced-scale toxicity test methods against full-scale room fire data is reviewed. The agreements and disagreements obtained thus far are summarized. The current NIST research program for systematizing the validation process itself is also reviewed.

HYPOTHESIS

The simplest hypothesis that can be used in the validation of bench-scale toxicity data against full-scale data is the following: Is the yield of all toxicologically important gas species similar in the bench-scale tests and in the full-scale studies? We note that the definition of yield is that yield of gas X = kg X produced/kg fuel burned. To this end, several test series of data can be examined.

THE DATA EXAMINED

During the last few years, opportunities arose at NIST to complete 3 different test series where the objective was to investigate the relation between full-scale fire toxicity data and the data from reduced-scale test methods. The first two projects were conducted under the sponsorship of the Consumer Product Safety Commission (CPSC) – these will be referred to as the 1987 report [1] and the 1988 report [2]. Also reported on in 1988 was work sponsored by the Fire Retardant Chemicals Association (FRCA) [3]. Detailed data on all three of these projects have been published. In the present paper we will merely point out some of the most salient conclusions.

The two CPSC projects differed primarily in the large-scale test arrangements. The first series used a complex three-room layout, where most of the measurements were made in a room remote from the fire. The second test series focused on a single room, with measurements being made within that same room. For practical reasons, also, while the first series used mockups of entire upholstered chairs as the test item, the second series was simplified to using just a single chair cushion. The test specimens for both series were constructed of the same materials, and were two in number: cotton upholstery fabric paired with fire-retardant (FR) polyurethane foam, and the same fabric paired with a non-fire-retardant (NFR) polyurethane foam. The full-scale tests comprised three different scenarios: flaming, smoldering, and smoldering-to-flaming transition.

In addition to room fire tests, less-than-room-size tests were conducted. These included the furniture calorimeter [4], where the specimens can be of full, end-use size, but are tested in the

open, not inside in room. Smaller-scale tests were conducted using the Cone Calorimeter [5] and the NBS Toxicity test [6].

An important objective of these studies was to find if yields of various toxic gases are similar between bench scale and full scale. Table 1 shows a summary of the results; details of the measurements made are all given in the original references cited. For a given test exposure (flaming, smoldering, or transition), the different tests often show an order of magnitude agreement, but not much closer. The smoldering and the transition exposures would especially be expected not to show good agreement, since neither the Furniture Calorimeter, the Cone Calorimeter, nor the NBS toxicity test were actually designed for the purpose of simulating cigarette smolder exposures. All could be modified to better represent such fire conditions, but such modifications were not undertaken as part of these studies.

The FRCA studies comprised a wider range of materials – 5 different types of materials were examined, each in a fire retarded and a non-fire-retarded formulation. The exposures examined were simpler, however, and only a flaming fire was studied. Table 2 shows the results for the FRCA test specimens in the less-than-room-size tests. For the room fire test portion of this program, the specimens were not tested individually. Instead, all FR commodities were tested together in one series of tests, while all NFR commodities were tested together in a second series of tests. Table 3 shows these results.

The above data are certainly not conclusive. Taken together, however, they to suggest that the yields of CO_2 and of the acid gas species ($HC\ell$, HBr) are similar among the tests to within a factor of 5. The data for HCN are inconclusive. For CO, it is clear that the bench-scale data do **not** predict the full-scale, except in the roughest order-of-magnitude sense. It is evident that a dedicated research program is needed to develop procedures which would predict the full-scale CO yields. Pitts [7] has outlined some of the steps that will need to be taken to achieve this predictability.

NEW WORK

The above considerations suggest that a simple hypothesis of all gas yields being scaled successfully is not appropriate. Thus, there has been started at NIST a new project in this area. For the Fiscal Year 1989, Congress provided a special appropriation so that a pilot study could be produced on the *methodology* required for validating reduced-scale toxicity test methods against full-scale room fires. The project itself includes only a limited amount of experimental work; its objective, however, has not been to provided lists of validated or invalid bench-scale tests, but, rather, to lay the groundwork for systematic future validation efforts. The work is now being completed and will be reported upon shortly [8].

To arrive at this improved methodology, the present situation can be summarized as follows. Even when a special CO prediction technique becomes available to solve the specific problems associated with that gas, it is clear that yields for the remaining gases will not be identical for all scales. This is not surprising when viewed in light of the actual combustion phenomena. Typical full-scale room fires show a progressive history: first ignition, then a small, spreading fire, later possibly reaching flashover, eventually burning mostly at charred surfaces, then dying out. Both

the condition of the specimen and the external conditions (type of heating, oxygen concentration) will, in consequence, vary throughout the fire. A modern bench-scale test, by contrast, exposes the specimen to one set of combustion conditions throughout the burning. We emphasize here the 'modern.' Older fire test of various types often did try to create a time-varying exposure to the specimen. These were much less useful than today's tests, however. The modern test methods attempt to create simple exposure conditions, so that basic material fire properties of the specimen could be deduced. The older, simulation type of tests created an exposure history which did not correspond to actual full-scale conditions. Thus, such data had utility neither as material fire properties, nor as an assessment of hazard.

The proposed validation methodology being explored is based on recognizing this fact that a single bench-scale test cannot fully capture the essence of a full-scale scenario where the fire does not burn in a steady state. This is posed as the question: **Does the bench-scale test show the same primary toxic gases as the full-scale test?** If a given bench-scale test does this successfully for a suitably wide range of test materials or products, then it has been validated. Conversely, if it shows primary toxic gases which are not the same as in the full-scale tests, then the results of the proposed bench-scale test cannot be used to assess hazard for this fire scenario. Note that it is not required in this definition that yields or the ratios of the primary toxic gases be the same in the bench-scale test as in full scale. To insist on such equality would assure that only a single, unique combustion condition could be matched. (In the above, by 'primary gases' we mean gases that contribute an amount to the fractional effective dose, FED, which is greater than the uncertainty interval of the FED determination; a fuller discussion of the FED concept is contained in [3].)

Finally, our current understanding of CO production poses a unique difficulty in test design. The indications are that the quantity of CO produced depends at least as much on the full-scale ventilation and geometry as it does on any 'material properties' of the test specimen. This suggests that the proper way to take this aspect into account will be a combination of physical, bench-scale testing and a numerical calculation of expected CO yields. The exact mechanisms for doing this have not yet been worked out.

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Table 1

Summary of yields found in NIST tests on upholstered chair specimens

Material	Test	Exposure	CO yield	CO_2 yield	HCN yield
NFR	Room test	flaming	0.09	1.9	0.002
	Furniture calorimeter	flaming	0.04	1.9	0.0006
	Cone Calorimeter	flaming	0.01	2.3	N.A.
	NBS Toxicity test	flaming	0.02	1.6	0.0017
	Room test	sm.-to-fl.	0.07 - 0.08	0.4	0.003
	Room test	sm.-to-fl.	0.11 - 0.12	2.2 - 2.6	N.A.
	Furniture calorimeter	sm.-to-fl.	0.12	3.6	0.001
	NBS Toxicity test	ramped	N.A.	N.A.	0.0105
	Room test	smolder	0.08 - 0.11	0.3 - 0.4	N.A.
	Furniture calorimeter	smolder	0.24	N.A.	< 0.0014
	Cone Calorimeter	smolder	0.03	1.7	N.A.
	NBS Toxicity test	non-flaming	0.03	0.2	0.0004
FR	Room test	flaming	0.10	1.3	0.004
	Furniture calorimeter	flaming	0.05	1.8	0.0018
	Cone Calorimeter	flaming	0.05	1.9	N.A.
	NBS Toxicity test	flaming	0.05	1.5	0.0057
	Room test	sm.-to-fl.	0.11 - 0.15	2.1 - 2.2	0.001
	Room test	sm.-to-fl.	0.11 - 0.14	0.6 - 0.7	N.A.
	Furniture calorimeter	sm.-to-fl.	0.13	1.9	0.007
	NBS Toxicity test	ramped	N.A.	N.A.	0.0130
	Room test	smolder	0.08 - 0.11	0.5	N.A.
	Furniture calorimeter	smolder	0.35	N.A.	< 0.0005
	Cone Calorimeter	smolder	0.03	1.7	N.A.
	NBS Toxicity test	non-flaming	0.04	0.3	0.0003

N.A. - not available

Table 2

FRCA series – Summary of yields found in less-than-room-size tests

Specimen	NFR /FR	CO (kg/kg) Cone Cal.	CO (kg/kg) Furn. Cal.	CO (kg/kg) Tox. Test.	CO_2 (kg/kg) Cone Cal.	CO_2 (kg/kg) Furn. Cal.	CO_2 (kg/kg) Tox.[d] Test.	HCN (kg/kg) Cone Cal.	HCN (kg/kg) Furn. Cal.	HCN (kg/kg) Tox. Test.	HBr (kg/kg) Cone Cal.	HBr (kg/kg) Furn. Cal.	HBr (kg/kg) Tox. Test.	HCl (kg/kg) Cone Cal.	HCl (kg/kg) Furn. Cal.	HCl (kg/kg) Tox. Test.
TV Cabinet H	NFR	0.015	0.12	0.084	2.28	1.39	2.09	—	—	—	—	—	—	—	—	—
TV Cabinet G	FR	0.109	0.37	0.18	0.67	0.74	0.78	—	—	—	0.069	0.082	0.017	—	—	—
Bus. Machine F	NFR	0.037	0.13	0.17	2.21	1.61	1.98	—	—	—	—	—	—	—	—	—
Bus. Machine A	FR	0.055	0.29	0.30	1.60	1.45	1.53	—	—	—	—	—	—	—	—	—
Chair T	NFR	0.020	0.01	—	1.62	1.89	—	0.002	0.001	—	—	—	—	—	—	—
Chair S	FR	0.051	[a]	—	0.964	[a]	—	0.005	—	—	—	—	—	0.023	—	—
Chair T[b]	NFR	0.016	—	0.025	1.71	—	2.05	0.002	—	0.0007	—	—	—	—	—	—
Chair S[b]	FR	0.055	—	0.15	0.81	—	1.19	0.0023	—	0.0032	—	—	—	0.022	—	—
Cable D	NFR	0.041	0.12	—	1.77	1.61	—	—	—	—	—	—	—	0.112	0.121	—
Cable K	FR	0.060	0.10	—	1.34	1.04	—	—	—	—	—	—	—	0.131	0.133	—
Cable D[c]	NFR	0.029	—	0.050[e]	2.19	—	2.38	—	—	—	—	—	—	ND	—	—
Cable K[c]	FR	0.135	—	0.13	1.00	—	1.26	—	—	—	—	—	—	0.093	—	—
Circuit Bd. C	NFR	0.014	0.10	0.075[e]	2.07	1.71	2.13	—	—	—	—	—	—			
Circuit Bd. L	FR	0.103	0.10	0.15	0.87	1.36	1.24	—	—	—	0.022	—	0.0043			

[a]Could not be determined reliably.
[b]Foam only, no cover fabric.
[c]Wire insulation only.
[d]Determined only from those tests where animals were not used.
[e]Excludes data from the highest mass loading tested, since presumed unrepresentative.
—Not run
ND Not detected

Table 3

FRCA series – Comparison of CO yields to room fire data
CO yield (kg/kg)

Specimens	Room test	Cone Calorimeter	Furniture Calor.	NBS Toxicity test
NFR	0.18	0.02	0.09	0.074
FR	0.23	0.06	N.A.	0.155

N.A. – not available

Note: the specimens tested in the room tests comprised all 5 types of commodities (as described in Table 2) tested in two arrangements: one all-NFR, the second all-FR. For the other tests, the values reported are appropriately weighted sums.