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Comparison of Several Compartment Fire Models: An Interim Report

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U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
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Abstract

A substantial number of mathematical models for compartment fires have been developed in the past decade. This report analyzes and compares in depth three such models. This is done with particular emphasis on the needs of the Nuclear Regulatory Commission and Sandia National Lab, for their Risk Methods Integration and Evaluation Program. The models examined are: (1) the Harvard family of models, Mark 5, 5.2, 5.3, and 6; (2) COMPBRN; and (3) FAST. The capabilities of a model can be understood in terms of the answers to a series of questions; these are formulated, placed into categories, and then answered. The answers are given in brief form in a table (section 4); the bulk of the report consists of elaborations and discussions of these points.

A number of conclusions emerge from this study: first, there is at present no one model which will do everything which is wanted by an arbitrary user - some have certain capabilities; others, different capabilities. Therefore each user must look for a model which does what he (she) wants, and does it well. Second, from the point of view of the NRC, Harvard Mark 5.3 may be the best choice, because it is the only one which has all of the following characteristics: it is time-dependent; it considers forced ventilation; it has good numerics; and it takes into account heating and ignition of target objects. The last section of this report briefly outlines which developments would be desirable, for each model.

Keywords: compartment fires, fire models, mathematical models, comparison.

1. INTRODUCTION

The Nuclear Regulatory Commission (NRC) decided several years ago to update its estimates of risks and hazards in nuclear power plants. It commissioned Sandia National Laboratory to carry out this analysis; to this end, Sandia established a Risk Methods Integration and Evaluation Program (RMIEP). One of the major hazards in nuclear facilities is the occurrence of fire; a cost-effective method for quantitatively determining the fire hazards is <u>via</u> reliable mathematical models of how fires develop in nuclear facilities.

A substantial number of mathematical models for compartment fires have been developed in the past decade. This paper analyzes and compares in depth three such models which might be of use to the NRC and SANDIA in their RMIEP process: the Harvard model(s)*, COMPBRN (developed at UCLA), and FAST (developed at NBS). Limitations of time have precluded the consideration of other possible candidate models, such as DACFIR [32]. There have been a number of other analyses such as this one, to which the reader may wish to refer: see [27-30].

An attempt has been made to be as objective as possible in this analysis; however, there are two obstacles to complete objectivity: first, many of the comparisons involve judgements, rather than quantifiable criteria. Second, the writer of this report is also one of the authors of the Harvard models, and so is most familiar with them.

It is understood that all these models are still evolving, and that limitations or inadequacies which exist today may be removed tomorrow. However, this report addresses itself strictly to what is available today.

In section 2, a brief summary of the main good and bad features of the models is given, with emphasis on NRC's needs.

Section 3 begins the detailed analysis of the models, in the form of a series of questions; these are grouped into six categories (Numerics, Documentation, Physics, Validation, Structure, and Other Factors). The brief answers to these questions, for each model, are given in Table I in section 4, for quick and easy reference. Section 5 consists of extensive annotations to the Table, so that various points can be clarified; this is the heart of the report. In the subsection on Physics, an effort has been made to indicate the validity of each algorithm; this is in addition to a separate subsection on Validation.

Since this is not a research report, and the author has explicitly eschewed making any conclusions, there is no CONCLUSIONS section. Section 6 briefly indicates what developments are needed in each model to make it more useful to NRC/SANDIA.

2. GENERAL IMPRESSIONS

A caveat for the reader: As pointed out in the Introduction, the author has been responsible to a large degree for the development of the Harvard programs, and is therefore much more familiar with them than with the others. For this reason, somewhat more detailed comments are made about them than about the other programs. Moreover, although efforts have been made to avoid bias in this analysis, complete objectivity is of course not possible. One way the author has tried to minimize bias, is to have the principal authors of the other models review the rough draft of this paper, and to include their comments.

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*Although the Harvard model is here referred to in the singular for convenience, it is in fact a family of models (at present), of which the basic single-room model is Mark 5. Mark 6 is a multi-room version. Versions Mark 5 and 6 were developed at Harvard; Mark 5 was enriched at NBS to version 5.2, and to 5.3 at Harvard and NBS. Mark 6 was debugged and partially improved at NBS.

There is at present no mathematical model that is ideal for all users, nor even one which is ideally suited to any single user, such as the NRC. Among Harvard, COMPBRN, and FAST, the Harvard model is the most comprehensive one, the best documented, and the most validated*. It calculates the hot layer temperature and depth, and the radiative and convective fluxes to a target object (all as functions of time), reasonably well. The resulting heating up of that target, therefore, is reliably calculated. Perhaps the most significant drawback of the Harvard models, as of this writing, is that the ability to simulate forced ventilation and the ability to follow the heating of the lower layer appear in two different versions, Mark 5.3 and Mark 5.2. (Work is now underway towards merging 5.2 and 5.3.) Mark 6, on the other hand, while having the capacity to deal with several rooms, has neither of the enrichments mentioned above. A difficulty with the Harvard models, as well as all the others, is that of finding the thermophysical data needed to run them. This has been addressed and partially solved in Mark 6 (see "Other Factors", item 4).

COMPBRN is simpler, less detailed, and less (physically) reliable, but it is more flexible in its treatment of the fuel-bed and of targets, and it is much faster. Perhaps its greatest drawback is that it is a (quasi)static model, so that if the fire is developing rapidly, the results will be inaccurate. Another feature of COMPBRN is that the user must specify (as input) a good deal of information which is <u>not</u> thermophysical data to be found in handbooks or in the literature. Examples are: the degree of "porosity" of a given fuel-bed, the amount of feedback from the compartment, and the fractions of a forced flow which enter the upper and lower layers, respectively. Although this permits a good deal of flexibility, it also permits a fair amount of arbitrariness.

FAST has the most reliable numerics, and is a multi-room model. It also includes heating of the lower layer(s), and does the most complete job of calculating species concentrations. Its principal drawbacks from Sandia's point of view are that it does not calculate the heating or ignition of target objects, nor does it incorporate forced ventilation.

3. QUESTIONS TO BE ADDRESSED IN ANALYZING A COMPARTMENT FIRE MODEL

The capabilities of a model can be understood in terms of the answers to a series of questions. These questions are here separated into six general categories:

I. Numerics
II. Documentation
III. Physics
IV. Validation
V. Structure
VI. Other Factors

The starred items below (*) are of special interest to NRC/SANDIA. The rest are of more general interest, and are listed in what is estimated to be decreasing order of importance.

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*A good deal of validation work has been done on FAST in the past year, however.

I. Numerics

1. How robust are the numerics? i.e., are the numerical computations stable, and convergent 98% of the time?

2. How accurate is the numerical method? Can a certain level of accuracy be guaranteed?

3. Can the desired accuracy be prescribed?

4. Can a different "math pack" be substituted if desired?

II. Documentation

1. Is there good documentation to support the program?

2. Is there a good user manual?

3. Is the internal documentation (in the program) good?

III. Physics

*1. Does it give the variation of the depth and temperature of the hot gas layer?

*2. Does it handle temperature gradients in the hot gas layer?

*3. Does it handle forced ventilation? How well?

*4. Can it handle multiple rooms? How many?

*5. Modeling of fuel source(s):

a. How many fuel sources does it permit? Simultaneously?
b. crib fire
c. wall fire
d. corner fire
e. slab (horizontal) fire, growing
f. solid pool
g. liquid pool
h. burner
i. moving source

*6. Does it determine when a second source ignites? How?

*7. Does it give species concentrations in the hot layer? In particular:

a. O_2
b. CO_2
c. CO
d. THC (total hydrocarbons)
e. unburnt fuel
f. smoke
g. H_2O

h. HCl
i. other

*8. How well does it handle different target configurations?

*9. Does it adequately treat the convective and radiative heat transfers to an object immersed in the hot gas layer, which cannot "see" the flame?

*10. Does it consider the mixing of (hot and cold) layers at vents? How well?

*11. What is the effect of beams or partitions on the modeling accuracy?

*12. Can it handle oddly-shaped rooms? How well?

*13. What is the number of dimensions handled by the program? (is it two-dimensional or three-dimensional)?

14. Does it permit the user to prescribe an arbitrary fire?

15. Can it handle fires other than prescribed ones?

16. Is the model static or dynamic (time-dependent)?

17. Does it determine radiative heat transfers? How well?

18. Does it determine convective heat transfers? How well?

19. Does it give the spread rate of a fire on an object?

20. Does it determine the heating of objects? How well?

21. Does it determine the heating of the ceiling?

22. Does it determine the heating of the walls?

23. Does it determine the heating of the floor?

24. Does it predict fire detection?

25. Can it handle burnout? How well?

26. Does it consider the temperature and composition of the lower layer?

27. Does it consider burning in vitiated air?

28. Does it handle ceiling venting?

29. Does it give ceiling ignition?

30. Does it predict layer ignition?

31. Does it predict ignition in a room other than the room of origin?

32. Can it handle charring fuels?

33. Does it consider different ignition modes? How well?

34. Can a vent be opened or closed <u>during</u> the fire?

35. Can it handle rooms on more than one floor? How well?

36. Does it describe fire suppression?

37. Can it handle leaning plumes (which are inclined because of wind)?

38. In general, how much of the important physics involved is included?

39. How well does it treat the physics it <u>does</u> consider?

IV. <u>Validation</u>

*1a. How thoroughly has the <u>overall model</u> been tested ("validated") against real fires?

*1b. How well did it perform?

2. How well have the algorithms for <u>each physical process</u> been validated? (see item III. 39)

V. <u>Structure</u>

1. How modular is the program?

2. How easily can it be modified? With:

   a. New algorithm(s)
   b. New variable(s)
   c. Changes in I/O
   d. Changes in numerics

3. How transportable is it?

4. How well has it been "idiot-proofed"?

VI. <u>Other Factors</u>

*1. What is the "computer power" required? i.e. how large a machine is required?

*2. What are typical run times?

*3. What are the parameter limits within which it is <u>valid</u>?

*4. What is the quality and availability of required input data?

5. Is it user-friendly? How easy is it to use?

6. What are the parameter limits within which it will converge?

7. What are the principal advantages of the model?

8. What are the principal drawbacks of the model?

9. Can it be run interactively?

10. Can it be run in batch mode?

11. Does it have graphics capability?

4. Table 1. Brief answers to the points and questions raised in items I to VI, for the several compartment models considered. The symbols have the following meanings: C = see comments following Table. D = dynamic. E = excellent. F = fair. G = good. M = maybe. NA = not applicable. P = poor. QS = quasistatic. U = unknown. VG = very good. √ = yes. x = no.

			Mark 5	Mark 5.2	Mark 5.3	Mark 6	COMPBRN II	FAST
I. Numerics	1	Stable & convergent?	√	√	√	√	√	√
	2	Accurate? Guaranteeable?	G,√	G,√	G,√	E,√	F-G,x	G,√
	3	Is accuracy prescribable?	√	√	√	√	x	√
	4	Other "math packs"?	x	x	x	M,C	x	M,C
II. Documentation								
	1	Program documentation?	E	VG	VG	G	P-F	F-G
	2	User manual?	F	F	F	G	G	G
	3	Internal documentation?	G	G	G	F	P	G
III. Physics	*1	Depth & T of layer?	√	√	√	√	√	√
	*2	Temp. gradients?	x	x	x	x	x	x
	*3	Forced ventilation?	x	x	√VG	x	√P	x
	*4	Multiple rooms?	x	x	x	√E,5	x	√E,11
	*5a	No. of fuel sources?	5	5	5	5	≥25	1
	* b	crib fire?	P	P	P	P	√	x
	* c	wall fire?	P	F	P	P	√	√,C
	* d,i	corner fire? moving?	x	x	x	x	x	√,x,C
	* e	growing horizontal fire?	√	√	√	√	x	x
	* f,h	solid pool, burner?	√	√	√	√	√	x
	* g	liquid pool fire?	√	√	√	√	x	x
	*6	Ignition?	√	√	√	√	√	x
	*7	Species concentrations:	√	√	√	√	x	√
		O_2, CO_2, CO, smoke H_2O	√	√	√	√	x	√
		THC, unburnt fuel	x	x	√	x	x	√
		HCl, other	x	x	x	x	x	√
	*8	Complex targets?	F	F	F	F	G	x
	*9	Heat transfers to immersed object?	√	√	√	√	F	x
	*10	Layer mixing?	x	√	x	U	x	√G
	*11	Effect of beams?	C	C	C	C	C	C
	*12	Odd-shaped rooms?	√P	√P	√P	√E	√F	M
	*13	2D or 3D?	3D	3D	3D	3D	3D	3D
	14	Prescribed fire?	x	√	√	√	x	√
	15	Non-prescribed fires?	√	√	√	√	√	x

Table 1, cont'd

			Mark 5	Mark 5.2	Mark 5.3	Mark 6	COMPBRN II	FAST
III. Physics	16	Dynamic?	D	D	D	D	QS	D
	17	Radiation heat transfer?	E	E	E	E	F	C
	18	Convective heat transfer?	G	G	G	G	F	G
	19	Fire spread rate?	✓	✓	✓	✓	✓	x
	20	Object heating?	E	E	E	E	E	x
	21,22	Ceiling, wall heating?	✓	✓	✓	✓	C	✓
	23	Floor heating?	C	C	C	C	C	✓
	24	Fire detection?	x	x	✓	x	x	x
	25	Burnout?	G	G	G	G	P	M
	26	Lower layer T?	x	✓	x	x	x	✓
	*27	Burning in vitiated air?	x	x	x	x	x	x
	28	Ceiling venting?	F	F	F	F	x	x
	29	Ceiling ignition?	C	C	C	C	C	x
	30	Layer ignition?	x	x	x	x	x	x
	31	Second-room ignitions?	x	x	x	✓	C	x
	32	Charring fuels?	x	x	x	x	x	✓
	33	Different ignition modes?	x	x	x	x	x	x
	34	Vent opening?	x	✓	x	x	x	✓
	35	Multiple floors?	NA	NA	NA	M	x	✓
	36	Fire suppression?	x	x	x	x	x	x
	37	Leaning plumes?	x	x	x	x	x	x
	38	Comprehensive physics?	G	VG	VG	G	F	G
	39	Adequacy of physics?	F-E	F-E	F-E	F-E	F	G
IV. Validation								
	*1a	Degree of validation?	G,C	G,C	G,C	G,C	F	G
	*1b	Performance?	----------P To E; generally, G---------				P-G	F
	*2	Algorithm validation?	G	G	G	G	F	G
V. Structure	1	Modular?	G	G	C	E	G	E
	2a	Add new algorithms?	F-G	F-G	F-G	F-G	P-G	G
	b	Add new variables?					G	G
	c	Can change I/O?	G	G	G	F	U	P
	d	Can change numerics?	P	P	P	F	U	P
	3	Transportable?	E	E	G	G	G-E	E
	4	Idiot-proofed?	G	F	E	F	P	F

Table 1, cont'd

		Mark 5	Mark 5.2	Mark 5.3	Mark 6	COMPBRN II	FAST
VI. Other Factors							
*1	Computer Power?						
*2	Run times?	C	C	C	C	C	C
*3	Parameter limits?						
*4	Input data?						
5	User-friendly?	P-G	G	G	G	P	G
6	Convergence limits?						
7	Principal advantages?	C	C	C	C	C	C
8	Principal drawbacks?						
9	Run interactively?	√	√	√	√	x	x
10	Can it run in batch?	P	P	P	P	√	√
11	Graphics capability?	x	√	x	√	x	E

5. DISCUSSIONS OF THE ANSWERS

These are elaborations to the entries in Table 1. Note that entries are commented on only where it is appropriate.

I. Numerics

1. How robust are the numerics? i.e., are the numerical computations stable, and convergent 98% of the time?

   Mark 5 is single precision, and converges about 85% of the time. Mark 5.2, 5.3, and Mark 6 are double precision, and converge about 98%, 98%, and 99% of the time, respectively. COMPBRN II converges most of the time, though it hasn't been "stretched" to consider large fires [Siu, private communication]. (Also see sections VI.3 and VI.6.) FAST is very stable; it has always converged, although occassionally convergence may be very slow.

2. How accurate is the numerical method? Can a certain level of accuracy be guaranteed?

   The Harvard Mark 5 series are (numerically) reasonably accurate: at any one time step, all significant variables should be correct to 300 parts per million. The accumulated errors in a 500-sec run are a few percent. The numerics in Mark 6 were designed to <u>guarantee</u> a prescribed accuracy; it does not always succeed in that, for subtle reasons; but it is at least as accurate as Mark 5.n. COMPBRN is less accurate: it requires, as a convergence criterion, that the hot layer temperature be converged within <u>one</u> Celsius degree (an accuracy of order 1% per time step), and "a few" cm. for layer height. The other variables are then presumed to be comparably accurate. It does not guarantee any prescribed degree of accuracy. In FAST, the variables converge to one part in a thousand <u>per time step</u>, comparable to the Harvard simulations.

4. Can a different "math pack" be substituted, if desired?

   <u>In principle</u>, Mark 6 should permit one to substitute another "math pack", because of its modularity. This has not been tried, however, and would be unlikely to be easy to do. The same answer holds for FAST, though the author (Jones) claims it would be relatively easy to do.

II. Documentation

1. Is there good documentation to support the program?

   In the author's estimation, the published documentation for FAST [18,34] is fair. In Jones' estimation, on the other hand, they constitute good documentation, when taken together with the comments written into the program itself.

   The documentation for Harvard Mark 5 is excellent [1]; it includes a description of all the physics algorithms, the numerics, the input/output, and the structure of the program. Mark 5.2 and 5.3 are <u>enriched</u> versions of Mark 5, and hence differ little from it in structure and numerics; therefore the same documentation applies, except of course that it does not include descriptions of the new physics algorithms. There is also documentation which validates the program -- see Section IV.

Mark 6 now has some documentation as well [2], but it is nowhere as complete as that for 5: it mostly discusses the structure of 6. However, it could be used as an adjunct to reference [1], since the physics in 6 is virtually the same as in 5. The documentation for COMPBRN is somewhat scattered ([3], [4], [5]), and not nearly so detailed as that for Mark 5. Some of the algorithms are discussed, in general terms.

2. Is there a good user manual?

There is no separate "user manual" for Mark 5, 5.2, 5.3, though Section VIII in ref. [1] gives a brief explanation and description. Morita [6] has written a draft of a user manual for Mark 6, but it is not yet available. The documentation for COMPBRN [3] includes a good section on the use of the program. Similarly, that for FAST [18] contains an appendix which is the user manual; it is sufficiently detailed that a knowledgeable engineer could run FAST without further help (Jones, private communication). Moreover, a user manual is about to appear: see ref. [33].

3. Is the internal documentation (in the program) good?

COMPBRN's internal documentation has received "mixed reviews", according to its author. It is not very easy to follow. Mark 5 (and 5.3) have fairly good internal documentation (especially if used in conjunction with the published documentation, ref [1]). However, it needs updating. This author has not examined the internal documentation for FAST, but its creator says that it is good (see item 1, just above).

III. Physics

*3. Does it handle forced ventilation? How well?

Mark 5.3 has a good algorithm for prescribed ventilation into or out of a room. However, it neglects the mixing of gases at vents. It also is primitive in that it requires the user to prescribe the volumetric flow rate at the vent (as a function of time - such as due to an HVAC system), rather than specifying the fan characteristic and power setting. Vent locations are prescribed by the user. For its validation, see Section IV, 1 and ref. [13]. COMPBRN II mixes a user-prescribed fraction of the forced ventilation inflow into the hot gas layer, and extracts a (possibly different) fraction from the layer, in the spirit of a one-node model. The different fractions (as well as the volumetric flow rates) must be specified by the user. This makes it more crude than the Mark 5.3 algorithm.

*4. Can it handle multiple rooms? How many?

FAST is multiroom, and can handle up to 11 rooms, at present. Moreover, it is a multistory model. For validation, see refs. [12] and [18]. COMPBRN, Mark 5, 5.2 and 5.3 are all single-room models. Harvard Mark 6 is a multi-room model, and does that well. It can handle up to 5 rooms, at present. (There is no limitation, in principle - the number of rooms allowed was arbitrarily DIMENSIONED to five). It is not a multi-story model, however.

*5. Modeling of fuel sources:

a. The Harvard models were (arbitrarily) DIMENSIONed to handle no more than 5 objects. This could easily be changed, but would require going into the program. COMPBRN can handle some 30 "modules", and each module can itself be subdivided into a number of pieces. As with the Harvard codes, more objects can be modeled simply by increasing the dimensions of the arrays. FAST only has (by design) the original fire.

b. Crib fires.

COMPBRN has an explicit algorithm for cribs, based on correlations explicitly found for cribs. It prescribes whether there is feedback of energy from the layer, etc. and how much. It also specifies a "porosity factor", which is an additional parameter permitting greater flexibility in describing of the fuel configuration. However, it is not impressive in its predictions. (see ref. [5], p. 73). The Harvard programs do not have a crib fire, though Mark 5.2 and 5.3 can be preprogrammed to mimic typical crib behavior. FAST also can be preprogrammed to mimic crib behavior.

c. Wall fires.

Of the Harvard codes, only Mark 5.2 has a wall fire algorithm, but it need to be debugged. They all can be programmed to mimic a wall fire with a horizontal growing fire, by choosing a larger effective fire growth parameter, A. This should be adequate for many purposes. COMPBRN, too, has a wall-fire algorithm; the same remarks apply. However, at least one sample calculation shows fairly good agreement with experiment, for the variation of pyrolysis rate with height for a PMMA fire. (See ref [5], p. 76). FAST only deals with prescribed fires, but it handles wall fires and corner fires in the sense that it associates an appropriate plume with each.

d. Corner fires.

None of the Harvard codes considered here has a corner fire algorithm (although, again, it could be mimicked by a judicious choice for the fire growth parameter, A, (see 5c)). Nor does COMPBRN, but one can use the feedback model which is incorporated into it, to specify how "the wall" affects burning. The fire plume coefficients are user-input in COMPBRN, so the plume can be "tuned" to account for a wall or corner. This is an ad hoc procedure, however, and useless for prediction unless the user manual instructs the user how to modify the coefficients. (It does not do so at present). FAST uses the plume entrainment coefficient found experimentally by Zukoski (see paragraph 5c, above).

e. Growing horizontal fires.

Mark 5 & 6 have an analytic expression for the rate of growth of a fire set on a horizontal surface. The growth rate is quasi-exponential, and agrees with a large class of fires (see ref. [8]). Acceleration of growth/spread rate due to the feedback of energy from the hot layer, ceiling, and other flames is explicitly and automatically computed.

f. Solid pool fires.

In the Harvard codes, it is assumed that a pool fire "turns on" very quickly (in a matter of seconds) -- it is otherwise quite similar to a growing fire. Once it has reached its maximum radius (i.e. area), the pyrolysis rate depends on the net heat flux entering the surface, again using the feedback from other sources (for validation, see ref [8]). COMPBRN makes no distinctions among these categories; it simply assumes everything is a solid. The user specifies $\dot{m}''$, the pyrolysis rate. COMPBRN also accounts for the increase in burning rate due to feedback from other flames, the ceiling, etc.

g. Liquid pool fires.

COMPBRN treats liquid pools essentially the same way it treats solid ones; it can probably do a fair job of predicting this burning mode by choosing the relevent parameters appropriately. The Harvard program(s) does not have an explicit algorithm for liquid pools. However, the various relevant physical effects - radiation blocking, reflection, transmission losses, etc. - can all be crudely taken into account by utilizing an <u>effective</u> heat of vaporization, in the <u>solid</u> pool algorithm.

h. Burner fires.

COMPBRN does not have a burner algorithm, but can mimic one, with the algorithms it <u>does</u> have; the user must choose a fuel element of some size, and prescribe $\dot{m}''$. Validation is essentially irrelevant, of course. Mark 5 has a burner algorithm which prescribes a user-chosen, constant gas flow rate. Mark 5.2, 5.3, and 6 have a more general algorithm (see item 15). FAST is similar to Mark 6 in this respect.

i. Moving source.

None of the programs has a moving-source algorithm. Both the Harvard and COMPBRN codes can easily mimic one, however, by judicious choices of growth and burnout of multiple objects. COMPBRN has a greater capacity for this, because it permits (right now) a larger number of objects.

*6. Does it determine when a second source ignites? How?

All of the Harvard variants, as well as COMPBRN, have a very simple ignition criterion: the surface reaches an "ignition temperature",

T_{ig}. The correctness and adequacy of the algorithm for calculating the surface temperature are well established. There is no target ignition in FAST.

*7. Does it give species concentrations in the hot layer?

All the Harvard variants give the mass concentration of O_2, CO, CO_2, smoke, and H_2O in the hot layer. Mark 5.3 gives total hydrocarbon (THC) (and therefore also unburnt fuel) as well. Note that other species could be monitored, even within the current constraints, by replacing H_2O (for example) by another, more interesting species (e.g. a radioactive one). The concentration of the radioactive species would then be labeled "H_2O", but would be that of the desired one. The validity of the calculation is demonstrated in [8], [9], and [1] (fig. 41). FAST gives the concentrations of all the above, and HCℓ, HCN, N_2, and NO_x as well. Moreover, it gives the optical depth for smoke. Finally, the source fractions can be given as prescribed functions of time (whereas they are only constants in the Harvard models).

*8. How well does it handle different target configurations?

In part, this question overlaps nos. 5, 17, and 18. As far as heating of targets is concerned, the radiative fluxes are reasonably well calculated, for simple geometries (e.g. horizontal or vertical slabs), in the Harvard models. The convective contributions are done more crudely, but reasonably adequately, too. Similar comments apply to COMPBRN, though the heat transfer algorithms are perhaps a bit cruder. On the other hand, more complex geometries are permitted in COMPBRN, via a "communication matrix" which allows the user to specify which objects can "see" which other objects. Moreover, if the target ignites, then much greater "fuel-bed discretization" (see #5) can be carried out, with greater flexibility.

*9. Does it adequately treat the convective and radiative heat transfers to an object immersed in the hot gas layer, which cannot "see" the flame?

COMPBRN and the Harvard models all treat this case. COMPBRN, however, does not take the attenuation of radiation through the hot gas layer (due to smoke, etc.) into account. (Also see item 8). For FAST, the answer would be "yes", if it included target objects (other than walls, floor, ceiling).

*10. Does it consider the mixing of (hot and cold) layers at vents? How well?

FAST considers mixing; it uses Quintiere's correlation for mixing into the lower layer, McCaffrey's correlation for mixing into the upper layer. The only one of the Harvard family of models which considers mixing of layers at vents is Mark 5.2. (There is some question, as to how well it does this, as the experimental correlations themselves are not entirely satisfactory). COMPBRN does not do it at all.

*11. What is the effect of beams or partitions on the modeling accuracy?

Single-room models do not recognize the existence of beams or partitions. Generally, this will not make a significant difference for beams as the "hot" layer usually rapidly drops below the level of the beams, and they are "inundated" by the layer. However, the magnitude of the effect depends entirely on the geometry and the fire size. For example, consider a room whose dimensions are 2.5 m high, 4 m wide, and 200 m long, with a one-foot deep beam running down the center of the room, making two channels. Thus the beam segregates two volumes, each 200 x 0.3 x 2 = 120 m^3. For a 100 kw fire, the plume will pump something like 500 gm/sec of gas into the upper space. Hence it will take about two and a half minutes to fill the first volume with hot gas (assuming the gas temperature = 300°C). After that time, the layer would have gotten deeper, and gas would begin to spill into the next space. This is a very significant period of time, however, and

(a) the gas trapped in the first channel is hotter than it would be without the beam,

(b) the other volume in the room is clear of hot gases for 2.5 minutes (or more, if there are other such partitions). If there were a smoke detector in the adjoining space, it would be delayed in its response by about 2.5 minutes; if there were sensitive equipment, it would be protected.

(c) The sensible way to solve the problem, then, would be to take the partitioned section as "the room", and follow that until significant spillage of hot gas occurs into the adjoining section(s).

This is an admittedly unrealistic example, but it serves to illustrate the point that when there are beams, the use of a single-room version may compromise modeling accuracy. A steady-state model such as COMPBRN will give incorrect results, since it will give the equilibrium layer depth, which is automatically greater than the deepest beam, for all times.

Partitions which project upward from the floor (and run the length or width of the room) are much more significant; they essentially break up the room into more than one compartment. Hence COMPBRN and the other single-room models are useless. For multi-room models such as Mark 6 and FAST, on the other hand, this presents no problem at all (in principle), since the partitions can simply be considered to divide the room into several end-to-end rooms.

*12. Can it handle oddly-shaped rooms? How well?

The single-room Harvard models - i.e. Mark 5, 5.2, 5.3 - can handle odd-shaped rooms to some extent. It is hard to say how well, since this would be done by taking an equivalent-volume rectangular parallelepiped. In general, the surface/volume ratio will be different, and so the convective heat loss to the walls will be different. If the ceiling is flat, the results may be expected to be better then for an inclined roof. In that case, too, Mark 6 (the multi-room version) should in principle do an excellent job, so long as the rooms are rectangular parallelepipeds. An L-shaped room, for example, can then be considered as two rooms, connected by a "doorway", with unit vent coefficient. COMPBRN has the same basic limitation as the single-room Harvard models, but should be able to do better from the point of view of which walls see which flames, etc. (*via* the communications matrix). But the hot gas layer algorithm will not treat it any better. (It will treat the room as a rectangular parallelepiped).

FAST can handle odd-shaped rooms better than either Harvard or COMPBRN, because it takes explicitly into account the fact that the room may not be a parallelepiped. It does this by allowing the cross-sectional area of the room to be a function of height. This permits the consideration of a peaked-roof house, or of an atrium. (Or even of the existence of furniture in the compartment.) Like Harvard, however, it still cannot describe the increase in resistance to fluid flow resulting from an L-shaped room, nor the changes in view factors (nor the changes in convective heat transfer due to inclined walls). But it will do about as well as Mark 6, in this regard.

*13. What is the number of dimensions handled by the program? (is it 2d or 3d)?

This question only applies to field models, where the complexity of the calculations is such that all early models were two-dimensional; that is still largely (though not entirely) true. The zone models are all effectively three-dimensional.

14. Does it permit the user to prescribe an arbitrary fire?

FAST handles prescribed fires by having the user specify $\dot{m}(t)$. Similarly, Mark 5.2, 5.3, and 6 handle it by specifying the fuel flow rate, $\dot{m}_f(t)$; i.e., they have a variable-burner algorithm built in. The resulting burning rate and power output are then calculated internally. Neither Mark 5 nor COMPBRN have provisions for a prescribed fire.

15. Can it handle fires other than prescribed ones?

All the Harvard models can handle pool fires and growing fires (see No. 5). COMPBRN also handles fire spread over a surface, and therefore handles non-prescribed, growing fires.

16. Is the model static or dynamic (time-dependent)?

All the models but COMPBRN are dynamic - i.e., time-dependent (or "transient"). COMPBRN is a quasi-equilibrium model; the driving forces are the fire size (i.e. the power output) and the rate of loss of energy to the walls.

17. Does it determine radiative heat transfers? How well?

The Harvard programs all determine most of the heat transfers. The calculations are essentially identical in all variants, and they are very good: most of those are as good as or better than is warranted by the rest of the modeling accuracy. The absorption coefficient of a layer is calculated as a function of time, as conditions change; i.e. as the concentrations of smoke, CO_2, and H_2O change with time. There are two algorithms to calculate the absorption coefficient: a simple one which considers smoke only, and a more complex one which takes the absorption/emission from the CO_2 and H_2O molecular bands into account explicitly. For Mark 5, 5.3, and 6, only the hot layer is considered. In Mark 5.2, mixing is taken into account, and therefore absorption and emission from the lower layer comes into play as well. Some validation of the radiation calculations has been done: see ref [1], fig. 42. COMPBRN also includes radiation heat transfers, but generally in a cruder way - e.g. attenuation in the hot layer is not taken into account; the emission from the layer is assumed to occur only from an equivalent thin layer at the ceiling; the absorption coefficient of the gas is taken to be a prescribed constant. FAST also considers radiative heat transfers, with the approximation that each volumetric (i.e., gaseous) source is a point source, and attenuation is either via a modified mean beam length approximation using a sphere, or assuming an infinite slab. The absorption coefficient is assumed to be 0.1 m^{-1} for the upper layer, and the lower layer is assumed to be transparent.

18. Does it determine convective heat transfers? How well?

The expressions for convective heat transfers in the Harvard programs are very simple, but seem to work reasonably well. Better algorithms have been written for them, but have not yet been incorporated. COMPBRN uses a better algorithm for the convective heat transfer from the plume to the ceiling than the Harvard codes do: Alpert's correlation for the ceiling jet [22] with Zukoski's expression(s) for the heat transfer coefficient (h) [23]. For the layer, however, the user must prescribe (a fixed value for) h - whereas Harvard computes a mean convective heat transfer from the upper layer to the ceiling, and uses a heat transfer coefficient which is a programmed function of upper layer temperature.

FAST uses different expressions than either Harvard or COMPBRN: it uses the Turner approximations [25] for convective heat transfer from vertical and horizontal (up-facing and down-facing) surfaces.

19. Does it give the spread rate of a fire on an object?

COMPBRN computes the ignition of objects adjacent to the fire (and hence, "fuel cells" adjacent to a burning section of an object partially involved in the fire) in the same manner as it treats ignition of distant objects, except that conduction gains are accounted for. Fire spread occurs (in COMPBRN) in jumps, rather than in a continuous manner. In the Harvard programs, the spread rate is not prescribed at run time. Rather, an experimental value is obtained for the spread rate in the open, which gives a "spread rate parameter". Then the effect of feedback in the enclosure is factored in. Validity: it is reasonably good for non-charring or melting fuels.

20. Does it determine the heating of objects? How well?

COMPBRN II corrected a deficiency in COMPBRN I, and now does this (as far as this author can tell) in about the same way as is done in the Harvard codes (via one-dimensional heat transfer) - and therefore, quite well. As for its validity, see item #6. For FAST, the answer is the same as in item 9: if objects were considered, this could be done.

21. Does it determine the heating of the ceiling?

All the Harvard programs determine the heating of the ceiling in the same way as the heating of objects is determined. COMPBRN will determine it only if it is explicitly entered as a separate object ("module"); however, that should not be difficult to do. FAST also does it, essentially as the Harvard programs do.

22. Does it determine the heating of the walls?

All three models do. Mark 5, 5.2, 5.3, and 6 all consider the part of the walls which are in contact with the hot layer, to be extensions of the ceiling, so there is no separate calculation. As in COMPBRN, however, the walls could be considered as separate objects, and have the temperature(s) determined separately. The lower parts of the walls are considered as extensions of the floor.

Just as for the upper part of the walls (the "extended ceiling"), COMPBRN will find the wall temperatures only if the wall is entered as a separate object(s). FAST treats the upper part of the walls precisely as Harvard does, i.e., as extensions of the ceiling. The lower part of the walls are treated separately, however, rather than as extensions of the floor. Under some circumstances (e.g., thin walls and a carpet on the floor) this may be a very useful feature. Moreover, multilayer walls can be modeled.

23. Does it determine the heating of the floor?

Mark 5.2 has a floor-heating algorithm, but it is (as of this writing) still being debugged. The other variants of the Harvard code do not have it at all; just as for COMPBRN, however, they could calculate the floor temperature if it is included as a separate object. FAST has a floor-heating algorithm which does work.

25. Does it handle burnout? How well?

COMPBRN is "hard-wired" to snuff out the flame over any fuel element which has burned out by 70%. This may help to mimic the burning of wood and other charring materials, but it is not correct for liquids nor for most solids. This does, however, allow the reduction of fuel surface area over time (in discrete steps). As for the 70% figure, this can now be changed by simply increasing or decreasing the amount of available fuel. The Harvard models handle burnout reasonably well: when a massive object burns down to 200 gm, the (model) flame height is designed to decrease in a way which mimics the reduction of surface area (and therefore flame volume) which is observed. This reduces radiation to other objects, ceiling, etc. (An alternative procedure is used for objects whose initial mass is < 200 gm.) There is also a burnout parameter, t_b, which specifies how the burning rate decreases near the end. In Mark 5.2 and 5.3, t_b can be user-specified, which extends the flexibility available for describing the burning rate. FAST will "handle" burnout, only if it is specified by the user at run time (in the fuel vapor input rate).

28. Does it handle ceiling venting?

COMPBRN can treat forced ventilation injection into and extraction out of the hot gas layer (see comment #3). It cannot handle buoyancy-driven flow out of a ceiling vent. None of the Harvard variants has a ceiling-venting algorithm built in; however, in the cases where the ceiling vent is not the sole vent for the compartment, one should be able to do adequately by substituting for it a thin horizontal slit of the same total area, in a wall(s), at ceiling height. Since such venting is given very well (see [26], fig. 5), this should work well. FAST can handle ceiling venting in the same way as Harvard does.

None of the programs can handle buoyancy-driven ceiling venting if it is the sole vent: that is an unsolved theoretical problem.

29. Does it give ceiling ignition?

All of the Harvard variants, as well as COMPBRN, will let the ceiling ignite only if it is considered as a separate object, with an ignition temperature. FAST does not ignite targets. See items 6 and 20.

31. Does it predict ignition in a room other than the room of origin?

This is evidently only applicable to multiroom models, and only to Mark 6. However, radiation from one room to another has not been incorporated there. On the contrary, COMPBRN can handle ignition of external objects by radiation from sources within a room, whereas the hot gas model employed is only for one room. FAST never considers ignition.

32. Can it handle charring fuels?

Neither Harvard nor COMPBRN can handle charring fuels. Mark 5.3, however, can mimic it (albeit crudely), by choosing a very large value for the burnout parameter, t_b. FAST can handle it in the sense of specifying the amount of carbon (C) left over (which is assumed to be char - the carbon in smoke is specified separately).

34. Can a vent be opened or closed during the fire?

FAST takes this into account. The opening (or closing) must be preprogrammed, however, just as the fire strength is.

35. Can it handle rooms on more than one floor?

FAST does handle the multi-story situation. The algorithms used in FAST are reasonably satisfactory, in that a 4-story calculation has been made and the results compared with experiments in Japan [19]. The predicted values of mass and enthalpy flows into the upper floors agreed with experiment within 20%. A difficult problem is in the treatment of plumes (especially time-varying ones) emerging from rectangular vents and going up a shaft, especially a "rough" inclined one, such as a stairway. Harvard Mark 6 was not designed to handle multi-story configurations. Because a second room can have a higher ceiling than the burn room, however, it is possible to (crudely) simulate some two-story configurations.

38. In general, how much of the important physics involved is included?

Naturally, each model contains what its creator considered to be the most important phenomena. However, there still are many significant phenomena which have not yet been included, in each of them. For example, ignition of the upper layer, and a liquid pool fire, are not included in any of the models, and wall fires are not addressed in FAST or in the Harvard models. There is no point in listing all of the items which are missing, here (indeed, this very report gives some insight into what is missing); suffice it to say that almost every time a new problem is addressed, some lacuna in the model(s) becomes immediately apparent.

39. How well does it treat the physics it does consider?

This varies from "very crudely" to "excellently", depending on the model and the phenomenon. The adequacy of treatment for each phenomenon is addressed in detail in the discussions above.

IV. Validation

*la and b. How thoroughly has the overall model been tested ("validated") against real fires? How well did it perform?

The Harvard family of models has been tested against a substantial number of real, full-scale fires: Factory Mutual Research Corp. ran a series of tests in 1977, which were simulated by Mark 5 (see references [1], [7-9]). A number of full-scale fires were run at NBS, and comparisons made with Mark 5, 5.2 and 6 (references [10-12]). A series of forced-ventilation tests was made at Lawrence Livermore National Laboratory, and Mark 5.3 attempted to simulate these [13]. The predictions for a variable range from "poor" (the peak CO concentration is underpredicted by a factor of 5, sometimes), to "excellent" (the pyrolysis rate for a PU foam slab; the air inflow rate (through the free vent) in the forced ventilation runs). The hot layer temperature is generally very well predicted, but the peak temperature is usually underpredicted (by 50-100°C for large fires). On the average, the calculated variables deviate from experimental measurement by some 10-15%. COMPBRN II: A number of full-scale tests was run at Underwriters' Labs. for the NRC in 1982-3 (ref. [14]), and simulated by COMPBRN [15]. Just three variables were examined by them - the hot layer temperature, (total) heat fluxes to cables (the target items), and cable surface temperatures. The results are shown in figs. 8-26 of ref. [15].

The gas layer temperature is taken to be constant throughout the run, and therefore greatly overpredicts the temperature, initially. On the other hand, the asymptotic (peak) temperatures are underpredicted by varying amounts, from 0°C to 130°C. The average is perhaps 50°C. The resulting cable temperatures are generally overpredicted, by quite significant amounts = sometimes by as much as 150°C. In one case (experiment 2) a reasonable choice for χ_A (the burning efficiency, which they choose *a priori*, rather than from experiment) gives the surface temperature very well (though the layer temperature there is underpredicted by 130°C). When C_e = 0.7 and χ_A = 0.85 the average error for the three variables is about 25%.

COMPBRN has also been tested against some crib fires, with comparable (or slightly better) results. Siu (private communication) also makes the important point that uncertainties (or errors) in input parameters influence how well a model simulation predicts the actual behavior.

FAST has been validated by two sets of experiments [20,21]. The predicted and observed values of T_L, T_u, and H_L (upper layer temperature, lower layer temperature, and layer height) for each was compared, as a function of time. The agreements were quite good; on the average, these variables were predicted within 10%. The review of validation tests suggests that the "overall accuracy" is approximately:

HARVARD models → 10-15%
COMPBRN II → 25%
FAST → 10%

2. How well have the algorithms for each physical process been validated?

In COMPBRN, the algorithms for the subroutines have been taken from, or compounded out of, other people's models - the validation was assumed to have already been carried out by those others. The linear dependence of burning rate on external heat flux has been reported for a number of plastic fuels, as discussed in [5] (see Appendix E in that reference). More recent work by A. Tewarson at Factory Mutual (for cable insulation) seems to show this also, at least over the ranges of heat flux examined. The (sort of) linear dependence of burning rate on height for vertical fires is not factored in *a priori* into COMPBRN, but is a function of feedback heat flux.

Essentially the same comments apply to some of the Harvard program algorithms. For the growing fire algorithm, validation was against Orloff's work on polyurethane foam slabs, at FMRC. For every algorithm, basic physics was used wherever possible, rather than empirical correlations. The vent flow algorithms were validated by Steckler's ([17],[31]), extensive work at NBS. The plume algorithm was of course initially validated by the work of Morton *et al* [16] (though it is often being used in a regime for which it was *not* validated).

In FAST, the plume algorithm has been "validated" very well, in the sense that the algorithm is an explicit representation of experimental work [24]. Some others are equally good. Still others are cruder, such as the radiation algorithms; these have not been independently checked, e.g. with a radiometer. Also see section III, items 17 and 18.

V. Structure

1. How modular is the program?

Since there is no way to quantify this attribute, the answers are subjective. The relative ranking between Mark 6 and Mark 5.n, however, is unambiguous. In this context, the symbols mean:

E = very modular = it would be hard to make it more modular.

G = fairly modular = all of the physics subroutines are modular, and can be replaced. "Fairly modular" is the adjective used by Siu for COMPBRN [personal communication].

The author is not familiar with the FAST program, but its creator (W. Jones) feels [personal communication] that it merits an E ranking. The Harvard models 5.n all deserve at least a G rating, and Mark 6 (perhaps) an E.

2. How easily can it be modified?

Same comments apply here as for question V.1 (above). The meanings here are

E = extremely simple - practically anyone could do it in a day
G = pretty easy; a novice programmer could do it in a day or two
F = a mediocre programmer could do it in a few days
P = pretty hard to do; a good programmer would need a week.

Siu [private communication] says that some parts of COMPBRN are easy to modify, some are hard. His hot-layer model, for example, is "hard-wired" into the program and therefore can not be easily modified. Jones [personal communication] avers that FAST is easily modified, except that the input/output is tedious. The numerics should be straightforward. It is estimated that modifications in Harvard are F to G, new algorithms are G, insertion of a new variable, F.

4. How well has it been "idiot-proofed"?

The Harvard models have a substantial number of input-error-checking features; moreover, if a (non-syntactical) error slips through, there are a number of opportunities for correction.

COMPBRN II now has some input-error-checking routines (however, it is not clear to the author whether these are only in the latest version that Siu has, or in other versions currently in the hands of users, as well).

FAST has some internal checks (e.g., how many entries have been made) but not others: it permits the user to specify a vent width which is greater than the width of the wall in which it appears, or a vent height greater than the room height, for example.

VI. Other Factors

*1. What is the "computer power" required? i.e., how large a machine is required?

The Harvard Mark 5 series was developed on a PDP 10 and a VAX 11/780; it has also been run on a Perkin-Elmer 3242 and a HP9000 "super micro". The basic program is about 120 kilobytes, and so any minicomputer should be able to handle them. Indeed, many of the larger microcomputers should be able to handle them. Mark 6 is larger, but not very much so. COMPBRN is substantially smaller than Mark 5 (2000-3000 lines of code, vs 7200 lines for Mark 5), and hence it should be easy to run on any minicomputer (it has only been run on a large machine, because that is how it was developed). FAST is comparable in size to Mark 5: 110 kilobytes. Hence it can be run on any minicomputer, and on quite a few micros.

*2. What are typical run times?

The time required by FAST increases as n log n, where n is the number of rooms. On the PE 3242, a 500-sec run of a six-room case took about 530 CPU sec, and a two-room, 300-sec run took 35 CPU sec (and a one-room case should take approximately 15 CPU sec). On a Cyber 205, a six-room case took 8 CPU sec. For Mark 5: A 500-sec run with the standard case (one room, two objects, one vent) takes 84 CPU-sec on a VAX 780. The same problem with a non-optimized compilation of Mark 5.3 takes about 120 sec on the P-E 3242 for the single precision version, and between 80 and 240 CPU-sec on the HP 9000, depending on how "CPU time" is interpreted.* The 500-sec run with Mark 5.3 took 344 time steps, so that the average step size was 1.45 sec, and took 0.35 sec of CPU time per step. The same problem run with Mark 5.2 takes a little longer because it is in double precision. The same problem run with Mark 6 takes 12.8 CPU min on the P-E machine. A five-room, one-object simulation with Mark 6 takes 17.2 CPU min. One might expect that these times would be cut by an order of magnitude on a large mainframe computer. A two-room problem was recently run with Mark 6, taking about 18 CPU min (for a 500 sec simulation). The same problem run with FAST took about 12.5 min (with very similar results).

COMPBRN is smaller and simpler. A run takes only a few seconds on a mainframe; on a PRIME minicomputer, a typical job takes about 10 CPU sec. (The time steps are one minute apart, and runs are 9 to 30 minutes long).

*Private communication, P. diNenno (Oct. 1984).

*3. What are the parameter limits within which it is valid?

This is not a trivial question, since there are a great many parameters in each model, and the limits of validity for one may depend on the particular values of some or all the others. For example, the limiting fire size in a box will be made smaller than that in a warehouse. More specifically: the Harvard models assume that propagation of the plume is instantaneous; since the actual propagation velocity is finite, this can lead to a significant error in the time to smoke detector activation, in a very large room. Also, it is assumed that flow velocities are well subsonic - this restricts how small a vent we can have. Thus, a vent one mm on a side will be too small, for the "standard case" run. One cm on a side, however, is fine. Similarly, compression of the gases is not permitted, so that deflagrations will not be properly modeled. The plume model in Mark 5 and Mark 6 is only valid in the far zone of a flame, and therefore cannot be expected to be very good when the flame is very large (i.e. extends to the ceiling). Mark 5.2 offers a choice of several plume models, of which at least one is better in the flame zone. A configuration which may lead to difficulties is a single fire on a high base, in a room with a (natural) vent close to the floor. This is so, because the fire is assumed to be snuffed out, if the layer interface sinks below the fire base - even if the oxygen concentration in the hot layer is well above the flammability limit. (An algorithm for burning in the upper layer is currently being developed for Mark 5.3).

These are the major limitations on the values various physical parameters can take on. Of course there may be limitations the parameter values can take on, because of numerical instabilities = see item 4.

For FAST, the comments are generally similar to those made for the Harvard codes. Thus, the plume will probably not be correct in a very high building (if there is stratification within the room - as is likely). For COMPBRN, this question was not investigated at all. Just as for the Harvard models, however, at least one vent is always required (since ambient pressure is assumed).

*4. What is the quality and availability of required input data?

There are two kinds of data needed to run any model: first, geometric data about the enclosure, fuel and target location, vents, etc. This is of course to be supplied by the user and is automatically "available". Second, there is thermophysical data about the fuel, the walls, the targets, etc. Some of these (e.g. ρ, c, k, heat of combustion) are readily available from handbooks, and are reasonably reliable. However, they are usually only given for a single temperature, (ambient), and since ρ, c, and k are generally functions of temperature, the quality of these input data is not generally very good. The Harvard models and COMPBRN also require the heat of combustion, heat of vaporization, and burning efficiency. Most of that is also available in the literature, but does require some hunting. FAST and the Harvard models require some more esoteric items: the rate of production of combustion products - e.g. the mass of CO_2 produced per gram of fuel burned (in the open!).

Such data is given almost exclusively by Dr. A. Tewarson, at FMRC, and is of very variable quality (the measurement errors range from a few percent, to factors of 5 or more). For growing fires, the Harvard programs require an input, the spread-rate parameter A, which does not appear in the literature at all; it must be inferred from other data or estimated. In Mark 6 a table of parameters (for 22 materials, so far) has been built in, making the use of the program far easier: the user merely chooses which material to use, at run time (this makes no claims for the quality of these data, however).

FAST requires less overall data than the Harvard codes, but, in one respect, it is even more demanding: the mass fractions of various species which are emitted during combustion must be given as functions of time. Also, it permits a more general description of the room geometry - see item III.12.

COMPBRN does not require species generation data since it does not give species concentrations. It uses empirical correlations or empirical data for pyrolysis rate ($\dot{m}''_o$) or for spread rate.

5. Is it user-friendly? How easy is it to use?

For FAST, the input is simple. However, it is not interactive, and therefore extra care must be taken in typing in the data. The only other way to catch input errors is to verify the input data when they are printed as the first part of the output, and then start over again.

Probably the principal difficulty of the Harvard models is the lack of a comprehensive user manual. The Harvard models are very easy to use, in one way, difficult in another: Easy, because they are interactive, and the input required is obtained by answering unambiguous questions at the console. Once the input has been entered, the program runs. Moreover, it is fairly forgiving of errors in input syntax or format. On the other hand, all the single-room versions require up to 18 items of thermophysical data input for each material, some of which is difficult to obtain.

Mark 6 has had a "materials handbook" built in, so that the job of "inputting" the required thermophysical data is enormously simplified. Of course, if a material other than one of those in the material handbook is involved, the same problem will arise. (The same is now being done for Mark 5.3.)

As for COMPBRN, the author has had no experience with it, but its creator (Dr. N. Siu) says [private communication] that it is not particularly "user-friendly". Very little input is required, however, so once the user is familiar with the model, it is relatively easy to use. As noted in the table, some improvements have been made. The NAMELIST input formatting is very forgiving, but, as with the Harvard codes, a certain amount of thermophysical data for the various fuel elements is needed.

6. What are the parameter limits within which it will converge?

FAST has rarely had any difficulty converging. COMPBRN converges consistently in free burn scenarios. It has problems in some scenarios involving compartment fires, due to convergence problems in the hot gas layer submodel. Convergence is a function of the fire size, fire location, the door size, the room dimensions, and the forced ventilation rate. COMPBRN has difficulty converging when the fire source is "close" to the ceiling. Also when the fire is "large" compared to the room, or when the door is small (and there is no forced ventilation).

A study of Harvard 5, carried out some years back, indicated that the program begins to fail to converge when room dimensions approach 500 m on a side. It also fails for small boxes. For a burner of diameter D > 2 meters it also runs into difficulties. Mark 5.2 and 5.3 are in double precision and have no difficulty with these extremes; the programs have been tested assuming burners of diameter up to 20 m; with a burner of diameter 1 m and flow rates yielding up to 30 Mw; and for other extreme situations. They have converged for all these cases with no difficulty (though the accuracy/reliability of the results is questionable - see item 3). Mark 6, which is also double precision, has little difficulty in converging, but has not been tested so extensively.

7. What are the principal advantages of the model?

The Harvard models are quite comprehensive in their inclusion of many physical processes; they are time-dependent, and flexible. They are also reasonably reliable, both in their physics and numerics. The treatment of radiation transfer is significantly more sophisticated than that in the other models. They are modular, and allow for expansion and modification. The single-room versions (Mark 5 and 5.n) use a numerical scheme which is fast, so that individual runs are not too expensive. Mark 6 is slower, but guarantees accuracy and is numerically more robust.

COMPBRN is relatively simple, and since it uses a specified fire, requires much less input than the Harvard codes do. It is quick, and cheap to run. Its use of multiple fuel cells allows greater flexibility in specification of a fuel configuration than the Harvard codes do.

FAST has excellent graphics, is quite rapid, and is numerically robust and reliable. It is modular, and hence easy to modify.

8. What are the principal drawbacks of the model?

COMPBRN does not work for all situations; for example, a small vent gives trouble. Worse, it may not give trouble, but give nonsensical answers. This is a danger, since it may not always be apparent that results are incorrect!* Second, it is not (at present) very "user-friendly". Finally, the results are not very accurate, in general. The Harvard models do not have a simple user manual to guide the novice user; they are, in that sense, "user-unfriendly". Also, the data that is required to run them is not always readily available. Finally, they do not (at present) have a wall-fire algorithm built in (although the horizontal growing-fire algorithm can be - very crudely - used to mimic that, with an appropriately increased value for the growth-rate parameter).

For FAST, setting up the input is tedious, and the only fire it handles is a specified fire. It also does not heat up (or ignite) targets.

10. Can it be run in batch mode?

COMPRBN was designed that way, and FAST is designed to be run only in batch; see item 5. Contrary to these, the Harvard programs were designed to be run interactively. They can be run in batch mode, but that requires knowledge of the sequence of questions which would appear on the console screen. Since the user manual section does not describe all these, running in batch is not easy.

11. Does it have graphics capability?

FAST has superb graphics capacity. However, it is machine-dependent, at the moment. The Harvard models have a rudimentary graphics subroutine built in; moreover, the output file can be used to generate graphs of the results. COMPBRN has none.

6. DEVELOPMENTS NEEDED

Each of these models needs improvements of various kinds, some of which are easy to infer from glancing at the table of section 4. Consider first the Harvard models, Mark 5.2 and 5.3, since they are already enriched in desirable directions.

a. The enrichments in 5.2 and 5.3 should be merged.

b. Floor heating should be properly implemented in 5.2 and 5.3

c. Ignition and burning entirely within the vitiated layer must be allowed.

d. A good wall-fire algorithm should be incorporated.

e. The burning of a fuel which is long and narrow must be considered and incorporated.

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*These situations are now being "flagged out" by COMPBRN II, according to Siu, but it is not clear to the author how this can be done internally, if it is not apparent to the user, who is much more sophisticated than the program!

f. Ignition of the hot layer should be included.

g. Inclusion of a "materials handbook" which is built into the program, similar to what is now in Mark 6. This should include the thermophysical constants for at least two of the cable types most commonly used in nuclear plants.

h. A better treatment of multi-layered target objects, such as laminates or cables with several layers, should be included.

i. The effect of the ceiling jet on detectors, sprinklers, or cable trays should be explicitly incorporated.

j. A good user manual should be written for each of the "codes".

k. Ceiling burning should be included.

l. Modeling of fuel sources with a complex geometry should (eventually!) be done; preferably in a way which is better than that used in COMPBRN.

m. A liquid-pool fire algorithm should be explicitly written.

n. Ceiling venting should be included.

o. A "communications matrix" similar to that in COMPBRN would be a very useful adjunct, for radiation interchange in complex geometries.

p. Convective heat transfer algorithms should be improved.

q. The forced-ventilation algorithm should be improved by incorporating the fan characteristics and permitting the system to determine the flow rate (see discussion under item III.3.).

All of the above enrichments should also be incorporated into Mark 6, of course.

Next, consider COMPBRN.

a. The program should be made time-dependent.

b. A means of prescribing or guaranteeing a prescribed degree of accuracy should be installed.

c. The forced ventilation algorithm should be improved, so that (for example) the user does not have to specify the mixing into the upper and lower layers (which is essentially arbitrary).

d. Solid and liquid <u>pool</u> fires should be included.

e. The treatment of radiative heat transfer in (or through) the upper layer should be improved.

f. Mixing of layers at vents should be incorporated.

g. It should enable the user to prescribe an arbitrary fire.

h. The heating of walls, ceiling and floor should be automatically incorporated, since they affect (among other things) the actual layer temperature!

i. Burnout should be better treated.

j. The temperature of the lower layer should be calculated.

k. Burning in vitiated air should be considered.

l. Ceiling venting should be included.

m. Ignition of the hot layer should be included.

n. A proper calculation of the absorption in the layer should be made.

o. Items g, h, i, k, m of those listed above for the Harvard program, which have not yet been mentioned here, should also be included.

Although Jones [private communication] does not envision incorporating burning into FAST in the near future (it is meant to be a transport model only), it could easily do so. Thus for FAST, the NRC might want to see:

a. Burning of various kinds of fires should be incorporated (see items 5 a-i in Table I).

b. Forced venting should be included. (Work is in progress).

c. The heating of target objects should also be included.

d. The ignition of target objects should be included.

e. Fire detection might also be included.

f. Items c, d, f-i, k-m from the list of desirables for the Harvard models.

g. Items d, i, and n from the list of desirables for COMPBRN.

Finally, it must be remembered that as long as development continues, continued validation, both of new submodels as well as of the entire program, is very important. There are of course numerous other enrichments possible, but the above lists are already quite substantial; it will be some time before it is necessary to consider other points.

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☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)*

A substantial number of mathematical models for compartment fires have been developed in the past decade. This report analyzes and compares in depth three such models. This is done with particular emphasis on the needs of the Nuclear Regulatory Commission and Sandia National Lab, for their Risk Methods Integration and Evaluation Program. The models examined are (1) The Harvard family of models, Mark 5, 5.2, 5.3, and 6; (2) COMPBRN; and (3) FAST. The capabilities of a model can be understood in terms of the answers to a series of questions; these are formulated, placed into categories, and then answered. The answers are given in brief form in a table (section 4); the bulk of the report consists of elaborations and discussions of these points.

A number of conclusions emerge from this study: first, there is at present no one model which will do everything which is wanted by an arbitrary user - some have certain capabilities; others, different capabilities. Therefore each user must look for a model which does what he (she) wants, and does it well. Second, from the point of view of the NRC, Harvard Mark 5.3 may be the best choice, because it is the only one which has <u>all</u> of the following characteristics: it is time-dependent; it considers forced ventilation; it has good numerics; and it takes into account heating and ignition of target objects. The last section of this report briefly outlines which developments would be desirable, for each model.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

comparison; compartment fires; fire models; mathematical models

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