NBSIR 84-2934

A Model for the Transport of Fire, Smoke and Toxic Gases (FAST)

Walter W. Jones

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Engineering Laboratory
Center for Fire Research
Gaithersburg, MD 20899

September 1984

NBSIR 84-2934

A MODEL FOR THE TRANSPORT OF FIRE, SMOKE AND TOXIC GASES (FAST)

Walter W. Jones

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Engineering Laboratory
Center for Fire Research
Gaithersburg, MD 20899

September 1984

TABLE OF CONTENTS

A MODEL FOR THE TRANSPORT OF FIRE, SMOKE AND TOXIC GASES (FAST)

1. INTRODUCTION

In recent years there has been considerable research in the area of the spread of fire and smoke from a room of fire origin to connected compartments. The work is motivated by a need to understand and be able to predict the environmental conditions which occur as a fire develops and spreads. Much of the attention has focused on the development of numerical models which are able to make a reasonably accurate assessment of the environment from ignition. The motivation is two-fold. Being able to correlate laboratory scale experiments with full-scale tests is desirable from a cost standpoint. More important, however, from a life-safety and operational standpoint, the ability to make accurate predictions of the spread of fire, smoke and toxic gases opens up many possibilities for combating these problems, as well as taking effective preventive measures. The ability to prevent the hazards from developing becomes especially important as new and exotic materials become available.

This paper describes a model which allows one to predict the evolution of a fire in a room and the subsequent transport of the smoke and toxic gases which evolve from this fire. The numerical implementation improves on previous work, for a review see Jones (1983), in particular by retaining the conservation laws in their full differential form and solving them as a set of coupled ordinary differential equations (ODE's). Such a formulation takes advantage of the effort which has gone into solving such systems of equations. The result is a numerical scheme which is considerably faster and much more "rugged" than previous models.

The model is assumed to be in a world of uniform temperature T_a and reference pressure P_a, with the outside of a wall at T_e which may not be the same as the ambient. The discussion is broken down into the basic structure and fundamental assumptions which go into the model, followed by a derivation of the predictive equations, a discussion of the source terms, the numerical implementation and some calculations and comparisons with experimental data. The notation is given in Appendix A. The numerical implementation of the model is modular and straightforward. It is designed to be transportable.

2. STRUCTURE OF THE MODEL

The primary element of the model is a compartment. The primary interest lies in the composition of the gas layers in each of these compartments. As such, the model is structured around fluid transport phenomena. In this context, the predictive equations for the gas layers in each compartment result from conservation of mass, momentum and energy together with an equation-of-state for each compartment. The actual physical phenomena which drive the transport are then couched as source terms. Such a formulation allows the greatest flexibility in adding, modifying or deleting terms which are appropriate to the problem being solved.

Each compartment is subdivided into one or more "control volumes." These control volumes will be of sufficient size that we will require only a few to describe any system of interest. The choice is based on the premise that the details which occur within such a volume do not concern us (at present), but their mutual interaction does. Each of these control volumes is called a zone. The rationale for such a choice arises from the experimental observa-

tion that when a fire spreads, the gas layers in the compartments actually stratify into two distinct zones. This is a compromise between a network model and a finite difference model. The former is computationally fast but yields no information on the internal structure whereas the latter yields a great deal of information but requires more computational resources than is warranted. The two zones are referred to as "upper" and "lower", respectively. The basic equations describe the mass, momentum and energy transfer from zone to zone in a fire driven environment. A schematic is shown in figure 1.

In considering dynamic systems, it is necessary to solve a problem self-consistently. If such is not done, then some of the dynamics may be obscured or even lost. In particular, discussion of movement of the zone interfaces must be consistent.

The conservation equations for mass and energy can be written in the form

$$\frac{dm}{dt} = \sum_i \dot{m}_i \tag{1}$$

for mass and from the first law of thermodynamics we have

$$\frac{d}{dt}(EV) + p\frac{dV}{dt} = \dot{Q} + \dot{h} \tag{2}$$

together with an equation of state

$$P = \rho RT \tag{3}$$

which closes the set of equations, and with the definitions

$$E = c_v \rho \left(T - T_R \right)$$

$$\dot{h} = c_p \sum_i \dot{m}_{i,in} \left(T - T_R \right) - c_p \sum_i \dot{m}_{i,out} \left(T - T_R \right) + \sum_i h_{i,o} \left(T_R \right)$$

$$\dot{Q} = \dot{Q}_f + \dot{Q}_R + \dot{Q}_c = \text{net energy input}$$

$$i = \text{index of other compartments } (i \neq \text{volume of interest}).$$

The term $h_{i,o}(T_R)$ is relative to the temperature from which this mass parcel, $\dot{m}dt$, came. It includes enthalpy of formation. The equation of state for an ideal gas is usually used for closure of the system. More correctly it should be written

$$P = P \left(\rho, T, \{i\} \right), \quad \{i\} \equiv \text{set of species} \qquad (4)$$

especially for applications to fire problems which are not ideal gas problems. However, for the case of an ideal gas, the derivations and discussion are simplified, and generalizations can be discussed later. The sign convention is that positive fluxes on the right hand side of an equation will increase the quantity being calculated on the left hand side, that is, transfer into a volume is indicated by a positive flux on the right hand side.

The general form of the model is to divide each compartment into two zones: an upper zone which contains a hot layer, and a lower layer which is relatively cool. There may exist one or more fires and plumes in each compartment and these can usually be considered to be part of the upper zone. Mass and energy transfer between the zones is provided by the plumes, mixing

at the vents, radiation between layers and flow along the walls. In general a plume, once created, simply transfers mass and energy from one zone to another. Another set of equations could be written for the plume, but as long as it is in quasi-steady equilibrium, considering it to be part of the upper zone is sufficient. Another way of the looking at the plume is to consider it so small in mass, energy content and volume that it can be ignored except as a transfer mechanism. For some problems, however, the plume must be considered a separate zone along with the concomitant conservation equations. An example would be when the rise time of the plume is of interest or when the actual size and composition of the plume is important.

Since the conservation equations are written in terms of the volumes of these entities, a relationship between the height and the volume is needed, such as

$$V_u = \int_{Z_\ell}^{H_R} ZA(Z)\,dz \tag{5}$$

to calculate the layer depths. This removes the usual restriction that the compartments be rectangular parallelepipeds, and allows calculations for circular crosssections (aircraft) and trapezoids (atria).

The radiation transport scheme used is fairly simple and derives from the work of Siegel and Howell [1981]. The view factors which are used in the calculation of solid angles are concomitant with surfaces which are planes or discs. The relationship is shown schematically in figure 2. The simplification used here and discussed in more detail by Jones (1983) is retained, but the actual areas are used, and the exact view factors are used wherever

possible, Kusada (1976). For example, in calculating the area of the upper wall, allowance is made for any vents which exist by subtracting their area from the total wall area. In addition, ceiling and upper wall, lower wall and floor are treated separately (as pairs). This is necessitated by the possible use of different materials for the respective surfaces which may have different radiative properties, as well as the different types of convective flow which occur over each of these surfaces. More correctly, we should consider three surfaces, ceiling, wall and floor. This is under development. A problem arises in treating vertical convection as the layer depth tends to zero.

Actual closure of the model is obtained by assuming that the size of the compartment is fixed so that

$$V = V_u + V_\ell \tag{6}$$

and that there is a single reference pressure

$$P_u = P_\ell \tag{7}$$

at the boundary (interface) of the zones.

The set of equations which is necessary to describe fully such a physical system can be reduced by considering the physical impact of some of the terms. In particular, the pressure should be a general function of position, $P(X,Y,Z)$, in the compartment, which would require us to include a differential equation for the conservation of momentum explicitly. A general form for the perturbed pressure might be

$$\bar{P}\,(x,y,t) = P(t) - \int_{0}^{Z} \rho(t)dz + \delta P\,(X,Y,Z,t) \qquad (8)$$

where P is a reference pressure and is usually the pressure at the base of the compartment. In the spirit of the "control volume" formulation

$$\delta P \rightarrow 0.$$

This implies that acoustic waves are filtered out and that internal momentum need not be calculated. The hydrostatic term is small in absolute value in comparison with the reference pressure, so it is not necessary to carry this calculation through the equation of state. Finally, the time dependent portion of the hydrostatic term deals with the movement of the interface, and thus can be ignored if we limit ourselves to problems where the momentum associated with the discontinuity (alternatively the velocity) is not significant. Dropping the momentum equation for internal waves increases the computational time step a great deal since we are not limited by the Courant time step criterion (time step α grid size/speed of sound). This prohibits us from considering problems such as deflagration waves and explosions. With these considerations in mind, we will assume

$$P_u = P_\ell = P. \qquad (9)$$

The pressure in eqn. (9) is the reference pressure at the floor. This simplification is carried through the conservation equations and greatly simplifies the resulting predictive equations. However, it is necessary to retain the hydrostatic term for the flow field calculations at vents. As we are considering only small changes in the absolute pressure, differences of these terms will be comparable to the hydrostatic pressure change, eqn. (8).

For example, for eqn. (22)

$$\delta P \sim 1 - 1000 \text{ pa}$$

whereas

$$\int \left(\rho_1 T_1 - \rho_2 T_2 \right) dz \sim 100 \text{ pa}$$

where the integration is over a vent opening. So the flow can be dominated by the hydrostatic term whereas the $\delta P/P < 1\%$.

3. DERIVATION OF THE CONSERVATION EQUATIONS

A zone model describes a physical situation in terms of integrals of extensive physical quantities. Thus we deal with total mass rather than mass density, total energy rather than energy density but temperature is used as before (an intensive quantity). The integrals are volume integrals whose boundary surfaces enclose the Euclidean space of interest. The space with which we are concerned usually is a compartment with zones including a hot upper gas, a cool (relatively) lower layer, objects, plumes and fires. The connections occur at the boundary of these zones. Examples of possible connections are the vents connecting compartments, the radiation from a fire to the compartment walls, etc. With this basis we can mold the conservation equations into a form which describes a fire in terms of the quantities which are appropriate to the control volume approach, intuitively understandable and lend themselves to measurement.

3.1 Fluid Transport

The conservation equations for each compartment of a two layer model are

$$\frac{dm_u}{dt} = \sum_i \dot{m}_{u,i} + \dot{m}_u \tag{10}$$

$$\frac{dm_\ell}{dt} = \sum_i \dot{m}_{\ell,i} + \dot{m}_\ell \tag{11}$$

$$\frac{d}{dt}\{c_v m_u (T_u - T_R)\} - V_u \frac{dP_u}{dt} = \dot{Q}_u + \dot{h}_u \tag{12}$$

$$\frac{d}{dt}\{c_v m_\ell (T_\ell - T_R)\} - V_\ell \frac{dP_\ell}{dt} = \dot{Q}_\ell + \dot{h}_\ell \tag{13}$$

In writing these equations, we will make two assumptions. First, that the fire will not feed mass directly into the lower layer. Second, we will write the upper layer equation as if there is only one fire. If more than one fire exists, then a sum over such sources is necessary and if none are present, then this term vanishes. The source term $\dot{Q}$ includes all energy transfers due to radiation and convection and $\dot{h}$ includes the enthalpy flow. We can rewrite the energy conservation equations as predictive equations for temperature, in which case they become

$$m_u c_p \frac{dT_u}{dt} - V_u \frac{dP_u}{dt} = \dot{Q}_u + \dot{h}_u - c_p T_u \frac{dm_u}{dt} + c_v T_R \frac{dm_u}{dt} \tag{14}$$
$$+ \dot{E}_u$$

and

$$m_\ell c_p \frac{dT_\ell}{dt} - V_\ell \frac{dP_\ell}{dt} = \dot{Q}_\ell + \dot{h}_\ell - c_p T_\ell \frac{dm_\ell}{dt} + c_v T_R \frac{dm_\ell}{dt} \,. \tag{15}$$
$$+ \dot{E}_\ell$$

The right hand side of eqn. (14, 15) can be rewritten in a simpler form. The reference temperature (T_R) is chosen arbitrarily. If the only phase change occurs in pyrolysis of the fuel, then we can set the reference pressure to zero and include the pyrolysis energy as a sink term in the energy release rate. As $T_R \to 0$ we obtain

$$\dot{E}_u = \dot{Q}_f(u) + \dot{Q}_R(u) + \dot{Q}_c(u) - Q_p \dot{m}_f + c_p \dot{m}_p \left(T_v - T_u\right)$$
$$+ c_p \sum_i \dot{m}_{i,u} \left(T_i - T_u\right) \tag{16}$$

and

$$\dot{E}_\ell = \dot{Q}_f(\ell) + \dot{Q}_R(\ell) + \dot{Q}_c(\ell) + c_p \sum_i \dot{m}_{i,\ell} \left(T_i - T_\ell\right). \tag{17}$$

The equations and assumptions necessary to close this set are

$$P = \rho RT \tag{18}$$

$$\rho_u RT_u = \rho_\ell RT_\ell \tag{19}$$

with

$$m = \rho V \tag{20}$$

and $V = V_u + V_\ell = \text{constant.} \tag{21}$

The energy source terms $\{\dot{E}_\ell, \dot{E}_u\}$ are shown schematically in eqns. (16, 17) but can be much more complex and depend upon the configuration. Combining eqns. (10-11) and (14-17), together with the closure relations, we obtain

$$\frac{dP}{dt} = \frac{\dot{s}}{(\beta-1)V} \tag{22}$$

$$\frac{dT_u}{dt} = \frac{1}{\beta} \left(\frac{T_u}{PV_u}\right)\left(\dot{E}_u + \frac{V_u}{(\beta-1)V} \dot{s}\right) \tag{23}$$

$$\frac{dT_\ell}{dt} = \frac{1}{\beta} \left(\frac{T_\ell}{PV_\ell}\right)\left(\dot{E}_\ell + \frac{V_\ell}{(\beta-1)V} \dot{s}\right) \tag{24}$$

$$\frac{dV_u}{dt} = \frac{1}{P\beta} \left(c_p \dot{m}_u T_u + \dot{E}_u - \frac{V_u}{V} \dot{s}\right) \tag{25}$$

where

$$\dot{s} = c_p \dot{m}_u T_u + c_p \dot{m}_\ell T_\ell + \dot{E}_u + \dot{E}_\ell \tag{26}$$

and $\beta = c_p/R = \gamma/(\gamma-1)$ \hfill (27)

It should be pointed out that the equations are written in this form for the sake of clarity and simplicity. In a numerical implementation there are better ways to express the source terms which minimize the problem of the small difference of large numbers.

4. SOURCE TERMS

Equations (22-25) are written so that physical phenomena which affect the environment are source terms and appear on the right-hand-side. Sources which appear directly are:

1. radiation between the gas layers and walls, fires and other objects,

2. convective heating,

3. flow in plumes,

4. flow in vent jets,

5. mixing at vents.

Phenomena which are included but do not show up explicitly are:

1. radiation between objects,

2. conduction through walls and objects.

4.1   Source Terms: Radiation

In order to calculate the radiation absorbed in a zone, a heat balance must be done which includes all objects which radiate to the zone. Clearly, in order for this calculation to be done in a time comensurate with the other sources, some approximations are necessary.

The terms which contribute heat to an absorbing layer are the same (in form) for all layers. Essentially we assume that all zones in these models are similar, so we can discuss them in terms of a general layer contribution.

Radiation can leave a layer by going to another layer, to the walls, exiting through a vent, heating up an object or changing the pyrolysis rate of the fuel source. Similarly a layer can be heated by absorption of radiation from these surfaces and objects as well as from the fire itself. The formalism which we will employ for the geometry is that used by Siegel and

Howell (1981) and is shown in figure 2. The radiative transfer can be done with a great deal of generality; however, as with most models we assume that zones and surfaces radiate and absorb like a grey-body with some constant emissivity ($\epsilon \leq 1$).

A further assumption consonant with the stratified zone assumption is that emission and absorption are constant throughout a gas layer. In application to a growing fire, a further assumption is made that the lower layer is mostly diathermous. Although not a necessary assumption, this reduces the computation time for this term by 50%. For smoke propagation some distance from the fire(s) such an assumption will not be valid, but the temperature will be so low that radiation will not be the dominant mechanism for heat loss. Flames, plumes, fires, objects and bounding surfaces have some average shape from which the view factors can be calculated. The walls of compartments are usually flat and rectangular. The gas layers are spheres with an equivalent radius of

$$L = 4V/A \tag{28}$$

and an effective emissivity of

$$\epsilon_g = 1 - \exp(-\alpha L). \tag{29}$$

The terms which contribute to heating of a layer are:

1. fires and plumes,

2. walls,

3. other layers,

4. vents (radiation from other compartments),

5. nonburning objects.

The radiation balance of items 2-5 can be dealt with using the following notation:

F_{jk} – geometrical view factor of surface (j) by surface (k)

σ – Stephen-Boltzman constant = 5.67×10^{-8} W/m^2K^4

α – absorption coefficient of the upper gas layer m^{-1}

L – mean beam length of the equivalent sphere (m), defined in eqn. (28)

$\epsilon_{u,\ell}$ – emissivity of the upper/lower walls

ϵ_g – emissivity of the upper gas layer

Using the formalism of Siegal and Howell (1981) we have

$$D = \{1 - (1-\epsilon_u)(1-\epsilon_g)F_{uu}\}\,\{1 - (1-\epsilon_\ell)F_{\ell\ell}\} \tag{30a}$$
$$- \{(1-\epsilon_u)(1-\epsilon_\ell)(1-\epsilon_g)^2\,F_{u\ell}F_{\ell u}\}$$

$$\Pi_u = [\{1 - (1-\epsilon_g)F_{uu}\}\,\{1 - (1-\epsilon_\ell)F_{\ell\ell}\}$$
$$- \{(1-\epsilon_\ell)(1-\epsilon_g)^2\,F_{u\ell}F_{\ell u}\}]\sigma T_{uw}^4 \tag{30b}$$
$$- (1-\epsilon_g)F_{u\ell}\epsilon_\ell\sigma T_{\ell w}^4 - [1 + (1-\epsilon_\ell)\{(1-\epsilon_g)F_{u\ell}F_{\ell u} - F_{\ell\ell}\}]\epsilon_g\sigma T_g^4$$

$$\Pi_\ell = [\{1 - (1-\epsilon_u)(1-\epsilon_g)F_{uu}\}(1-F_{\ell\ell}) - (1-\epsilon_u)(1-\epsilon_g)^2 \, F_{u\ell}F_{\ell u}]\sigma T_{\ell w}^4$$
$$- (1-\epsilon_g)F_{\ell u}\epsilon_u\sigma T_{uw}^4 \qquad\qquad (30c)$$
$$- [\{1 - (1-\epsilon_u)(1-\epsilon_g)F_{uu}F_{\ell u} + (1-\epsilon_u)(1-\epsilon_g)F_{\ell u}]\epsilon_g\sigma T_g^4$$

Finally,

$$\dot{Q}(\text{upper}) = A_u \epsilon_u \Pi_u/D$$

$$\dot{Q}(\text{lower}) = A_\ell \epsilon_\ell \Pi_\ell/D.$$

To this must be added the energy radiated by the fire. A heat transfer balance with the fire is not necessary simply because the amount of heat radiated by the fire is usually much greater than that absorbed by the fire. In order to investigate flashover, however, this calculation must be generalized to include the fire and lower layer absorption in the radiative heat balance equation rather than relying on the postulate that superposition of the terms is sufficient.

A simple example of the results can be given for the case

$$\epsilon_u = \epsilon_\ell = 1,$$

for which we have

$$\dot{Q}_g = -\sigma[\epsilon_g T_u^4 A + (1-\epsilon_g)T_{uw}^4(A_u+A_{uv}) - T_{uw}^4 A_u - \epsilon_g T_{\ell w}^4 A_d - T_a^4 A_{uv}] + F_f \dot{Q}_f \qquad (31)$$

where A_d = area of the upper/lower layer discontinuity

A_{uv} = area of vents which the gas layer "sees"

A_u = area of the upper wall (including ceiling)

F_f = fraction of the fire which radiates times its view factor for the gas layer.

$A = A_u + A_d$

4.2   Source Terms: Convective Heating

Convection is the mechanism by which the gas layers lose (or gain) energy to walls or other objects. Conduction is a process which is intimately associated with convection but as it does not show up directly as a term for heat gain or loss, it will be discussed here.

Convective heat flow is energy transfer across a thin boundary layer. The thickness of this layer is determined by the relative temperature between the gas zone and the wall or object surface, Schlichting (1955) and Turner (1973). We can write the heat flux term as

$$\dot{Q}_c = h_c \left(T_g - T_w\right) A_w \tag{32}$$

where the transfer coefficient can be written as

$$h_c = \frac{k}{\ell} C_v \left(Gr \cdot Pr\right)^{1/3}.$$

The terms are:

A_w = area of wall(s) in contact with the zone

Gr = Grashoff number = $g\ell^3 \left|T_g - T_w\right|/\nu^2 T_g$

Pr = Prandtl number ≈ 0.7

k = thermal conductivity of the gas = $2.7 \times 10^{-7} \left(\dfrac{T_g + T_w}{2}\right)^{4/5}$

ℓ = length scale $\simeq \sqrt{A_w}$

C_v = coefficient which depends on orientation, Turner (1973)

N_u = Nusselt number

ν = $7.18 \times 10^{-10} \left(\dfrac{T_g + T_w}{2}\right)^{7/4}$

For the cases of interest

Orientation	Coefficient	Condition
Vertical	0.130	$Gr \times Pr > 10^8$
Horizontal	0.210	$T_g > T_w$
Horizontal	0.012	$T_g < T_w$

The coefficients for horizontal surfaces apply to a slab over the zone. For the inverse of this situation the coefficients should be reversed.

4.3 Source Terms: Plumes

A fire generates a plume which transports mass and energy from the fire into the upper layer. In addition, the plume entrains mass from the lower layer and transports it into the upper layer. The former generally increases the upper zone internal energy whereas the latter will have a cooling effect. For a fire which is consuming mass at a rate $\dot{m}_f$, heat addition will be

$$\dot{Q} \cong \chi_e \dot{m}_f \cdot H_c.$$

Some fraction, χ_R, will exit the fire as radiation and the remainder will be left to drive the plume. We can emperically devide the heat transfer into actual combustion and simple gasification. The former, denoted by χ_c, is the relative fraction of pyrolysate which participates in the combustion. Also, once combustion occurs, a fraction of the energy leaves the fire as radiation ($\chi_R \dot{Q}$) and convective energy ($\{1-\chi_R\}\dot{Q}$). The former is a function of such external effects as radiation, e.g., other fires, and vitiation. The latter efficiencies relate to sootiness and Froude number. The mass flow in a plume comes from a correlation of experimental data given by McCaffrey (1983). This correlation divides the flame/plume into three regions:

flaming: $\qquad \dot{m}_p = 0.011 \ Q \ (z/Q^{2/5})^{0.566} \qquad z/Q^{2/5} < 0.08$

intermittent: $\qquad \dot{m}_p = 0.026 \ Q \ (z/Q^{2/5})^{0.909} \quad 0.08 \leq z/Q^{2/5} < 0.20$ $\qquad$ (33)

plume: $\qquad \dot{m}_p = 0.124 \ Q \ (z/Q^{2/5})^{1.895} \quad 0.20 \leq z/Q^{2/5}.$

Entrainment in the intermittent region agrees with the work of Cetegen et al. (1982) but yields greater entrainment in the other two regimes. This difference is particularly important for the initial fire as the upper layer is far removed from the fire. In this formulation, the total mass flow in the plume is given by the above correlation and the fuel pyrolysis is related to it by

$$\dot{m}_p + \dot{m}_v = f \ (mz, \ Q) \qquad\qquad (34)$$

given above.

4.4 Source Terms: Door Jets

Flow at vents is governed by the pressure difference across a vent. In the control volume approximation the general momentum equation for the zones is not solved. Instead, the momentum transfer at the zone boundaries is included by using Bernoulli's solution for forced flow. This solution is augmented for restricted openings by using "flow coefficients." The modification deals with the problem of constriction of velocity streamlines at an orifice.

There are two cases which apply to these models. The first, and most usually thought of in fire problems, is for air or smoke which is driven from a compartment by buoyancy. The second type of flow is due to a piston effect which is particularly important in the early stages of a fire. Rather than depending on density difference between two gases, the flow is forced, for example, by volumetric expansion when combustion occurs.

The results used for this model are those of Bodart and Jones (1984) and will not be duplicated here. The notation used is:

S = smoke

A = air

ij = flow from compartment (i) to (j)

P = floor pressure (reference)

The order of the letters indicate the type of atmosphere from which the fluid is coming and to which it is going. As many as three neutral planes can exist for such flows. Two mixing phenomena which occur at vents are similar to entrainment by plumes. For the case when hot gas leaves a compartment and is driven by buoyancy into the upper layer of a second compartment, a door jet exists which is analogous to a normal plume. Mixing of this type occurs for flow

.

$$SA_{ij} > 0$$

and is discussed in detail by Zukoski (1982) and Tanaka (1980). The other is much like an inverse plume and causes contamination of the lower layer as cold gas from a compartment flows through a hot layer in a second compartment and is driven by buoyancy (negative) into the lower layer. Quintiere et al. (1981) discuss this phenomena for the case of crib fires in a single room and deduce the relation

$$SA_i(u \rightarrow \ell)/AS_{ji} = 0.5 \left(\frac{T_{\ell j}}{T_{ui}}\right)\left(\frac{N - Z_i}{N}\right) . \tag{36}$$

This term is predicated on the Kelvin-Helmholz shear flow instability and requires shear flow between two separate fluids. The instability is enhanced if the fluids are of different density since the equilibration distance is proportional to $\nabla \rho$. A schematic of this type of flow is shown in figure 3. As can be seen, mixing into the lower layer of a room occurs under the same conditions for which the "door-jet" mixing to the upper layer occurs.

4.5 Source Terms: Fire

Currently we can deal with two types of fires. The first is a specified fire. Then the mass pyrolysis rate is specified and the heat release rate becomes

$$\dot{Q}_f = h_c \dot{m}_f - c_p \left(T_u - T_f \right) \dot{m}_f - Q_p \dot{m}_f \tag{37}$$

whereas the mass loss rate, $\dot{m}_v$, is related to the pyrolysis rate by

$$\dot{m}_v - \dot{m}_f = \left(1 - \chi_f \right) \dot{m}_v .$$

As the burning efficiency becomes 100%, all of the volatiles are burned, and nothing remains for sooting. The heat release goes into radiation and enthalpy flux

$$\dot{Q}_R(\text{fire}) = \chi_R \dot{Q}_f$$

$$\dot{Q}_c(\text{fire}) = \left(1 - \chi_R \right) \dot{Q}_f .$$

The term $\dot{Q}_c(\text{fire})$ then becomes the driving term in the plume flow equation (see eqns. (33, 34)).

This approach is extended for a pool fire. A pool fire is basically the same except that it is driven self-consistently by reradiation from the compartment and the flame itself. From Rockett (1983) we have

$$\dot{Q}_f = \dot{Q}_R(\text{ext}) + \dot{Q}_{\text{flame}} - \dot{Q}_{RR} + \dot{Q}_{\text{conv}} - \dot{Q}_{\text{cond}}. \tag{38}$$

where $\dot{Q}_R$ = external radiation to the fuel source

$\dot{Q}_{\text{flam}}$ = radiation from the flame back to the fuel

$\dot{Q}_{RR}$ = fuel surface reradiation

$\dot{Q}_{\text{conv}}$ = enthalpy flux away from the fire

$\dot{Q}_{\text{cond}}$ = conductive heat loss from the fuel to the surroundings

4.6   Source Terms: Conduction

Conduction of heat through solids is not a source term in the sense
mentioned earlier. That is, loss or gain of energy from solids occurs by
convective heating, which in turn is influenced by subsequent gain or loss
through the solids. However, as much of the net heat loss from a compartment
occurs through loss to the walls, as well as heating of interior objects, the
form of heat propagation in solids will be discussed here.

The equation which governs the heat transfer in solids is

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c} \nabla^2 T \tag{39}$$

and is a linear parabolic equation. As such, it must be solved by a different
technique than is used for the ordinary differential equations which describe
mass and enthalpy flux. In order to couple these systems in a reasonable way,
we appeal to the principle of time splitting. Simply stated, we have two
systems of equations which are decoupled as long as the time step used is
short compared to the characteristic time scale for either set of equations.

Wall temperatures change and the characteristic time for energy flux through a solid is characteristically on the order of minutes. By using a time step of no more than one second the applicability of time splitting is assured.

Currently the model assumes two walls, the upper wall (and ceiling) which is in contact with the upper layer, and the lower wall (and floor) which is in contact with the lower layer. A refinement will be to separate the ceiling and upper wall, and the lower wall and floor. This will be useful since walls are generally constructed of materials whose thermal properties are different than the ceiling and floor. A further assumption is that conduction is one dimensional only. That is, the heat equation is

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c} \frac{\partial^2 T}{\partial x^2} \tag{40}$$

and the solid behaves as an infinite slab in the other two space dimensions. A corollary to this is that the wall in contact with the gas layer changes temperature instantaneously as the layer interface moves up and down. Such a formulation is not entirely satisfactory as there is a finite equilibriation time for the solid. An additional refinement will be to extend this equation to two dimensions to track the layer as it moves up and down. So far, the only zone model to attempt to include this effect is discussed by Jones (1983) and Mitler and Emmons (1981). Even in this case the attempt was made only to include heat loss from the upper layer as it moves down and comes in contact with cool lower walls. However, the phenomenon is important, as is discussed by Quintiere et al (1983), especially as the thermocline in the wall will influence the direction in which the wall boundary flow propagates.

Conduction through solids occurs in two places: the compartment walls and interior objects. The technique used is the same in both cases, although the boundary conditions on the equation may be different. Generally a slab is cut into N intermediate slices (N+1 nodes). Then eqn. (40) is solved for each slice. The actual finite difference used is a time centered, implicit scheme which is symmetric about the nodes. For the interior nodes we have

$$T'_i[1+\eta] = \frac{\eta}{2}\left[T'_{i+1} + T'_{i-1}\right] + \left\{T_i + \frac{\eta}{2}\left[T_{i+1} - 2T_i + T_{i-1}\right]\right\}\tag{41a}$$

where

$$\eta = \frac{\Delta t}{\Delta x}\frac{k}{\rho c}$$

and for the edge nodes

$$T'_i\left[1 + \frac{\eta}{2}\right] = \frac{\eta}{2}\left[T'_{i+1} \pm \frac{\dot{Q}_c}{k}\right] + \left\{T_i + \frac{\eta}{2}\left[T_{i+1} - T_i \pm \frac{\dot{Q}_c}{k}\right]\right\}\tag{41b}$$

The temperature at the starting time at node "i" is T_i and at time $t+\delta t$ it is T'_i. The number of nodes is chosen to reduce the residual error to some reasonable value, say less than 1%. Use of $N > 20$ will improve precision with no concomitant increase in accuracy. This technique would allow one to use different constituents for each slab, although such is not done in the current implementation. Each time step requires both an initial condition and one boundary condition. We start with the internal temperatures in each case, and the flux on the "hot" side. The usual scheme is to set the far side boundary condition to zero heat flux (which allows heat build up in the interior) or to approximate the far side exterior as a constant temperature bath. Either

technique is satisfactory unless this far side happens to be the interior
boundary for another compartment.

5. NUMERICAL INTEGRATION

The problem of the spread of fire, smoke, etc. has been formulated as a
set of differential equations. These equations are derived from the conserva-
tion of mass and energy. As a result, most of the equations are non-linear
and first order ordinary differential equations (ODE). The exception to this
rule is the heat conduction equation which is a linear parabolic equation, in
one or two dimensions. The former can be solved using implicit predictor-
corrector methods, Conte (1965), and the latter successive over-relaxation
(SOR), Mitchell and Griffiths (1980).

In the numerical implementation, we have relied on the validity of a
technique called time splitting. Simply stated, we have decoupled equations
which have greatly differing relaxation times, that is

$$\frac{1}{n} \frac{dn}{dt} = L_n$$

where L_n varies by more than an order of magnitude for each process. Except
for the driving program which invokes the hydrodynamics, species transport and
thermal conductivity, the various modules which incorporate the physical
processes are exercised separately and interact as source terms. This
splitting technique is standard but the inherent assumptions should be checked
when implementing a new numerical model. In addition, a check should be made
at each time step to insure that the relevant stability criterion (similar to
a Courant condition for fluid flow) is not violated.

For both types of equations the solution at each time step is found by an implicit scheme. The implicit method allows us to implement the numerical solution as a time centered algorithm. This insures reversibility in the physical phenomenon, at least for non-diffusive systems. A test of this assertion is to exclude thermal conduction, integrate from an initial condition to some final time, and subsequently, by changing the sign of the time step, we should be able to return to the starting position. A time reversal calculation is an important step in assuring ourselves that the integration scheme itself is not dissipative and thus will not relax to an incorrect final state. This is a real property in non-dissipative physical systems and should be mirrored as closely as possible in a numerical model. When conductivity is included, such reversibility ceases to be strictly valid, of course.

An additional virtue of the time centered scheme is avoiding the bifurcation which can occur in pure leapfrog schemes. The disadvantage is the one additional source calculation required at each time step. This time appears to be short, however, in comparison with the "corrector" phase of the implicit scheme.

The order of the integrations is as follows:

(1) Estimate the values for pressure, etc. at $t_o + \delta t$.

(2) Find the source terms for eqns. (22-25) based on the time centered values $(t_o + 1/2\ \delta t)$.

(3) Integrate eqns. (22-25) using the source terms defined at the time
     centered positions.

(4) Repeat steps (2) and (3) until convergence is reached.

(5) Integrate the conduction equation using the SOR technique.

The following illustration shows where each of these time-step points is,
in relation to steps (1-5):

(1) t_0 --------------------> $t_0 + \delta t$ estimate values at $(t_0 + \delta t)$

(2) t_0 --------->x<---------> $t_0 + \delta t$ find sources at $(t_0 + \delta t)$

(3) t_0 ----->$t_0 + \delta t/2$-----> $t_0 + \delta t$ integrate from (t_0) to $(t_0 + \delta t/2)$

(4) t_0 --------------------> $t_0 + \delta t$ repeat steps (2) and (3)

(5) t_0 --------------------> $t_0 + \delta t$ integrate conduction equation

Since each step is of at least second order accuracy, the overall scheme
will also be second order accurate $(0(\delta t^3))$. The relative error allowed at
each time step is $\sim 10^{-3}$. Thus the precision is greater than the precision of
the computer being used (at least as long as these calculations are being done
in single precision).

As for the integration scheme itself, it is derived from an Adam-Bashford
backwards difference scheme, Conte (1965), of order k=1. This yields a single
step predictor and second order corrector, $0(\delta t^3)$. These equations become
"stiff" if the individual source terms are large, which leads to a short time
step, yet the total source function may be tightly coupled if the solution is

-27-

being approached asymptotically. Another possibility is that the source terms

for the various equations differ by more than an order of magnitude. In

either case, the usual time step criterion would require a time step which is

prohibitively short. It is possible to modify the Taylor expansion used in

obtaining the predictor-corrector scheme to use the asymptotic nature of the

equations to enhance the speed of the solver, Young and Boris (1977).

The general form of an equation is

$$\frac{dn}{dt} = q - \ell n \equiv f.$$

Using the notation $n(0)$, $q(0)$, $\ell(0)$, $f(0)$ are the initial values at time (t_0),

and $n(1)$, $q(1)$, $\ell(1)$, and $f(1)$ are the values at the new time $(t_0 + \delta t)$, we

obtain first for the normal equations

$$\text{predictor } n(1) = n(0) + \frac{\delta t}{2} f(0) \tag{42a}$$

$$\text{corrector } n(1) = n(0) + \frac{\delta t}{2} \left(f(0) + f(1) \right) \tag{42b}$$

and for the stiff equations

$$\text{predictor } n(1) = n(0) + \frac{\delta t}{1 + \delta t \ell(0)} f(0) \tag{43a}$$

$$\text{corrector } n(1) = n(0) + \frac{2 \delta t}{1 + \delta t \{\ell(0) + \ell(1)\}} \left\{ f(0) + q(1) - \ell(1)n(0) \right\}. \tag{43b}$$

The corrector must be iterated until some specified error criterion is reached. If the specified error can not be reached in a small number of iterations, say two or three, then the time step must be reduced. It turns out to be advantageous to half the time step for each instance that a reduction is required, and increase it by only 10% for each subinterval that the error criterion is satisfied.

One technique which has been used in previous work to reduce the solution time for these equations is to convert them to an algebraic form. The conversion is done by noting that the final state of the equations at each timestep is a pseudo equilibrium. Thus the transient term can be dropped. For a number of reasons, simultaneous ODE's are generally easier to solve than the corresponding algebriac equations unless one is exceedingly close to the solution. Such an assertion is difficult to prove in the general case but two examples should suffice to indicate the difference in the nature of the root finding procedure. One of the simplest nonlinear algebraic equation is

$$A \, B = C$$

with A, B, and C being integers. Until recently this nonlinear decomposition was thought to be unsolvable (in finite time) for an arbitrary value of C. Also, a straight comparison of this method (embodied in a model) with other models using the algebraic scheme, has shown a reduction by at least a factor of ten in the time required for a given calculation. A detailed timing comparison of several models is given elsewhere, Jones (1982).

6. COMPARISON WITH EXPERIMENTAL DATA

The series of tests which serve as a data-base for this analysis are based on a two-room fire scenario by Cooper et al. (1981) and an ongoing series of full scale validation tests at the National Bureau of Standards. The former was a two-room configuration, consisting of a burn (or fire) room and a corridor. It is referred to as the "Nike Site" in later discussions. The latter is a three room configuration with the additional room being a target room for testing high density occupancy, referred to as "Building 205." The geometry of each of these configurations is shown in Table I.

Comparisons between the model and experimental data are for fires of 100 kW. Figures 4 and 5 show the comparison for the Nike Site tests for the upper layer temperatures in the burn room and corridor, and the interface height in the corridor. Figures 6 and 7 show a similar comparison to the current experiments in B205, a full scale facility at NBS. It is apparent from a comparison of Fig. 4-7 that plume entrainment is estimated very well but that the door jet entrainment is underestimated. We can see this from the good agreement between experiment and theory in any compartment which contains a primary plume whereas in other compartments the predicted temperature is too high and the layer depth too small in comparison with experimental values. This underestimation occurs in the regions which McCaffrey (1983) calls the flaming and far field regions. In the intermittent region, where the results of McCaffrey (1983) and Cetegen et al. (1982) agree, the entrainment rate appears to be correct.

Another factor which gives rise to disparity between theory and experiment is the assumption, in the model, of known and uniform wall materials. In the experiments, walls consist of several materials in a composite such as calcium-silicate board over gypsum. Allowing for these factors, the agreement seems quite good. As research continues, these discrepancies will be resolved.

Table I.

		Burn	Vent	Corridor	Vent	Target
Nike Site	Depth[2]	4.3	–	11.1-20.2	–	
	Width	3.3	1.07	2.4	0.95	
	Height	2.3	2.00	2.3	0.15	
	Area	14.2	2.14	26.6-48.4	0.14	
	Volume	32.2	–	61.2-112.3	–	
		Burn	Vent	Corridor	Vent[1]	Target
Bldg. 205	Depth	2.3	–	12.2	–	2.3
	Width	2.3	1.0	2.4	1.0/1.0	2.3
	Height	2.2	1.9	2.4	1.9/2.0	2.2
	Area	5.5	1.9	29.7	1.9/2.0	5.5
	Volume	11.8	–	72.6	–	11.8

Note 1: V1/V2: V1 is from corridor to target room and V2 is from corridor to the ambient.

Note 2: Lengths are in meters, areas in square meters and volumes in cubic meters.

7. STABILITY AND COMPLETENESS

There are a number of phenomena which are either not included or need additional work. They are:

1. Wall effect – two dimensional, unsteady heat flow
2. Separation of flow – vents
3. Ceiling jet – transit time

The first refers to the finite thermal inertia of the wall as the hot layer moves down (or possibly up). There will be a two dimensional thermocline in the wall which differs from that in the compartment. Although this has only a small direct effect, it can lead to flow along the walls which can subsequently contribute to contamination of the lower layer. Such effects become particularly important as the smoke travels further from the fire source and temperature differentials become small.

The second problem is quite important for asymptotic predictions, especially near the room of fire origin. Currently we assume that hot gas mixes with hot gas or cold with cold gas as it traverses a vent. This was a reasonable approximation while the lower layer was assumed to be ambient. Now that we calculate the lower layer temperature, we find that the recirculating gas may have a temperature on the order of the lower layer of the room into which it enters. A particular example will demonstrate the effect. In a two compartment calculation, Jones and Quintiere (1983) found that the layer outside of the burn room is lower than that in the compartment of fire origin. As there is no source of heat in this second compartment and cooling occurs

due to mixing, the upper layer in this adjacent space is cool relative to the upper layer in the fire room, and even comparable in temperature with the lower layer. Currently we assume all of the hot gas in the adjacent room, which flows into the fire room, will be deposited in the fire room upper layer. As can be seen in figure 8, Evans (1983) this assumption leads to discrepancies in prediction versus experiment. A better approach is to divide the incoming flow into two components: for flow into compartment (i) from compartment (j), we have a component into the upper layer $= \left(\dfrac{T_{uj} - T_{\ell i}}{T_{ui} - T_{\ell i}} \right) \dot{m}_{j \rightarrow i}$, with the remainder going into the lower layer. This occurs only after an interface discontinuity has been established.

The third problem will only be important for very long corridors (20 m) or very tall compartments or shafts. Also, it is only a transient phenomenon. For purposes of siting smoke detectors, for example, this transient may be important.

8. CONCLUSIONS

The fire and smoke transport model, as described in this paper, is quite detailed and complete as far as our current understanding of fire phenomenology is concerned. It draws on a great deal of the research into fires which have occurred over the past ten years, pulling together much of the best work which has been done in the field. The numerical implementation is of particular interest because it is extremely durable. The problems discussed in the section "Stability and Completeness" need to be addressed if we are to carry this work further, such as to fires in high rise hotels or on aircraft carriers.

9. ACKNOWLEDGMENTS

Two NBS cooperative students, Alicia Fadell and Charles DeWitt have contributed to this effort. Ms. Fadell was instrumental in implementating the "BUILD" program which generates the configuration and description files for the "FAST" model. Mr. DeWitt is responsible for "FASTPLOT", a routine which enables one to analyze rather easily the extensive output available from "FAST."

A machine readable copy of the model is available through NTIS. The tape includes the data file listed in the appendices.

10. REFERENCES

Carslaw, H.S. and Jaeger, J.C., Conduction of Heat in Solids, Oxford University Press, London (1959).

Cooper, L.Y., Harkleroad, M., Quintiere, J. and Rinkinen, W. (1981), An Experimental Study of Hot Layer Stratification in Full Scale Multiroom Fire Scenarios, ASME 81-HT-9, Milwaukee.

Cetegen, B.M., Zukoski, E.E. and Kubota, T., Entrainment and Flame Geometry of Fire Plumes, Ph.D. Thesis of Cetegen, Cal. Tech. (1982).

Conte, S.D., Elementary Numerical Analysis, McGraw-Hill, New York (1965).

Evans, D., private communication (1983).

Jones, W.W., An Improved Numerical Method for Fire Models, Fall Technical Meeting of the Eastern Section of the Combustion Institute, Atlantic City (1982).

Jones, W.W., A Review of Compartment Fire Models, National Bureau of Standards (USA) IR 83-2684 (1983).

Jones, W.W. and Fadell, A., A Device Independent Graphics Kernal, to be published as an NBSIR.

Jones, W.W. and Quintiere, J.G., Prediction of Corridor Smoke Filling by Zone Models, Comb. Sci and Tech 11, 111 (1983).

Kusada, T., NBSLD, The Computer Program for Heating and Cooling Loads in Buildings, National Bureau of Standards (USA) BSS 69 (1976).

McCaffrey, B.J., Momentum Implications for Buoyant Diffusion Flames, Comb. and Flame 52, 149 (1983).

Mitchell, A.R. and Griffiths, P.F., The Finite Difference Method in Partial Differential Equations, J. Wiley & Sons, New York (1980).

Mitler, H.E. and Emmons, H.W., Documentation for CFC V, The Fifth Harvard Computer Fire Code, Home Fire Project Tech. Rep. #45, Harvard University (1981).

Quintiere, J.G., Steckler, K. and Corley, D., An Assessment of Fire Induced Flows in a Compartment, submitted for publication in Fire Science and Technology (1984).

Quintiere, J.G., Steckler, K. and McCaffrey, B.J., A Model to Predict the Conditions in a Room Subject to Crib Fires, First Specialists Meeting (International) of the Combustion Institute, Talence, France (1981).

Rockett, J.A., Experimental Determination of the Heat Flux to a Burning Surface, to be published in Fire Science and Technology.

Schlichting, H., Boundary Layer Theory, Pergammon Press, New York (1955), translated by Kestin, J.

Siegal, R. and Howell, J.R., Thermal Radiation Heat Transfer, McGraw Hill Book Co., New York (1981).

Steckler, K.D., Quintiere, J.G. and Rinkinen, W.J., Flow Induced by Fire in a Compartment, Nineteenth Symposium (International) on Combustion (1982).

Tanaka, T., A Model of Multiroom Fire Spread, National Bureau of Standards (USA) IR 83-2718 (1983).

Tanaka, T., A Model of Fire Spread in Small Scale Buildings, Building Research Institute (Japan) RP #84 (1980).

Turner, J.S., Buoyancy Effects in Fluids, Cambridge University Press (1973).

Yokoi, S., Study on the Prevention of Fire Spread Caused by Hot Upward Currents, Kenchiku Hokoku No. 34 (1960).

Young, T.R. and Boris, J.P., A Numerical Technique for Solving Stiff Ordinary Differential Equations Associated with the Chemical Kinetics of Reactive Flow Problems, J. Phys. Chem. 81, 2424 (1977).

Appendix A - Notation

A   area (m^2); A_u, A_ℓ, A_d are the upper and lower compartment surface areas in contact with the upper and lower gas layer, fig. (1), respectively. A_d is the interface area between the upper and lower layers. In section 4.4, "A" is used as a variable in the flow equations to indicate air.

B   width of a vent (m)

C, C'   flow coefficient $\simeq 0.6-0.7$ for both smoke and air

c   specific heat - c_p, c_v (J/kg/K)

$\dot{E}$ energy release rate (J/s)

E   internal energy of the gases - see eqn. (2)

F_{ij} view factor - relative area of "i" as seen by "j" (dimensionless)

g   acceleration of gravity (9.8 m/s^2)

H   height (m), H_u, H_ℓ, are the upper and lower limits of a vent - fig. (1)

h   enthalpy (J/kg/K)

h_c heat of combustion - theoretical (J/kg)

i,j   compartment indices

k   thermal conductivity (J/s/K)

L   mean beam length (m) equivalent opaque sphere

m   mass (kg)

$\dot{m}$ mass flow (kg/s): $\dot{m}_v$ - rate of release of volatiles

                                $\dot{m}_e$ - entrained into a plume

                                $\dot{m}_f$ - fuel burning rate = $\chi_e \dot{m}_v$

                                $\dot{m}_{ij}$ - mass entering room "i" from room "j"

                                $\dot{m}_p$ - flow rate in plume $\left(\dot{m}_p = \dot{m}_v + \dot{m}_e \right)$

N   height of the neutral plane (m)

P   pressure (pa): $\bar{P} + P$ - floor reference pressure

                            P_a - outside ambient pressure

$\dot{Q}$ rate heat is added or lost (J/s):

$$\dot{Q}_u, \; \dot{Q}_\ell \text{ - upper, lower zones, respectively}$$

$$\dot{Q}_f \text{ - fire } (h_c \dot{m}_v)$$

$$\dot{Q}_o \text{ - objects}$$

$$\dot{Q}_R \text{ - radiation}$$

$$\dot{Q}_c \text{ - convection by walls}$$

$$\dot{Q}_g \text{ - radiation added to upper gas layer}$$

$$\dot{Q}_k \text{ - radiation from surface "k"}$$

$$\dot{Q}_p \text{ - combustion energy lost by formation of volatiles}$$

R   gas constant for specific mixture

S   smoke - section 4.4

t   time (s)

T   temperture (k): T_a - ambient

                                      T_c - external wall

                                      T_u - upper wall

                                      T_ℓ - lower wall

                                      T_R - reference temperature for enthalphy flow

                                      T_g - upper zone temperature

                                      T_v - pyrolysis temperature

V   volume (m^3)

Z   layer thickness (m) - Z_i = interface height in compartment (i)

α absorption coefficient of upper gas layer (m^{-1}), thermal diffusivity (m^2/s)

γ ratio of specific heat (c_p/c_v)

ε emissivity (dimensionless): ε_i – surface "i"

ε_g – upper gas layer

ε_u – upper compartment surface

ε_ℓ – lower compartment surface

ρ_{ui} – density of the lower layer in

compartment (i)

ρ mass density (kg/m^3)

κ thermal conductivity (j/msK)

δ_{ij} Kronecker delta = 0 $i \neq j$

= 1 $i = j$

Δt time step (s)

Δx spatial discretization

Subscripts – In general "u" and "ℓ" indicate upper and lower gas layer,
            respectively. For area and emissivity variables, reference is to
            the compartment itself.

Appendix B

Shown in Table II is a sample input for FAST. The organization is that control is at the beginning, followed by component information, connections, wall properties, a description of the fire, species generation information and finally file descriptors for graphics and the dump file.

In general, the first word in each line is a key word and must be included. The explanation of this file will be by example:

Line	Meaning
1	version and title
2	time step information
	600 → number of seconds for the calculation
	120 → print interval
	120 → dump interval (requires files)
	1 → graphics interval (requires files)
	0 → hard copy counter
3	Number of floors — not used with this version, but retained for compatibility
4	Total number of compartments
5	Maximum number of openings between compartments (≤ 4)
6	ambient temperature,
7-10	compartment geometry, W x L x H x Floor (1 → NROOM)
11-16	connection configuration (outside is compartment NROOM + 1)
17	number of walls used in the calculation[1]
18-27	thermophysical properties of the upper and lower walls respectively (units are SI except energy (kJ) and power (kW)).
28	which compartment the fire is in
29	type of fire (currently only a gas burner is allowed)
30	number of intervals for production rate[2]
31	interior position of the fire to establish entrainment rate (1 → center)
32	fuel properties necessary for partial combustion
	1.0 → fraction of pyrolysis which burns
	0.0 → fraction of water in the fuel
	0.750 → fraction of carbon in fuel by weight
	0.25 → fraction of hydrogen in fuel by weight
	0.00 → fraction of oxygen in fuel by weight
	49758 heat release rate (kJ/kg)
	300. fuel inlet temperature
	0.0 fraction of heat which exits the fire plume in the lower layer as radiation

---

[1] Currently an upper and lower wall are used. This will change shortly to four walls to reflect the physical difference among the ceiling, walls and floor.

[2] Figure 9 shows a sample fire production curve.

33	mass loss rate at each end point (kg/s), LFMAX + 1$_e$
34	area of the fire at each end point (m^2)
35	height of the <u>base</u> of the flame (m)
36	duration of each time interval (LFMAX)
37-40	fractional production rate of species 3, 7, 9 & 10[3]
	first number is species (1 → 12)
	second number is a conversion factor
	third through LFMAX + 3 are fractional production rates[4]
41	termination label (required)
42-44	file descriptors
	DISFG = plan view[5]
	CONFG = layer information[5]
	DUMPR = dump file for FASTPLOT

There are two primary output files for the model. The first is binary (UNIT = 9) and is used by the routine "FASTPLOT" described in appendix D. The other is an ASCII file (UNIT = 6) and usually is displayed on the printer. Units are SI (MKS) except for energy which is in kJ. The meanings of the symbols, in the order which they appear, are:

Initial	-	reiterate the input parameter, generally in the order of input
Timestep Output	-	
TIME	-	simulated time (s)
U. TEMP	-	upper layer temperature (K)
L. TEMP	-	lower layer temperature (K)
U. VOLUM	-	upper layer volume (m^3)
U. DEPTH	-	vertical thickness of the upper layer (m)
C. TEMP	-	ceiling temperature at the surface (K)
F. TEMP	-	floor temperature (K)
EMS	-	flow into the upper layer from the plume (kg/s)
EMP	-	pyrolysis rate (kg/s)
ADS	-	area of the fire (m^2)
QF	-	enthalpy release rate of the fire (kW) to the upper and lower layer
QR	-	total radiant energy to the upper and lower layers (kW)
QC	-	total convective heating of the upper and lower layers (kW)
Pres	-	floor reference pressure (pa)
mass	-	vent flow from i → j (kg/s) - sec (section 4.4)

---

[3]Species 1-12 are N_2, O_2, CO_2, CO, HCN, HCL, ThHC, H_2O, smoke density, total % LC_{50}, smoke number density and HCL number density.

[4]Fraction of the mass burning rate at the corresponding endpoint (see line 33 and figure 9).

[5]Format for the graphics files is given in the NBSIR by Jones and Fadell.

Species concentrations listed by species:

mass	–	total mass of that species in the layer (kg)
M/V	–	mass per unit volume multiplied by the conversion factor shown in line 37-40 of the input fuel. Unity leaves this value in (kg/m^3).[6]
PPM	–	parts per million of the total molecules present
PPM-M	–	dosage which is an integral of (PPM) over time (PPM – minutes)

Table II

```
 1 - VERSION 15 Toxic hazard evaluation
 2 - Timesteps     600      120       120      1      0
 3 - NFLOR             1 NUMBER OF FLOORS IN THE CALCULATON
 4 - NROOM             5 TOTAL NUMBER OF ROOMS
 5 - NMXOP             1
 6   TAMB        300.
 7 - HI/F         0.0      0.0      0.0       0.0      0.0
 8 - WIDTH        3.3      2.4      2.9       2.4      3.3
 9 - DEPTH        4.3     18.8      9.9       9.9      4.3
10 - HEIGH        2.3      2.3      2.3       2.3      2.3
11 - HVENT          1        2              1.07      2.0      0.0
12 - HVENT          2        3              1.07      2.0      0.0
13 - HVENT          3        6              0.95      .15      0.0
14 - HVENT          2        4              1.07      2.0      0.0
15 - HVENT          4        6               .95      .10      0.0
16 - HVENT          2        5              1.07      2.0      0.0
17 - WALLS          2
18 - COND        .0012    .0012             .0012    .0012    .0012
19 - SPHT        .840     .840              .840     .840     .840
20 - DNSTY      2000.    2000.            2000.    2000.    2000.
21 - THICK       0.50     0.50             0.50     0.50     0.50
22 - EMISS       0.8      0.8              0.8      0.8      0.8
23 - COND        .0012    .0012             .0012    .0012    .0012
24 - SPHT        .840     .840              .840     .840     .840
25 - DNSTY      2000.    2000.            2000.    2000.    2000.
26 - THICK       0.50     0.50             0.50     0.50     0.50
27 - EMISS       0.8      0.8              0.8      0.8      0.8
28 - LFBO             1 ROOM OF FIRE ORIGIN
29 - LFBT             1 TYPE OF FIRE (GAS BURNER)
30 - LFMAX            6 NUMBER OF INTERVALS FO FIRE GROWTH
31 - LFPOS            1 POSITION OF THE FIRE (CENTER)
32                1.0      0.0      .750      .250     .00    49758 300.    .0
33 - FMASS       .002     .002     .002      .002     .002     .002    .002
34 - FAREA       .5       .5       .5        .5       .5       .5      .5
35 - PHIGH       .0       .0       .0        .0       .0       .0      .0
36 - FTIME      60.      60.      60.       60.      60.      60.
37 - SPECI  3    1.0      1.0      1.0       1.0      1.0      1.0     1.0     1.0
38 - SPECI  7    1.0      .025     .025      .025     .025     .025    .025    .025
39 - SPECI  9  3500.      .02      .02       .02      .02      .02     .02     .02
40 - SPECI 10    31.2     1.0      1.0       1.0      1.0      1.0     1.0     1.0
41 - ENDSP
42 - DISFG NIKE13A.DAT
43 - CONFG NIKE13B.DAT
44 - DUMPR TOXIC.DMP
```

---

[6]This conversion factor allows the user to convert this output to an optical density, LC_{50} or whatever.

41

Appendix C

The program BUILD is used to construct data files for configuration display. These files can then be used by FAST to display a decision tree either interactively or as a graphics streaming file. Both the configuration file for display as well as information on position and type of display for the decision tree are built by this program. The commands are:

ADD [VERTEX, EDGE, POLYGON]   (default = VERTEX)

     add vertex – create vertices by specifying three (x, y, z) coordinates;
             add vertices to the work file

       add edge – create edges by specifying two vertices; add edges to work
               file

     add polygon – create polygons by correcting vertices. A minimum of three
              vertices are required to define a polygon, and there is an
              internal maximum specified by NPVERT.

DELETE [VERTEX, EDGE, POLYGON]   (default = VERTEX)

    delete vertex – delete vertices and any edges or polygons which are
              connected to the deleted vertices

      delete edge – delete edges

    delete polygon – delete polygons

DISPLAY [ALL, VERTEX, EDGE, POLYGON]   (default = ALL)

       display all – display all edges and polygons in graphics mode

     display vertex – display all vertices and their line numbers in graphics
              mode .

      display edge – display all edges in graphics mode

    display polygon – display all polygons in graphics mode

DUPLICATE

    Duplicate a polygon at another location – askes for a displacement vector.

END

    End the program.

ERASE

    Erase the display screen.

GET [filename]   (default = INFILE)

    Open an existing file and assign the filename to INFILE; the elements of
    this file make up the new work file.

HELP

    List all the BUILD commands, their corresponding options, and the default
    values.

LIST [VERTEX, EDGE, POLYGON]   (default = VERTEX)

    list vertex - list the world coordinates, window coordinates, and the
                   vertices of the work file on the display screen

    list edge   - list the edges of the work file on the display

    list polygon - screen list work file's polygons on the display screen

MOVE [VERTEX, POLYGON]   (default = VERTEX)

    move vertex - move a vertex from its present location to a new
                  location - asks for a displacement vector

    move polygon - move a polygon from its present location to a new
                   location - asks for a displacement vector

PRINT [ALL, VERTEX, EDGE, POLYGON]   (default = ALL)

    print all - list the work file's world and window coordinates,
                vertices, edges, and polygons on the printer

    print vertex - list the world coordinates, window coordinates, and
                   vertices of the work file on the printer

    print edge - list the work file's edges on the printer

    print polygon - list the polygons of the work file on the printer

SAVE [filename]   (default = OUTFILE)

    Save the current file under the specified filename; assign the filename to
    OUTFILE.

STATUS

    List the filenames stored in INFILE and OUTFILE; indicate the current
    number of vertices, edges, and polygons and the maximum number of each
    element allowed.

WINDOW

    Create the work file's window space by specifying minimum and maximum x
    and y coordinates for display. Defaults to WORLD.

Create the work file's three-dimensional world space by specifying x, y, and z coordinates. All structures must be contained in this cartesian coordinate system.

FASTPLOT is a data analysis program which runs in conjunction with "FAST." The results for "FAST" are dumped to a data file after each prescribed desired time step. FASTPLOT has the capability to form a list of variables, read in their values at each time interval, list out the values in tabular form, graph the values (hard copy or screen), and save the variables in a file for future reference.

The FAST model models a fire in one of several compartments, or rooms, and follows smoke and toxic gases from one compartment to another. We are concerned with variables in both the upper and lower layers.

The list of variables presently available through FASTPLOT are:

AREA .... burning area of the fire (m^2)

CONCENTRATION .... species density in parts per million

CONVECTIVE .... heat loss from layer to solid surface due to convection (kw/m^2)

DOORJET .... bouyant mass flow through a vent (kg/sec)

DOSE .... species concentration integrated over time (ppm-min)

ENTRAINED .... mass entrained by a plume (from lower layer to the upper layer)

INTERFACE .... height of the two-zone discontinuity (m)

MASS .... mass density in a layer (kg/m^3)

MDOTFIRE .... mass loss rate of the fire source (kg/sec)

NEUTRAL 1
NEUTRAL 2 .... neutral planes (maximum of three) for each vent
NEUTRAL 3

PLUME .... total mass flow into the plume (kg/sec)

PRESSURE .... reference pressure at the floor of the compartment (pa)

QC .... total convective heat gain by a layer

QF .... total enthalpy increase from the fire source

QR .... total radiative heat gain by a layer

RADIATION .... heat loss from layer due to radiation (kw/m^2)

TEMPERATURE .... temperature of the layer (C)

VENTFLOW .... mass flow through a vent (kg/sec) -
                              bidirectional

VOLUME .... volume of the upper zone (m^3)

WALLTEMP .... temperature of the wall (C)

The CONCENTRATION, DOSE, and MASS also have associated with them a species number.

The main control of the program is carried out in the subroutine WHICHONE. It does the actual building of a list and the processing of the options. The possible options available to the user are:

ADD
CHANGE
CLEAR
DEFAULT
DELETE
END
HELP
LIST
PLOT
REVIEW
SAVE

Upon running the program, the first input encountered will be that of the dump file generated by FAST. Most of them will be of the form:

filename.DMP

Next, the user will be asked to input the option which he wishes to have performed. The following is a description of each of the options available. They are in the order that they usually will be encountered. However, some may be executed before the others without any problems. The minimum number of characters required to recognize an option is enclosed in the parenthesis at the beginning of each word.

1. (DE)FAULT

This enables the user to set his own default parameters for the following:

COMPARTMENT #
VENTFLOW DESTINATION
LAYER
SPECIES #
CHARACTER SET FOR PLOTTING

This option may be done at any time and if it is not done the defaults are set to "1, 2, upper, 9, and 4", respectively. The purpose of this option is to change the defaults available for other commands and data input.

2. (VA)RIABLES

The purpose of this option is to allow the user to recall the possible variables that are available for use. They will be listed on the screen.

3. (AD)D

This command is used to build a list of variables. When an option is requested ADD may be entered by itself or together with a list of variables that are to be added. If it is entered alone a message will be printed asking for the variables that are to be added to the list. For example:

```
> ADD
- INPUT VARIABLES TO BE ADDED >
              or
> ADD TEMP, PRES, ......
```

For each variable selected there is a series of questions that will be asked as to the type of that variable wanted. Questions asked about all variables are:

```
WHICH COMPARTMENT? ->
WHICH LAYER? ->
```

If VENTFLOW is chosen the compartment origin and destination will be requested; if CONCENTRATION, MASS, or DOSE are selected the species number of each will be requested.

The maximum number of variables allowed on the list at any one time is 25. If the list is full or the variable is presently on the list the addition will be disallowed and another option requested.

4. (DEL)ETE

When this option is entered the present list of variables will be printed out to the screen and the user will be asked to input the variables to delete by the number associated with them on the list. They must be entered on a single line separated by commas or blanks.

If the variable number that is input does not correspond to one that is currently on the list it will be skipped. After the deletions have been processed a new list is presented and another option requested. If the list is presently empty then that fact will be stated in an error message.

5. (HE)LP

This command may be input at any time that the user is asked for an option. It's purpose is to simply list out to the console a list of the available commands and a brief explanation after which another option will be asked for.

6. (RE)VIEW

At times the user may wish to see what is presently on his list before entering a command. This may be done with the REVIEW command. It will print out the current list along with the compartment number, species, and layer of each of the variables. After the printing of the entire list the option request is again displayed.

7. (LI)ST

After variables have been added to the list and their data values read in, the user may list out the values of any of the variables on the list to either the printer or the console. The user will input the device number (5 = CONSOLE, 6 = PRINTER), and the list of variables presently on the list will be displayed. He will then be asked to input the corresponding number(s) of the variable(s) to be listed out. They must be entered on a single line separated by commas or blanks. The maximum number of variables able to be listed at one time is 8 for the printer and 5 for the console.

8. (PL)OT

This option is central to the data analysis. After entering this command the current list of variables will be displayed along with their numbers. The user will be asked to input the number of the variable(s) to be plotted from the list. They should be entered in a string separated by a comma or a blank space. For example:

```
ENTER VARIABLES TO BE PLOTTED -> 1,2,3,4
                   or
ENTER VARIABLES TO BE PLOTTED -> 1 2 3 4
```

After entering the variable numbers, the number of the device which the graph is to be plotted on will be asked for.

The possible devices are:

1. CALCOMP
2. PRINTER
3. LEXIDATA
4. SCREEN

The maximum number of plots per call to PLOT is limited to 4. They will be printed in the following order on the device depending on the number of graphs per page:

```
-----------           -----------
|  1    2  |          |  1    2  |
|  3    4  |          |     3    |
-----------           -----------
   FOUR                   THREE
```

48

```
 -------------           -------------
|     1       |         |     1       |
|     2       |         |             |
 -------------           -------------
     TWO                     ONE
```

If more than 4 variables are input only the first four will be accepted
and the remaining ones disregarded. If a variable number not on the list is
entered, an error message will appear, the list will be reprinted and the
input will be asked for again. This will continue until all variables entered
are currently on the list.

Before the graphing is done the user is given the opportunity to change
the range of the X and Y axes. The maximum and minimum values of the X and Y
axes will be displayed, followed by a request for a change in each, which will
be of the form:

CHANGE (X or Y) AXIS TO? ->

If no change is desired simply enter a <RETURN> and the next axis change
will be displayed. If a change is made the value will be entered and the same
change request will be made again. This will be repeated until a <RETURN> is
entered.

When all the changes have been made, if any, the graph of that particular
variable will be plotted. After it has been completed the next variable's
maximum and minimum will appear and their changes input as before.

After the final graph has been completed the option request will be
displayed and a new option may be entered.

9. (SA)VE

This option allows the user to save the values of the variables on the
list in a file. The format used will make the data compatible with an experi-
mental data processing program designed for handling of data in the Center for
Fire Research.

The user will be asked for the name to be used for the file. A check
will be made to see whether that file presently exists or not. If it does the
user will be asked if he wants to write over the old file with this new data.
If his answer is NO, nothing will be placed in the file and another option
requested. If, however, he does want the file rewritten, or the file does not
already exist, the new file will be created and the data stored in it.

Each variable on the list will be dumped with the following format at the
beginning of each block of data:

I6,I6,A6, * ---------- COMMENT ----------

The first I6 will be for the number of data points for that variable, the
next I6 is for the number given to that variable on the list, and the A6 is
for the actual variable name. Everything after the * is a comment block and
will be filled with information relevant to that particular variable, such

49

things as species number, compartment number, layer, etc. The actual
numerical data will be dumped using the format 7E11.5.

10. (CL)EAR

The input of this command empties the variable list.
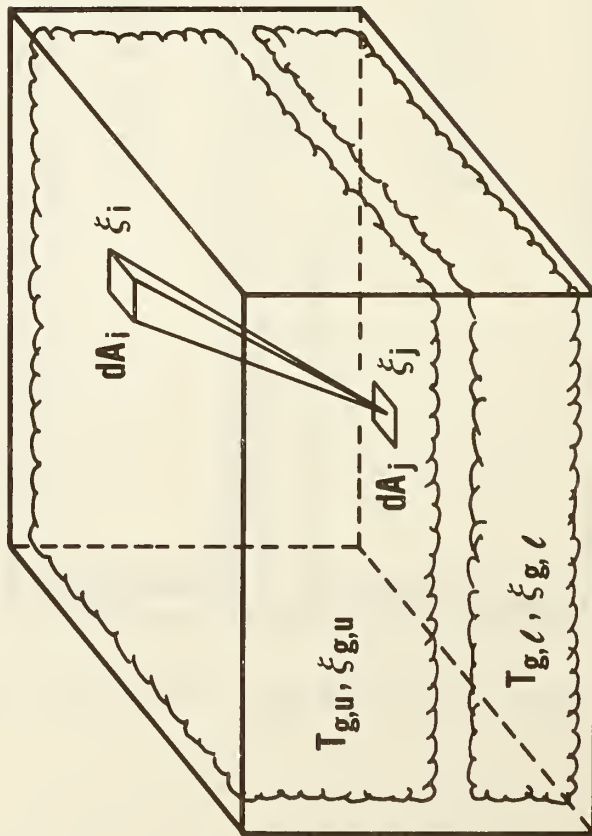
11. (CH)ANGE

This option restarts the program by asking for a new file and resetting
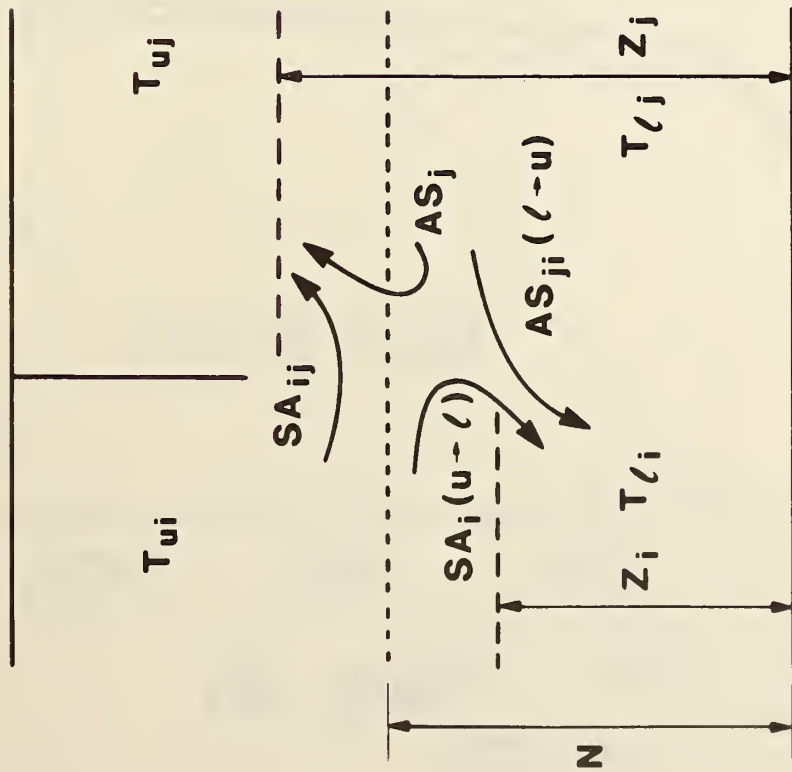all variable lists.

12. (EN)D

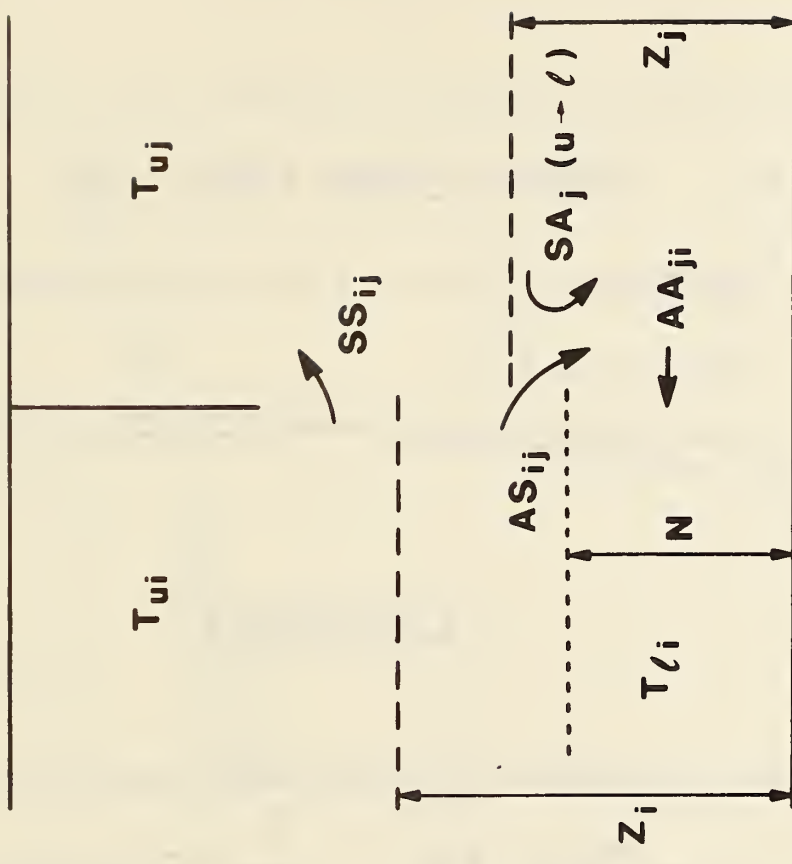This function terminates the execution of the FASTPLOT program.
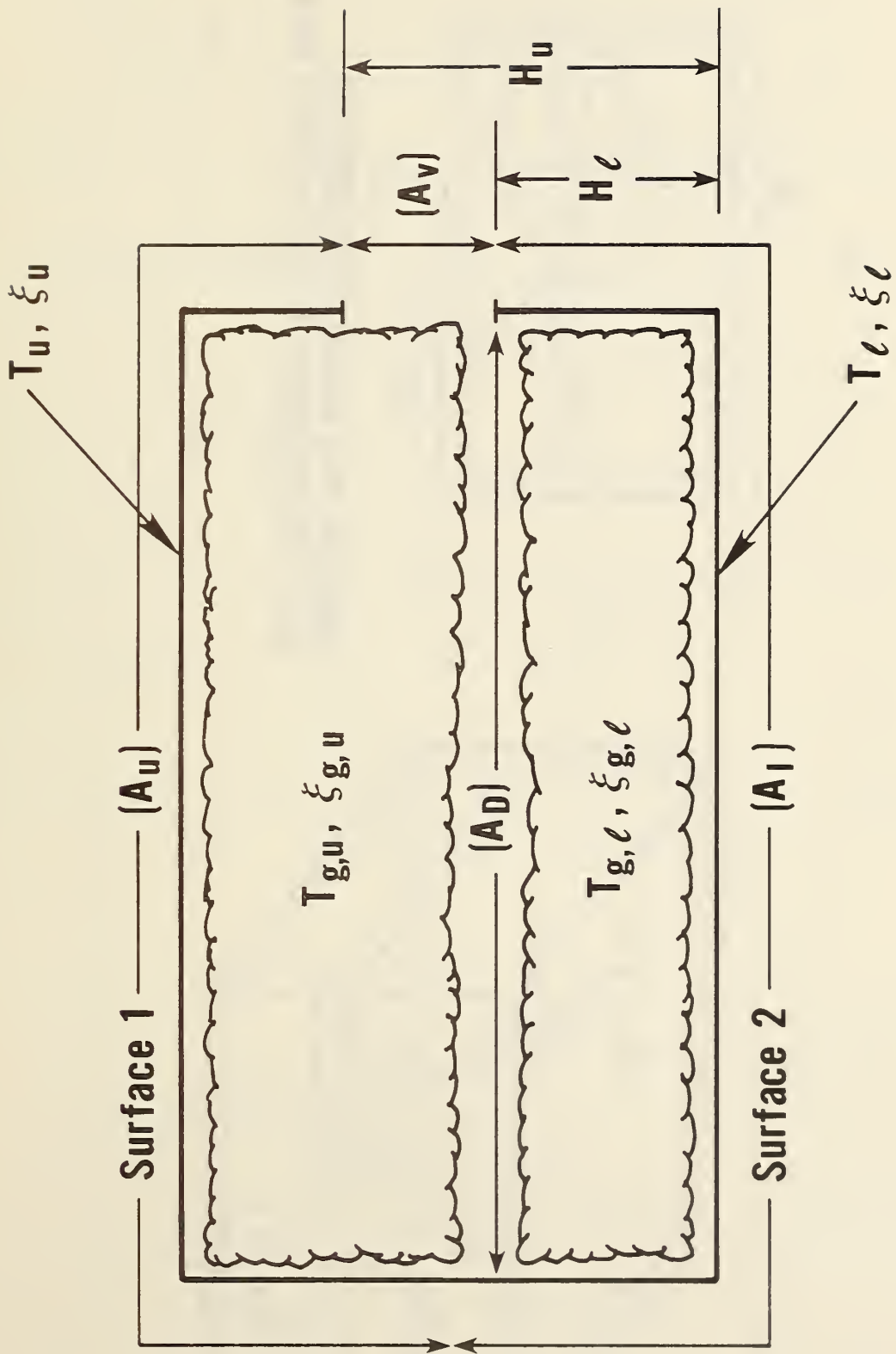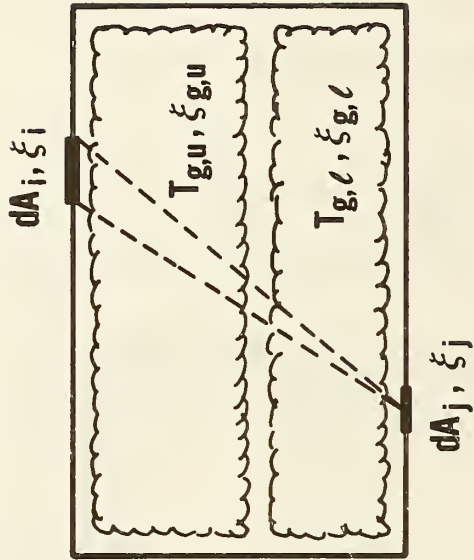
**RADIATION PATH BETWEEN TWO SURFACES
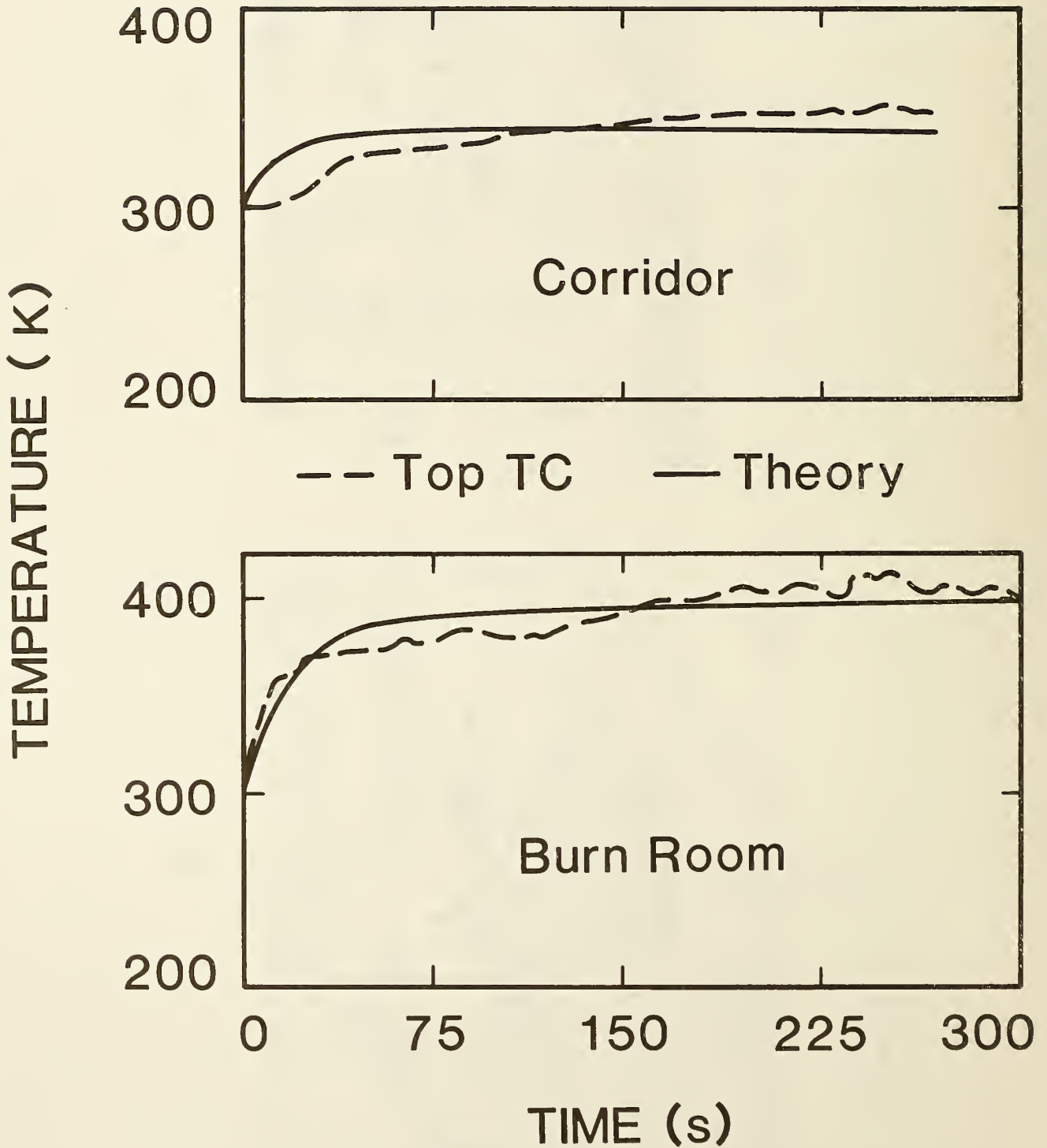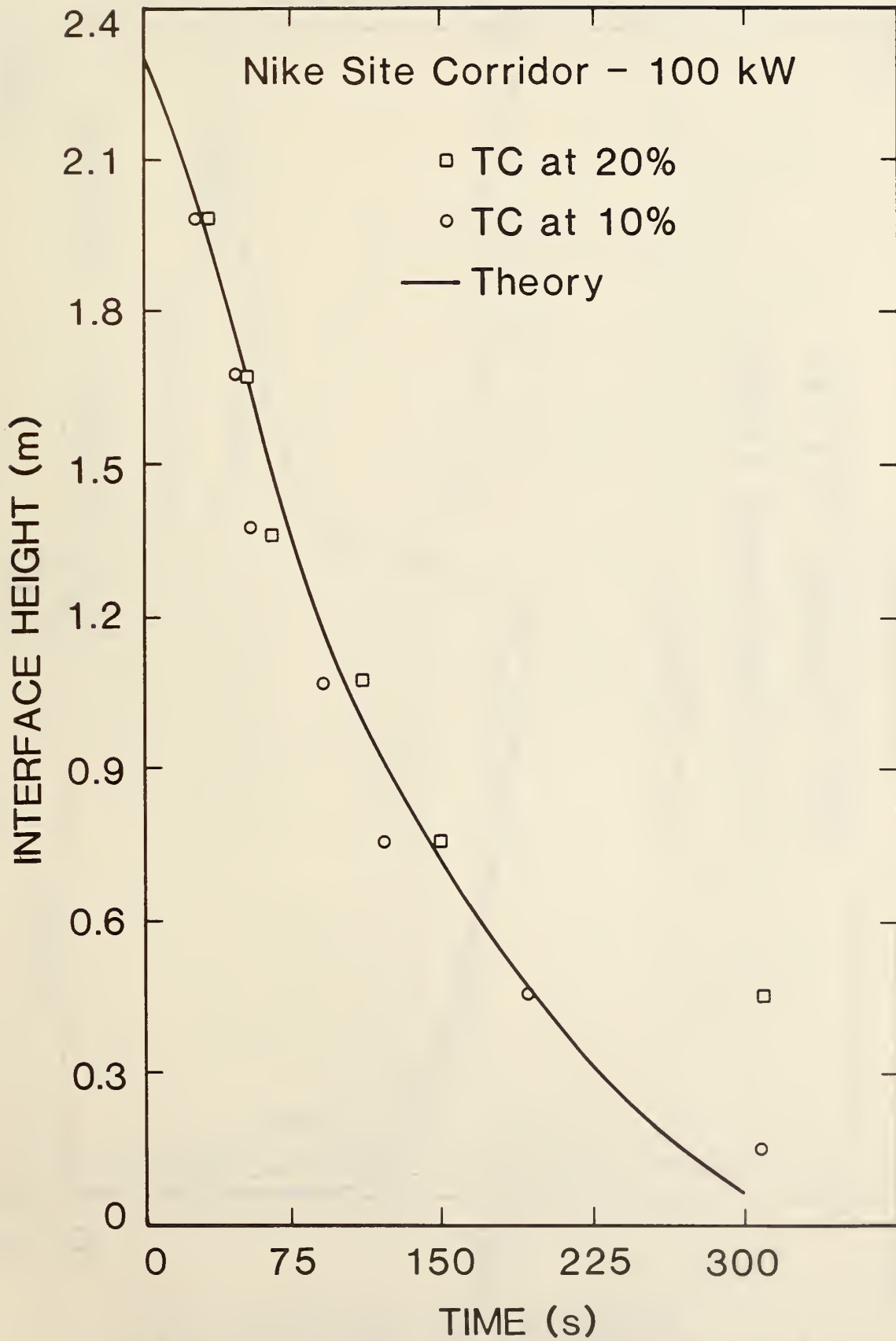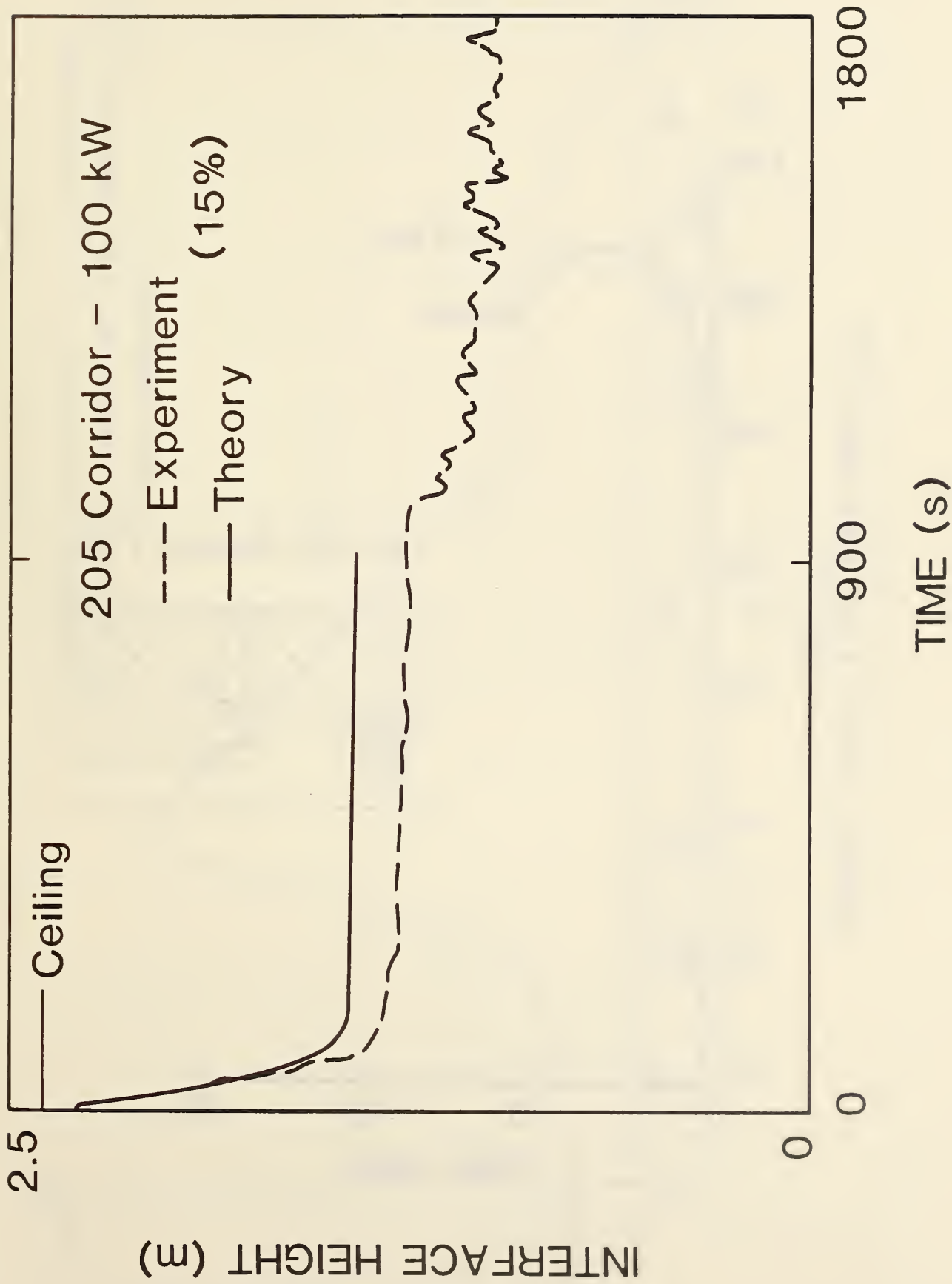WITH TWO ISOTHERMAL LAYERS BETWEEN THEM**

53

Nike site 100 kW

Corridor

-- Top TC   — Theory

Burn Room

Nike Site Corridor – 100 kW

□ TC at 20%
○ TC at 10%
— Theory

205 Corridor 100 kW
--- Experiment (15%)
—— Theory

UPPER LAYER TEMPERATURE (°C)

TIME (s)

INTERFACE HEIGHT (m)

TIME (s)

2.5

0

0   900   1800

Ceiling

205 Corridor – 100 kW

––Experiment

——Theory

(15%)

57
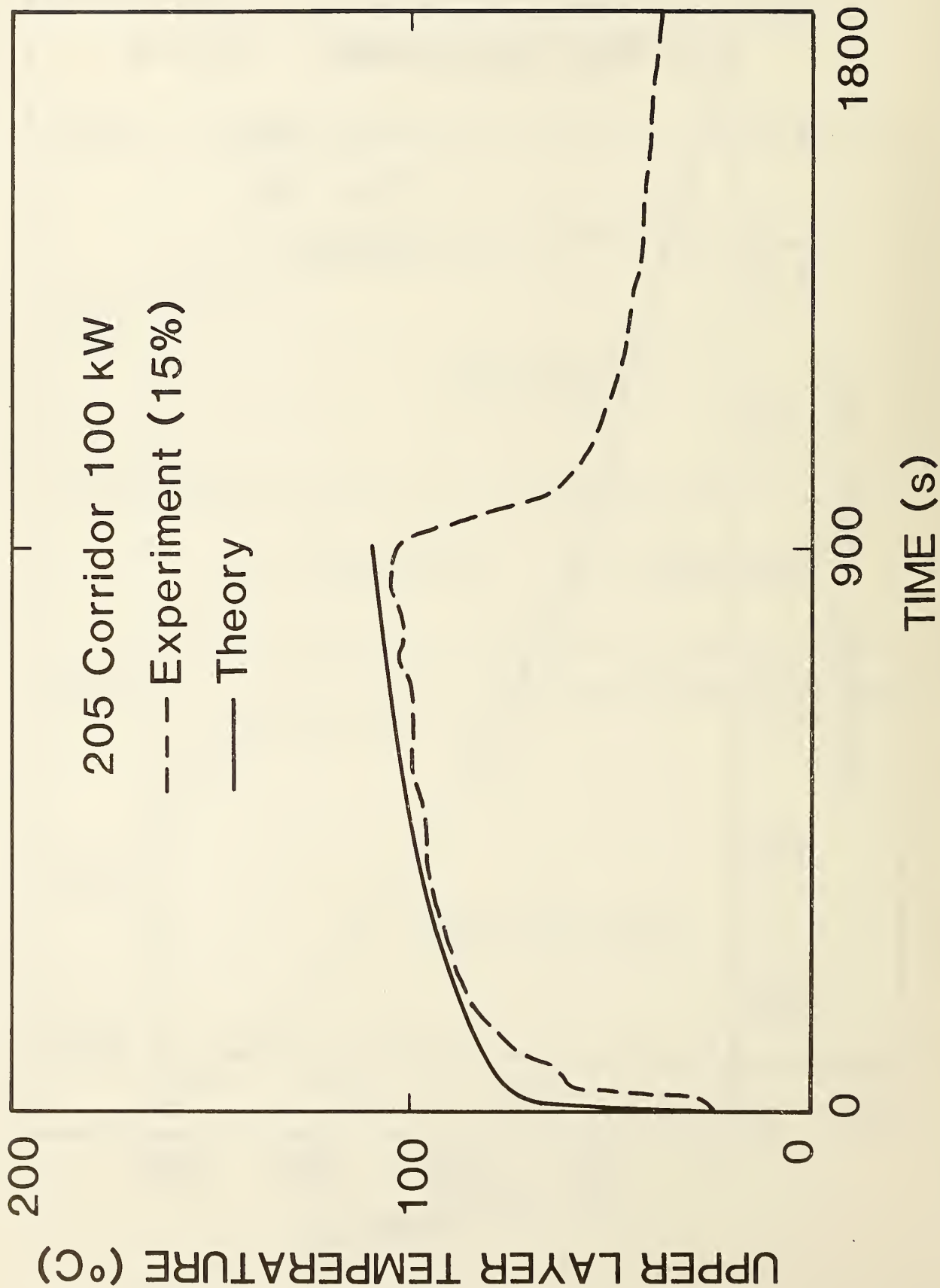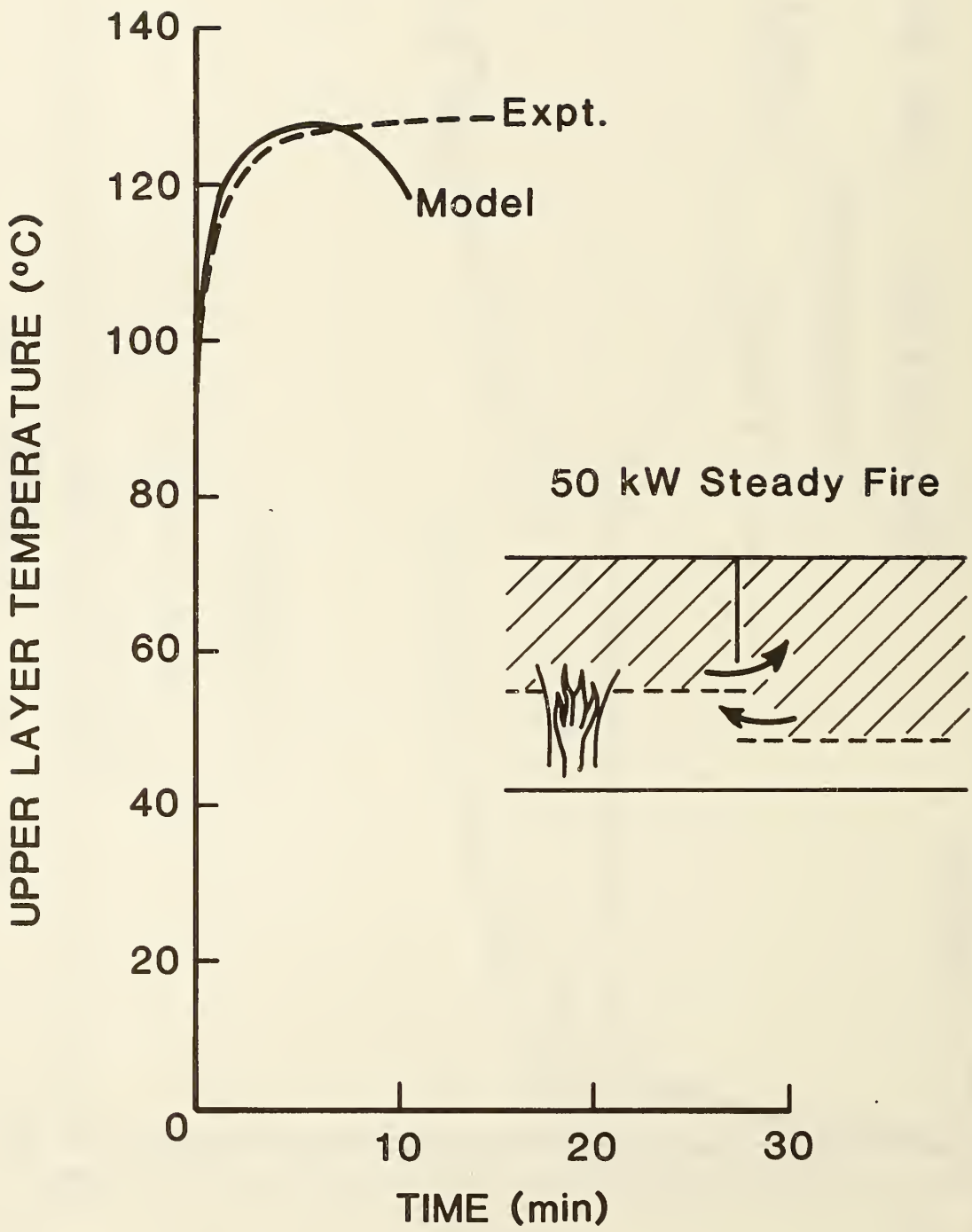
A sample fire interval ($I_1 - I_5$) production curve which requires six end points ($E_1 - E_6$) — See Appendix B

MASS LOSS RATE (kg/s)

1×10^{-4}

1×10^{-3}

TIME (s)

E_1 60 I_1 E_2 30 I_2 E_3 120 I_3 E_4 45 I_4 E_5 60 I_5 E_6

4. TITLE AND SUBTITLE

A Model for the Transport of Smoke, Fire and Toxic Gases (FAST)

5. AUTHOR(S)

Walter W. Jones

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 numerical implementation of a zone model which will transport fire, smoke and toxic gases in a multi-compartment structure is described. The areas covered are the equations which are solved, the numerical technique for the solution of these equations, species transport and the other relevant physical phenomena which govern fire growth and spread, and the transport of smoke. Also included in the model are the calculations necessary for a toxic hazard evaluation of a structure with a specific material loading. Forced ventilation is not yet included (version 15).

A machine readable copy of the model (FAST) is available through NTIS. The tape includes the data file listed in the appendices of this report.

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

Fire growth; mathematical models; smoke spread; toxic hazard; zone models.