



United States Department of Commerce National Institute of Standards and Technology

NIST PUBLICATIONS

NIST Technical Note 1282

Refinement of a Model for Fire Growth and Smoke Transport

Walter W. Jones

QC 100 .U5753 #1282 1990 C.2



NIST Technical Note 1282

Refinement of a Model for Fire Growth and Smoke Transport

Walter W. Jones

Center for Fire Research National Engineering Laboratory National Institute of Standards and Technology Gaithersburg, MD 20899

November 1990



U.S. Department of Commerce Robert A. Mosbacher, Secretary

National Institute of Standards and Technology John W. Lyons, Director

National Institute of Standards and Technology Technical Note 1282 Natl. Inst. Stand. Technol. Tech. Note 1282 50 pages (Nov. 1990) CODEN: NTNOEF

U.S. Government Printing Office Washington: 1990

For sale by the Superintendent of Documents U.S. Government Printing Office Washington, DC 20402

CONTENTS

1. INTRODUCTION	1
2. SOURCE TERMS 2.1 Hydrogen Chloride Deposition 2.2 Chemistry 2.3 Mechanical Ventilation	4 4 6 9
3. SOURCE MODULES 3.1 Hydrogen Chloride Deposition 3.2 Chemistry 3.3 Mechanical Ventilation	13 13 15 18
4. DESCRIPTION OF THE DATA FILE USED BY FAST	26
5. EXAMPLE OF HYDROGEN CHLORIDE DEPOSITION AND MECHANICAL VENTILATION	31
6. ERRATA for "Technical Reference Guide for FAST Version 18"	34
7. NOMENCLATURE	36
8. REVISION HISTORY	38
9. REFERÈNCES	45
10. ACKNOWLEDGMENTS	46
LIST OF FIGURES	
Figure 1. Fraction, (1.0-EXP(-10.0*O2INDEX)), as a function of oxygen and its limiting index. Figure 2. Node arrangement for example 2. Figure 3. Plan diagram of the geometry used in the HCl deposition calculation. Figure 4. HCl. concentration in the lower layer of compartments 2 and 3	29 32

THIS PAGE INTENTIONALLY LEFT BLANK

Refinement of a Model for Fire Growth and Smoke Transport

Walter W. Jones

Center for Fire Research
National Institute of Standards and Technology

This document describes the changes which have occurred in FAST, FASTplot, FAST_in and the distribution disks in the change from 18.3, the release for Hazard I, and the current release 18.5. Included are an errata section for the Technical Note 1262, a revision history that is distributed with the release disks, the addendum to the Technical Note for the new key words, and the description of the implementation of the physical routines.

Key words: compartment fires; fire growth; mathematical models; numerical models; room fires; smoke; toxicity

1. INTRODUCTION

This report describes additional features in the FAST model, and corrections to the Technical Reference Guide for FAST [1]. In addition, in the appendix there is a list of the revision history for this version of the model. This publication is not intended to stand alone. A presumption is made that the reader is familiar with FAST, the technical publications which describe the underpinnings, and the Technical Reference Guide.

The original Technical Reference Guide described the basis of the model, the data file used by the model, and described the ancillary modules which are used in conjunction with the model to provide a complete system for modeling fire growth and smoke spread. Since that publication, several algorithms have been added, and the purpose of this report is to document them. We have attempted to use a style similar to the earlier work.

Two phenomena which have been added are forced ventilation and deposition of hydrogen chloride on material surfaces. Also, a more general chemistry scheme is now included which allows for oxygen and chlorine in the fuel. There have also been a series of improvements and fixes in the software. These latter are documented in the section on the revision history. Mechanical ventilation was added in a manner similar to conduction of heat through surfaces and objects, and it will be described as a normal source term. The mechanical ventilation is based on a large body of knowledge and experience which is derived

from the extensive work on development of heating, ventilation and airconditioning systems. Likewise, the hydrogen chloride work is based on standard experimental techniques, but the actual number of such measurements is small. Thus data exist only for a few materials.

We have used the concept of time splitting in several places. With this concept, we can break out the phenomena which occur on widely varying times scales and solve them separately. We have used this concept in several places throughout the numerical implementation of FAST. For example, the time scale for a chemical reaction is normally much shorter than the time associated with gas flow, namely the number of air changes per hour in a compartment. This is reasonable in that typical kinetic time scales are on the order of milliseconds, whereas volumetric changes due to flow are on the order of tenths of seconds. It is certainly possible to violate these precepts. For example, we are precluded from modeling detonation. For a fan system, there is an implicit assumption that the inertia in the system, and the friction in the duct work will cause a significant delay between a pressure rise in a compartment and the effects on the ventilation system. The time step appropriate to this concept is 0.1 s, at least for this model. On such a time scale, wall temperatures will not change appreciably, and flow in ducts will not be altered very much.

In keeping with the original work, this document first describes the basis for the added phenomena and the equations which are used by the model. The second section is an annotated listing of the software used to implement these equations. The third section describes the changes in the data file as used by the "core" model. Finally, an example is shown which emphasizes the new features.

We have changed or added three features of the model: the chemistry, mechanical ventilation and the dynamics of a gas-surface interaction. These three phenomena represent extremes in phenomenology of modeling in general:

The chemistry algorithm results simply from a molecular balance. As such there is no assumption, nor any approximations. We have ignored species which are truly minor, such as argon. Also, the most difficult aspect of fire related kinetics has not been addressed in this implementation. The carbon monoxide-carbon dioxide ratio has been left as a parameter. It is incorporated in such a way that converting to an explicit scheme is easy, but as yet, there is not sufficient knowledge to do this.

For the mechanical ventilation, the formulae come from well established practice with ventilation systems. We have instantiated an ability to calculate ventilation much more precisely than measurements are made.

Finally, the wall deposition phenomena present in the hydrogen chloride algorithm has been established with only a few measurements. More experimental work needs to be performed to establish confidence in the coefficients, and indeed to established these coefficients for a wide range of materials.

One fact has become apparent. It is that we are able to predict, run parameter studies and so on much more readily and widely than can be calibrated experimentally. Indeed, one of the seductive features of such a model, is that it is possible to perform calculations for situations for which measurements are not practical. Thus validation of the various parts of the model is extremely important.

2. SOURCE TERMS

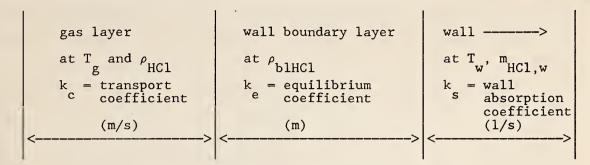
The conserved quantities, pressure, mass, etc., in each compartment are described by the set of predictive equations discussed by Jones [2] and Jones and Peacock [1]. The form of the equations is such that the physical phenomena are source terms on the right-hand-side of these equations. Such a formulation makes the addition (and deletion) of physical phenomena and changing the form of algorithms a relatively simple matter. We have added two phenomena by adding the appropriate source terms to the predictive equations. These are deposition of hydrogen chloride on surfaces and mechanical ventilation. The former has been added using an analogy with convective heat transfer.

Finally, the chemistry scheme has been changed to reflect more accurately the actual kinetics processes which take place. This change does not require any changes in external files, but it is important to understand what is taking place internal to the model, in order to interpret the results properly. In the previous version of the model, chlorine and "cyanide" were treated as minor species and the fuel was assumed to be devoid of oxygen. These simplifications have been remedied.

2.1 Hydrogen Chloride Deposition

Production of hydrogen chloride from a fire can result in a serious toxicity problem. It has been shown [3] that significant amounts of the substance can be removed by adsorption by surfaces which contact smoke. In our model, HCl production is treated like any other species (for details, see the section on chemistry). However, an additional term is required to allow for deposition on, and subsequent absorption into, material surfaces.

The physical configuration that we are modeling is a gas layer, either the upper or lower zone, adjacent to a surface, such as a wall. A gas layer is at some temperature T_g with a concomitant density of hydrogen chloride, ρ_{HCl} . The mass transport coefficient is calculated based on the Reynolds analogy with mass and heat transfer: that is, hydrogen chloride is mass being moved convectively in the boundary layer, and some of it simply sticks to the wall surface rather than completing the journey during the convective roll-up associated with eddy diffusion in the boundary layer. The boundary layer at the wall is then in equilibrium with the wall. The latter is a statistical process and is determined by evaporation from the wall and stickiness of the wall for HCl molecules. This latter is greatly influenced by the concentration of water in the gas, in the boundary layer and on the wall itself.



Schematic of hydrogen chloride deposition region

The rate of addition of mass of hydrogen chloride to the gas layer is given by

$$\frac{d}{dt}m_{HCl} = source - k_c \times (\rho_{HCl} - \rho_{blHCl}) \times A_w$$
 (1)

where source is the production rate from the burning object plus flow from other compartments. For the wall concentration, the rate of addition is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}_{\mathrm{HCl,w}} = \mathrm{k_c} \times \left(\rho_{\mathrm{HCl}} - \rho_{\mathrm{blHCl}}\right) - \mathrm{k_s} \times \mathrm{m_{HCl,w}} \tag{2}$$

where the concentration in the boundary layer, ρ_{blHCl} , is related to the wall surface concentration by the equilibrium constant k_e ,

$$\rho_{\text{blHCl}} = d_{\text{HCl},w} / k_e. \tag{3}$$

We never actually solve for the concentration in the boundary layer, but it is available, as is a boundary layer temperature if it were of interest. The transfer coefficients are

$$k_{c} = \frac{\dot{q}}{\Delta T \times \rho_{g} \times c_{p}} \tag{4}$$

$$k_{e} = \frac{b_{1} \times e^{\frac{1500}{T_{w}}}}{1 + b_{2} \times e^{\frac{1500}{T_{w}}} \times \rho_{hcl}} \times \left(1 + \frac{b5 \times \rho_{H_{2}O}^{b6}}{\left(\rho_{H_{2}O,sat} - \rho_{H_{2}O,g}\right)^{b7}}\right)$$
(5)

$$k_s = b_3 \times \exp^{-\left(\frac{b4}{R T_w}\right)}. \tag{6}$$

The only values currently available [4] for these quantities are

Surface	b ₁	b ₂	b ₃	b ₄	b ₅	b ₆	b ₇
units ->	m	m ³ /kg	s ⁻¹	J/g-mol	*		
Painted Gypsum	0.0063	191.8	0.0587	7476.	1.38	1.021	0.431
PMMA	9.6×10 ⁻⁵	0.0137	0.0205	7476.	0.19	1.0	0.431
Ceiling Tile	4.0×10 ⁻³	0.0548	0.123	7476.	0.2**	1.0	0.431
Cement Block	1.8×10 ⁻²	5.48	0.497	7476.	0.2**	1.0	0.431
Marinite tm	1.9×10 ⁻²	0.137	0.030	7476.	0.2**	1.0	0.431

These "b" coefficients are parameters which are found by fitting experimental data to equations (1) through (6). These coefficients reproduce the adsorption and absorption of HCl very well. The concept has not yet been tested in a wide variety of experiments, nor a wide variety of materials, so the accuracy of the general concept has not yet been determined.

2.2 Chemistry

The essence of the change in the chemistry scheme is to allow for a more realistic fuel composition, *i.e.*, include oxygen and chlorine as part of the fuel. The key words have not changed, but one of them has a new meaning. The oxygen parameter, O2, now refers to the ratio of the mass of oxygen in the fuel to the total fuel mass being pyrolized.

The fuel burning rate in terms of the carbon production is

$$\Delta m_f = \{-\} \times \Delta m_c \tag{7}$$

where {-} is the multiplier in the fuel production

$$\{-\} = \left(1 + \frac{H}{C} + \frac{HCI}{C} + \frac{HCN}{C} + \frac{O}{C}\right) \equiv f/C. \tag{8}$$

The following definitions are for the heat release rate as a function of the fuel pyrolysis rate, and the heat release rate based on oxygen consumption. H/C, HCl/C, HCN/C and O/C are the ratio of that species to carbon in the fuel. The key words [1] associated with these ratios are HCR, HCl, HCN and O2 respectively. The HCl and HCN key words refer to the ratio of that

^{*} $(m^3/kg)^(b_7-b_6)$

^{**} Very approximate - insufficient data for high confidence value

species to the fuel, that is HCN/f and HCl/f. The relationship will be discussed later. Note that the subscript "S" is used to designate soot, and we assume it consists primarily of carbon.

$$\Delta Q = \Delta m_f \times h_c \tag{9}$$

$$\Delta m_0 = -\frac{\Delta Q}{1.32 \times 10^7} \tag{10}$$

$$\Delta m_{O}(\text{needed}) = \Delta m_{O} - \Delta m_{O}(\text{in the fuel})$$
 (11)

$$\Delta m_0 = \Delta m_f \times \frac{h_c}{1.32 \times 10^7}, \text{ and}$$
 (12)

$$\Delta m_o(\text{actual}) - \text{minimum of } \{\Delta m_o(\text{available}), \Delta m_o(\text{needed})\}$$
 (13)

Essentially, we limit the amount of fuel that is burned, as opposed to the amount that is pyrolyzed, to the lesser of the amount pyrolyzed and that required to consume the *available* oxygen. The $\Delta m_O(actual)$ is the quantity used below. (See sect. 3.2 for an additional discussion whereby this term is calculated.)

We begin with the mass balance equation. The mass consumed as pyrolyzate plus oxygen must reappear as product. The terms in parenthesis are the ratios of the masses of the species shown. For example, (HCl/C) is the relative production rate of hydrogen chloride to fuel carbon pyrolysis.

$$\Delta m_{f} + \Delta m_{o} = \Delta m_{f} + \Delta m_{f} \times \frac{h_{c}}{1.32 \times 10^{7}} - \frac{\Delta m_{f}}{\{-\}} \times \left(\frac{O}{C}\right)$$

$$= \Delta m_{CO_{2}} + \Delta m_{CO} + \Delta m_{S} + \Delta m_{H_{2}O} + \Delta m_{HCI} + \Delta m_{HCN}$$
(14)

We then substitute the following definitions of mass produced of each species based on the amount of carbon (ala. fuel) consumed as

$$\Delta m_{HCl} = \left(\frac{HCl}{C}\right) \times \Delta m_C \rightarrow \left(\frac{HCl}{f}\right) \times \Delta m_f$$
 (15)

$$\Delta m_{HCN} = \left(\frac{HCN}{C}\right) \times \Delta m_{C} \rightarrow \left(\frac{HCN}{f}\right) \times \Delta m_{f}$$
 (16)

$$\Delta m_{H_2O} = \left(\frac{H_2O}{H_2}\right) \times \left(\frac{H}{C}\right) \times \Delta m_C = 9 \times \left(\frac{H}{C}\right) \times \Delta m_c \rightarrow 9 \times \left(\frac{H}{C}\right) \times \frac{\Delta m_f}{\{-\}}$$
(17)

$$\Delta m_{CO_2} = \left(\frac{CO_2}{C}\right) \times \Delta m_C \tag{18}$$

$$\Delta m_{S} = \left(\frac{S}{C}\right) \times \Delta m_{C} = \left(\frac{CO_{2}}{C}\right) \times \left(\frac{S}{CO_{2}}\right) \times \Delta m_{C} \rightarrow \left(\frac{S}{CO_{2}}\right) \times \Delta m_{CO_{2}}$$
(19)

$$\Delta m_{CO} = \left(\frac{CO}{C}\right) \times \Delta m_{C} = \left(\frac{CO_{2}}{C}\right) \times \left(\frac{CO}{CO_{2}}\right) \times \Delta m_{C} - \left(\frac{CO}{CO_{2}}\right) \times \Delta m_{CO_{2}}.$$
 (20)

Substituting the above definitions into the mass balance equation yields:

$$\left(\frac{\text{CO}_2}{\text{C}}\right) = \frac{\{-\} \times \left(1 + \frac{h_c}{1.32 \times 10^7} - \frac{\text{O/C}}{\{-\}}\right) - \left(\frac{\text{HCl}}{\text{C}} + \frac{\text{HCN}}{\text{C}} + \frac{\text{H}}{\text{C}}\right)}{\left(1 + \frac{\text{S}}{\text{CO}_2} + \frac{\text{CO}}{\text{CO}_2}\right)}.$$
(21)

With this definition, we can substitute back into the equation for carbon dioxide production, which yields

$$\Delta m_{CO_2} = \Delta m_f \times \frac{\left(1 + \frac{h_c}{1.32 \times 10^7} - \frac{O/C}{\{-\}}\right) - \left(\frac{HCl}{C} + \frac{HCN}{C} + \frac{H}{C}\right) \{-\}}{\left(1 + \frac{S}{CO_2} + \frac{CO}{CO_2}\right)}.$$
 (22)

We can now substitute this equation back into equations (19) and (20) to find the soot and carbon monoxide production. The form in which we cast these equations evolves naturally from the properties of combustion. Hydrogen, carbon and bound oxygen are properties of the fuel. They can be measured experimentally independent of the combustion process. Thus we use these ratios as the basis of the scheme. In a similar sense, hydrogen chloride and hydrogen cyanide are properties of the pyrolysis process. So hydrogen chlorine and hydrogen cyanide production are specified with respect to the fuel pyrolysis. Normally this is how they are measured, for example with the cone calorimeter, so we can use the measured quantities directly. Other than the cyanide, chloride and water production, hydrogen does not play a role. In general, hydrogen has much more of an affinity for oxygen than carbon, so almost all of the hydrogen will be utilized. This dictates our next choice, which is that soot is essentially all carbon. On a mass basis this is certainly true. On a molecular basis, however, it may not be so simple. Carbon dioxide is a direct product of combustion, and the assumption is that most carbon will end up here. Carbon monoxide and soot are functions of incomplete combustion. Thus they depend on the environment in which the burning takes place. They are in no case a function of the pyrolysis process itself. Thus the production of these products are specified with respect to the carbon dioxide. At present, we must rely on measured ratios, but this is beginning to change as we gain a better understanding of the

combustion process. So carbon goes to one of three final species, carbon dioxide, carbon monoxide or soot, with the particular branching ratio depending on the chemistry active at the time.

Equations (15) and (16) are used in terms of the carbon production. We now need to recast HCl and HCN in terms of fuel production rather than carbon production, since that is how they are measured. Since HCl and HCN are similar, we will just make the argument for one, and then assume that the derivation is the same. One simplification will be possible for the HCN though, and that is that its production rate is *always* much less than the pyrolysis rate.

Since {—} is just f/C,

$$\left(\frac{HCl}{C}\right) = \left(\frac{HCl}{f}\right) \times \left(1 + \frac{H}{C} + \frac{HCl}{C} + \frac{HCN}{C} + \frac{O}{C}\right). \tag{23}$$

Therefore

$$\left(\frac{HCl}{C}\right) = \left(\frac{HCl}{f}\right) \times \left(\frac{1 + \frac{H}{C} + \frac{O}{C}}{1 - \left(\frac{HCl}{f}\right)}\right),$$
(24)

and for hydrogen cyanide we have

$$\left(\frac{HCN}{C}\right) = \left(\frac{HCN}{f}\right) \times \left(1 + \frac{H}{C} + \frac{HCI}{C} + \frac{O}{C}\right). \tag{25}$$

In these latter cases, we assume that the cyanide ratio (HCN/C) is small compared to unity. It is the HCl/C and HCN/C ratios which are used by the model.

In summary, we can predict the formation of products of combustion, carbon dioxide, carbon monoxide, soot, water, cyanide, and hydrogen chloride given the branching ratios CO/CO₂, S(soot)/CO₂ and the composition of the fuel, H/C, O/C, HCl/f and HCN/f.

2.3 Mechanical Ventilation

The model for mechanical ventilation is based on the theory of networks. This is a simplified form of Kirchoff's law which says that flow into a node must be balanced by flow out of the node. There is a close analog to electrical networks for which the flow consists of electrons. In the case of ventilation, the flow is formed by molecules of air. The conservation equation differs slightly from that of an electrical system, but the basic ideas carry over. The former case, we have

voltage = current \times resistance.

In the present case we have

pressure change = mass flow \times mass flow \times resistance.

So the application of network theory is used, although the circuit laws are slightly different. In practice, as with the electrical analog, one solves the problem by summing all of the equations for the nodes, and require that the mass be conserved at each node. Thus we turn the equation around and put it into the form

mass flow = conductance \times (pressure drop across a resistance)^{1/2}.

For each node, this flow must sum to zero. There are several assumptions which are made in computing this flow in ducts, fans, elbow, etc. First, we assume unidirectional flow. Given the size of ducts, and the nominal presence of fans, this is quite reasonable. Second, in the conservation law for energy, there is a work term which describes compression or expansion of a volume. There is no such analogous term in the solution of the mass flow equations for ventilation. This is reasonable so long as a ventilation system is not being used to increase or decrease the pressure within a structure. It is still acceptable for connecting systems at different pressures. Further, the effect that a change in pressure within a duct has on the flow characteristics is likewise ignored. Once again, for most of the cases of interest this is a reasonable assumption. Finally, the particular implementation used here [5] does not allow for reverse flow in the duct system. The difficulty lies in describing how a fan behaves in such a case.

Given that we can describe mass flow in terms of pressure differences and conductance, the conservation equation for each node is

$$\sum_{\mathbf{j}} \dot{\mathbf{m}}_{\mathbf{i},\mathbf{j}} = 0. \tag{26}$$

The index "j" is a summation over connections to a node, and there is an equation "i" for each node. The remaining problem is to specify the boundary conditions. At each connection to a compartment, the pressure is specified. Then, given that flow is unidirectional, the mass and enthalpy flow into or out of a room can be calculated explicitly. Thus we end up with a set of equations of the form

$$f_{1}(P_{1},P_{2}, ...) = 0$$

$$f_{1}(P_{1},P_{2}, ...) = 0$$

$$f_{1}(P_{1},P_{2}, ...) = 0$$

$$f_{1}(P_{1},P_{2}, ...) = 0.$$
(27)

This is an algebraic set of equations that is solved simultaneously with the equations for flow in the compartments.

The equations describe the relationship between the pressure drop across a duct, the resistance of a duct, and the mass flow. The pressure can be changed by conditions in a compartment, or a fan in line in the duct system. Resistance arises from the finite size of ducts, roughness on surfaces, bends and joints. To carry the electrical analog a little further, fans act like constant voltage sources. The analogy breaks down, however, in that the voltage, current and resistance are related by the square of the current, rather than being linearly proportional. Since we are using the current form of the conservation equation to balance the system, recast the flow in terms of a conductance

$$\dot{\mathbf{m}} = \mathbf{G} \times \sqrt{\Delta \mathbf{P}}.\tag{28}$$

The conductance can be expressed generally as

$$G = \left(\frac{2 \rho}{C_0}\right)^{1/2} A_0 \tag{29}$$

where C_0 is the flow coefficient (usually a loss term), and A_0 is the area of the inlet, outlet, duct, contraction or expansion joint, coil, damper, bend, filter, and so on. Their values for the most common of these items are tabulated in the ASHRAE Handbook [6].

Ducts are long pipes through which gases can flow. They have been studied much more extensively than other types of connections. For this reason, eq (30) can be put into a form which allows one to characterize the conductance in more detail, depending on the type of duct, such as oval, round, square, and so on. The form derives from the Darcy equation and is

$$G = \left(\frac{F L}{2 \rho D_e A_0^2}\right)^{1/2},\tag{30}$$

where F is the friction factor and can be calculated from

$$\frac{1}{\sqrt{F}} = -2 \log \left(\frac{\epsilon}{3.7 D_e} + \frac{2.51}{R_e \sqrt{F}} \right). \tag{31}$$

For each node in the system, one has an entry of the form of eq (29). This set of equations is then solved at each time step. In the present form, the solution to the duct system is split from that of the buoyancy driven flow. This is justified based on the long time constant for change of the flow pattern in such a system. Implicit in this assumption is that there is only a very weak interaction between the systems of equations. When we begin to deal with the problem of flow reversal then the fan characteristics will be coupled much more closely with the buoyancy driven flow and we will have to reformulate the solution.

3. SOURCE MODULES

The routines described below come directly from the FAST program. The modules have been annotated to make them more understandable. For example, comments within the code which are directives for changing the routines are not included. There are also comments which appear here which are not shown in the actual code. The part that is strictly in upper case is FORTRAN code, whereas text in lower or mixed case are extra comments.

3.1 Hydrogen Chloride Deposition

```
SUBROUTINE HC1TRAN (LAYER, COMP, ARW, TG, TW, HWDOT, NWW)
       FAST COMMON BLOCK GOES HERE
C
       LAYER IS UPPER OR LOWER
С
       COMP IS THE COMPARTMENT NUMBER (1 to nr)
С
       ARW IS THE AREA OF THE WALL (DSOURC ACEILI, AUPPER, ALOWER, AFLOOR)
С
       TG IS THE RELEVANT GAS TEMPERATURE
С
       TW IS THE CORRESPONDING WALL TEMPERATURE
C
       HWDOT IS THE WALL CONCENTRATION DERIVATIVE
CCCCC
       THE GAS LAYER DERIVATIVE IS CALCULATED GLOBALLY AS NETMAS
       NWW IS THE WALL NUMBER 1=>CEILING,
       HC1G IS THE GAS PHASE DENSITY (KG/M<sup>2</sup>)
HC1W IS THE WALL DENSITY (KG/M<sup>2</sup>)
RK IS THE CONSTANT "kc" WHICH IS THE DEPOSITION COEFFICIENT (M/S)
RKE IS THE EQUILIBRIUM COEFFIENT BETWEEN THE GAS AND SOLID (WALL)
С
       H2OS IS SATURATION CONCENTRATION, AND H2O CURRENT CONCENTRATION
       INTEGER COMP
C
the following section sets the environment variables
       IF (LAYER. EQ. UPPER) THEN
           CVOL = P(COMP+N2)
       ELSE
           CVOL = MAX(VR(COMP) - P(COMP+N2), PMIN(COMP+N2))
       HClg = MASS(LAYER, COMP, 6) / CVOL
       HC1F = HC1G * TG * 2.25E-3
       HC1P = HC1F * 1.0E6
       HClW = HWJ(NWW,COMP)
       RHO = (RAMB(COMP) * TAMB(COMP)) / (PAMB(COMP) + POFSET)
            * (P(COMP)+POFSET)/TG
       FLUX = QSCNV(NWW, COMP)
       H2O = MASS(LAYER, COMP, 8) / CVOL
       TWC = TW - 273.15
```

the transfer coefficients are kept in the thermophysical data base, and are read in by NPUTT

```
B1 = HC1BF(1,NWW,COMP)

B2 = HC1BF(2,NWW,COMP)

B3 = HC1BF(3,NWW,COMP)

B4 = HC1BF(4,NWW,COMP)

B5 = HC1BF(5,NWW,COMP)

B6 = HC1BF(6,NWW,COMP)

B7 = HC1BF(7,NWW,COMP)
```

if properties are not specified, then we assume no deposition

```
IF (B1.LE.O) THEN
HWDOT = 0.0
RETURN
ENDIF
```

calculate HCl gas-surface partition coefficient, where H₂O is the saturation pressure of water and bcoef is the convective transfer coefficient

```
TWC2 = TWC * TWC
TWC3 = TWC2 * TWC
HC1F2 = HC1F * HC1F
HC1F3 = HC1F2 * HC1F
IF (TWC .LE. 40.) THEN IF (HC1P .GT. 10.) THEN
      H2OS = (1.8204 - 0.18890 * LOG(HC1P)
            + 0.06466*TWC + 1.650E-3*TWC2 + 7.408E-5*TWC3) / TW
   ELSE
      EXPTW = EXP(17.64262-5164.1/TW)
      BCOEF = (7.696E-5 + 3.5920E-6*TWC)
             + 9.166E-8*TWC2+4.116E-9*TWC3)
             / TW-1.E-7*EXPTW
      H2OS = 0.018 \times EXPTW + 1.8E4 \times BCOEF \times HClP
   ENDIF
ELSEIF ((TWC.GT.40.0).AND.(TWC.LE.60.0)) THEN
   HC1F4 = HC1F2 * HC1F2
   HC1F5 = HC1F4 * HC1F
   H2OS = (7.044 - 2.2416E3*HC1F - 3.874E-3*TWC2 + 2.328E-4*TWC3
        + 2.376E6*HC1F2 - 5.527E8*HC1F3 + 4.918E10*HC1F4
- 1.359E12*HC1F5 - 1.4033E2*TWC*HC1F + 2.431E4*TWC*HC1F2
         - 1.6023E6*TWC*HC1F3) / TW
ELSEIF ((TWC.GT.60.0).AND.(TWC.LE.80.0)) THEN
   HC1F4 = HC1F2 * HC1F2
   HC1F5 = HC1F4 * HC1F
   H2OS = (107.46 - 4.129*TWC + 5.096E-2*TWC2 - 3.1915E8*HC1F3
        + 1.0408E10*HC1F4 - 2.2793E11*HC1F5 - 5.8194*TWC2*HC1F
        + 7.6883E4*TWC*HC1F2 - 7.4363E2*TWC2*HC1F2
        + .059067*TWC3*HC1F + 1.8132E6*TWC*HC1F3) / TW
ELSEIF ((TWC.GT.80.0).AND.(TWC.LE.95.0)) THEN
   HC1F4 = HC1F2 * HC1F2
   HC1F5 = HC1F4 * HC1F
   H2OS = (2.583E2 - 8.0386*TWC + 1.739E5*HC1F + 7.608E-2*TWC2
         - 1.5492E7*HC1F2 + 3.956E9*HC1F3 - 2.065E11*HC1F4
        + 1.3747E13*HC1F5 - 4.086E3*TWC*HC1F + 24.06*TWC2*HC1F
        + 1.3558E5*TWC*HC1F2 - 3.076E7*TWC*HC1F3) / TW
ELSEIF ((TWC.GT.95.0).AND.(TWC.LE.110.0)) THEN
```

```
H2OS = (6.431E2 - 16.374*TWC + 2.822E5*HC1F + 0.12117*TWC2
               - 8.224E7*HC1F2 - 7.387E6*HC1F3 - 5.247E3*TWC*HC1F
               + 24.30*TWC2*HC1F + 1.5465E6*TWC*HC1F2
               - 7.250E3*TWC2*HC1F2) / TW
      ELSEIF (TWC.GT.110.0) THEN
         H2OS=0.2885*EXP(18.3036-3816.44/(TW-46.13))/TW
          STOP 'Error in hcltran - h2o out of range'
      ENDIF
      CALCULATE THE COEFFICIENTS, FIRST THE CONVECTIVE COEFFICIENT RK, THEN
С
      THE MASS TRANSFER (EQUILIBRIUM) COEFFICIENT, RKE
      IF (TW .GE. TG) THEN
         RK = 8.33E-3
      ELSE
         RK = ABS(FLUX/(MAX(0.001, TG-TW)*RHO*CP))
      ENDIF
      IF (H2OS.GT.H2O) THEN
          EXPTW = EXP(1500/TW)
         RKE = B1 * EXPTW/(1.+B2*EXPTW*HC1G)
              * (1.+B5*H20**B6/((H2OS-H2O)**B7))
      ELSE
         RKE = 1.0E4
      ENDIF
C
      CALCULATE THE DERIVATIVES
      HC1COF = RK * (HC1G - HC1W/(RKE+1.E-20))
      NETMAS(LAYER, COMP, 6) = NETMAS(LAYER, COMP, 6) - HC1COF * ARW HWDOT = HC1COF - B3 * EXP(-B4/(8.31*TW)) * HC1W
      RETURN
      END
```

3.2 Chemistry

CHEMIE is the routine which calculates the heat release rate and species production as described in section 2.2. It has been changed by incorporating the above formulae. The primary input is the mass pyrolysis rate, and the primary output is the heat generation rate. This routine is only used for a type 2 (constrained) fire.

```
SUBROUTINE CHEMIE (QPYROL, PYROL, ENTRAIN, NETFUEL, TARGET, LAYER, HCRATT, OCRATT, CCO2T, COCO2T, CLFRAT, CNFRAT)
```

"pyrol" is the mass pyrolysis rate from the PYROL routine, and apyrol the heat generation rate, "entrain" is the entrainment rate (we are dealing with diffusion limited combustion) and "netfuel" is the fuel *actually* burned as opposed to the possible "pyrol" value. "netxx" then are the species production rates, based on the formulae discussed in section 4.5.

FAST COMMON BLOCK GOES HERE

```
. NETCN, TMASS, NETFUL, XMASS(NS)
       EQUIVALENCE (NETO2, XMASS(2)), (NETCO2, XMASS(3)), (NETCO, XMASS(4)),
      . (NETFUL, XMASS(7)), (NETH2O, XMASS(8)), (NETC, XMASS(9)), (NETCD, XMASS(5)), (NETCL, XMASS(6))
       INTEGER SOURCE, TARGET
DATA XMASS/NS*0.0/, 02F/1.32E+7/, 02FI/7.578E-8/
"source" specifies the compartment of origin of the flow, and "layer" is the corresponding layer
from which the fuel and oxygen originate.
       SOURCE = TARGET
       TMASS = 0.0
       DO 2 LSP = 1, 9
     2 TMASS = TMASS + MASS(LAYER, SOURCE, LSP)
       TMASS = MAX (TMASS, MINMAS)
       O2FRAC = MASS(LAYER, SOURCE, 2) / TMASS
       O2ENTR = ENTRAIN * O2FRAC
       ALPHA = 1. / ( 0.207 - MIN(0.20, LIMO2))

02INDEX = MAX(0., (02FRAC-LIMO2)*ALPHA)

02MASS = 02ENTR * (1.0-EXP(-10.0*02INDEX))

00STOK = 13200000. / HCOMBA

QPYROL = MAX(0., MIN(PYROL, OOSTOK*02MASS)) * HCOMBA
       NETFUEL = QPYROL / HCOMBA
       THIS IS THE REAL KINETICS SCHEME AS DRIVEN BY DIFFUSION
       FIRST CONVERT CHLORINE AND CYANIDE PRODUCTION TO CARON BASED RATIOS
       CLCRAT = CLFRAT * (1.0+HCRATT+OCRATT)/(1.0-MIN(0.99999,CLFRAT))
CNCRAT = CNFRAT * (1.0+HCRATT+OCRATT)
       FCRATT = (1.0 + OCRATT + HCRATT + CLCRAT + CNCRAT)
       NETFUL = - NETFUEL
       NETO2 = - QPYROL * O2FI
       NOW DO THE "KINETICS SCHEME"
       NETH20 = 9.0 * NETFUEL * HCRATT / FCRATT
       FACTOR1 = 1.0 + HCOMBA*O2FI - OCRATT / FCRATT
       FACTOR2 = (CLCRAT + CNCRAT + HCRATT) / FCRATT
NETCO2 = (FACTOR1 - FACTOR2) * NETFUEL / (1.+COCO2T+CCO2T)
       NETCO = NETCO2 * COCO2T
                  NETCO2 * CCO2T
       NETC =
                  CLFRAT * NETFUEL
       NETCL =
       NETCN = CNFRAT * NETFUEL
     1 NETMAS(UPPER, TARGET, I) = NETMAS(UPPER, TARGET, I) + XMASS(I)
       NO POINT IN ENTRAINING FROM THE UPPER LAYER INTO THE UPPER LAYER
       IF (LAYER.EQ.UPPER) RETURN
       ADD IN THE FLOW ENTRAINED BY THE PLUME
       DO 8 LSP = 1, NS
```

REAL NETFUEL, NEWNET, NETH2O, NETCO2, NETCO, NETC, NETO2, NETCL.

*

C

С

C

IF (.NOT.ACTIVS(LSP)) GO TO 8

C PLUME CONTRIBUTION FOR ALL ENTRAINED GASES

NEWNET = ENTRAIN * MASS(LOWER, SOURCE, LSP) / OLDMAS(LOWER, SOURCE)
NETMAS(UPPER, TARGET, LSP) = NETMAS(UPPER, TARGET, LSP) + NEWNET
NETMAS(LOWER, TARGET, LSP) = NETMAS(LOWER, TARGET, LSP) - NEWNET
8 CONTINUE
RETURN
END

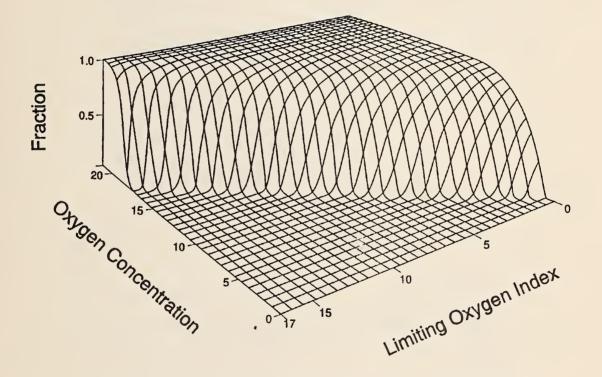


Figure 1. Fraction, (1.0-EXP(-10.0*O2INDEX)), as a function of oxygen and its limiting index.

The lines in the routine CHEMIE marked with an asterisk form the basis of the limit on the actual burning rate alluded to in section 2.2. The fourth line, for O2MASS, is a function of the limiting oxygen index and the percent of oxygen present in the environment. Figure 1 shows the fraction (1.0-EXP(-10.0*O2INDEX)). The oxygen concentration varies from 0% to 21%. The limiting oxygen index varies from 0% to 17%. Any cross section of this graph will be just like the curve discussed in the Technical Reference Guide [1]. Noteworthy, however, is the fact that as the two rates approach the high limit (21%), the curve steepens. This is an artifact of the approximation to the cutoff, and is not necessarily reflected in the reality of the chemistry being approximated.

3.3 Mechanical Ventilation

This is the internal part of the routine HVAC. It is the section that is called by the solver.

```
С
      GET STUFF FROM THE OUTSIDE WORLD
      CALL HVFREX
С
      DO THE MECHANICAL VENTILATION
      CALL HVMFLO
      CALL HVSFLO
C
      TELL THE WORLD WHAT HAS HAPPENED
      CALL HVTOEX
      RETURN
      END
      SUBROUTINE HVFREX
```

This routine retrieves data from the compartments and sets it up for the mechanical ventilation.

```
FAST COMMON BLOCKS GO HERE
   DO 10 II = 1, NEXT
      I = HVNODE(1, II)
      J = HVNODE(2, II)
      Z = ZZHLAY(I,LOWER)
      IF (HVELXT(II).LT.Z) THEN
          LAYER = LOWER
         ELSE
          LAYER = UPPER
      ENDIF
      ZL = MIN(Z, HVELXT(II))
XX0 = 0.0D0
      ZU = MIN(XXO, HVELXT(II) - ZL)
      RU = ZZRHO(I, UPPER)
      RL = ZZRHO(I,LOWER)
      HVP(J) = ZZRELP(I) - (RU*ZU + RL*ZL)*HVGRAV
IF (LAYER.EQ.LOWER) THEN
          HVEXTT(II) = ZZTEMP(I,LOWER)
          VLAYER = ZZVOL(I, LOWER)
         ELSE
          HVEXTT(II) = ZZTEMP(I, UPPER)
          VLAYER = ZZVOL(I, UPPER)
      DO 11 LSP = 1, NS
          IF (ACTIVS(LSP)) HVEXCN(II, LSP) = MASS(LAYER, I, LSP) / VLAYER
      CONTINUE
10 CONTINUE
```

11

RETURN END

SUBROUTINE HVTOEX

Assign results of hvac simulation to the transfer variables (hvextt, hvexcn).

```
FAST COMMON BLOCKS GO HERE
```

```
DO 10 II = 1, NEXT
       I = HVNODE(1, II)
       J = HVNODE(2, II)
       IB = ICMV(J, 1)
       Z = ZZHLAY(I, LOWER)
       IF (HVELXT(II).LT.Z) THEN
           LAYER = LOWER
           LLAYER = UPPER
          ELSE
           LAYER = UPPER
           LLAYER = LOWER
       ENDIF
       HVEFLO(LAYER, II) = HVFLOW(J,1)
HVEFLO(LLAYER, II) = 0.0D0
IF (HVFLOW(J,1) .GT. 0.0D0) THEN
           HVEXTT(II) = TBR(IB)
DO 11 K = 1, NS
               IF (ACTIVS(K)) HVEXCN(II,K) = HVCONC(IB,K)
11
           CONTINUE
       ENDIF
10 CONTINUE
   RETURN
   END
```

SUBROUTINE HVMFLO

Routine to calculate the mass flow thru a generic duct. The ducts have been "sanitized" by using coefficients from the ASHRAE handbook on ventilation, so all ducts,... look the same regardless of what the user thinks he is doing.

FAST COMMON BLOCK GOES HERE

```
LOGICAL CONV
INTEGER OUTITR, INITR, ITMAX
ITMAX=50
EPS=1.E-5
```

C CALCULATE AVERAGE TEMPERATURES AND DENSITIES FOR EACH BRANCH

```
DO 9 IB = 1, NBR
PAV = (HVP(NA(IB))+HVP(NE(IB)))/2. + POFSET
ROHB(IB) = PAV/(HVRGAS*TBR(IB))
9 CONTINUE
```

C START THE ITERATION CYCLE - ACTUALLY A PRETTY SIMPLE ITERATION SCHEME

```
OUTITR = 0
1 INITR = 0
irst section calcu
```

the first section calculates the resistivity due to various parts of the system - this assumes an electrical analog for flow in a network

```
INITIALIZE CONDUCTANCE - THIS IS THE ELECTRICAL ANALOG
      DO 11 IB = 1, NBR
   11 CE(IB)=0.
C
      CALCULATE CONTRIBUTION DUE TO DUCTS
      DO 10 ID = 1, NDT
      IB = IBRD(ID)
      VEL = BFLO(IB)/(ROHB(IB)*DA(ID))
RE = VEL*DE(ID)/HVVIS(TBR(IB))
      F = HVFRIC(RE,RR(ID))
      CDUCT=F*DL(ID)/(2.*ROHB(IB)*DE(ID)*(DA(ID)**2))
   10 CE(IB)=CE(IB)+CDUCT
C
      CALCULATE CONTRIBUTION DUE TO SIMPLE FITTINGS
      DO 20 IFT = 1, NFT
      IB=IBRF(IFT)
      CFIT=CO(IFT)/(2.*ROHB(IB)*(AO(IFT))**2)
   20 CE(IB)=CE(IB)+CFIT
      CONVERT FROM PRESSURE TO MASS FLOW RATE COEFFICIENTS
C
      DO 40 IB = 1, NBR
      IF (CE(IB).NE.O.O) THEN
         CE (IB) = SIGN(1./SQRT(ABS(CE(IB))), CE(IB))
      ENDIF
   40 CONTINUE
      CALCULATE HYDROSTATIC PRESSURE DIFFERENCE TERMS
      DO 70 I=1,NNODE
DO 70 J=1,NCNODE(I)
   70 DPZ(I,J) = ROHB(ICMV(I,J)) *HVGRAV*(HVGHT(IN(I,J)) - HVGHT(I))
      SOLUTION OF MASS FLOW EQUATIONS
```

This is the iteration section - go until the mass flow and pressure drop balance.

The inner iteration is for pressure drop with a given flow, whereas the outer iteration is for changing mass flow (velocity), and the effect is then reflected back in the friction,...

```
5 CONV=.TRUE.

DO 30 I=1,NNODE
IF(NCNODE(I) .GT. 1) THEN
DF=0.
F=0.
DO 25 J=1,NCNODE(I)
```

```
DP=HVP(IN(I,J))-HVP(I)+DPZ(I,J)
          IF(NF(\hat{I}CMV(\hat{I},\hat{J})) . EQ. 0) THEN
C
          RESISTIVE BRANCH CONNECTION
              ROOT=SQRT(ABS(DP))
              F = F + SIGN(CE(ICMV(I,J))*ROOT, DP)
              ROOT = MAX(1.E-9, ROOT)
              DF=DF-CE(ICMV(I,J))/(2.*ROOT)
          ELSE
C
          FAN BRANCH CONNECTION
              K=NF(ICMV(I,J))
              IF(NE(ICMV(1,j)) .NE. I)THEN
flow is at fan inlet
                F=F-HVFAN(I,J,K,DP,DFF)
                DF=DF+DFF
flow is at fan exit
                DP=-DP
                F=F+HVFAN(I,J,K,DP,DFF)
                DF=DF+DFF
              ENDIF
          ENDIF
   25
          CONTINUE
          HVP(I)=HVP(I)-F/DF
          IF(ABS(F) .GT. EPS)CONV=.FALSE.
       ENDIF
   30 CONTINUE
       INITR = INITR + 1
       IF (INITR.GT.ITMAX) STOP 'HVMFLO excessive inner iterations'
       IF (.NOT. CONV)GO TO 5
       END OF SOLUTION OF MASS FLOW EQUATIONS NOW CALCULATE MASS FLOWS
this is the outer iteration
       DO 60 I=1, NNODE
       F = 0.0
       DO 50 J=1, NCNODE(I)
       DP=HVP(IN(I,J))-HVP(I)+DPZ(I,J)
       IF(NF(ICMV(I,J)) .EQ. 0) THEN
ROOT = SQRT(ABS(DP))
          HVFLOW(I,J) = SIGN(CE(ICMV(I,J))*ROOT, DP)
BFLO(ICMV(I,J)) = ABS(HVFLOW(I,J))
F = F + HVFLOW(I,J)
       ELSE
C
       FAN BRANCH CONNECTION
          K=NF(ICMV(I,J))
          IF(NE(ICMV(1,j)) .NE. I) THEN
```

```
HVFLOW(I,J) = -HVFAN(I,J,K,DP,DFF)
            F=F+HVFLOW(I,J)
          ELSE
            DP=-DP
            HVFLOW(I,J)=HVFAN(I,J,K,DP,DFF)
            F=F+HVFLOW(I,J)
          ENDIF
      ENDIF
   50 CONTINUE
   60 CONTINUE
      OUTITR = OUTITR + 1
      IF (OUTITR.GT.20) STOP 'HVMFLO failed to converge'
      IF (INITR.GT.3) GO TO 1
      RETURN
      END
      SUBROUTINE HVSFLO
C
      ROUTINE TO CALCULATE SMOKE & HEAT FLOWS
      FAST COMMON BLOCK GOES HERE
      REAL HVCA(NS), HVTA
      CALCULATE TEMPERATURE & SMOKE FLOW AT THE CONNECTING NODES
      WE ASSUME THAT THE PRESSURE AND TOTAL MASS FLOW EQUATIONS
      HAVE BEEN SOLVED
      DO 30 I = 1, NNODE
      HVTA=0.
      FLOWIN=0.
      DO 19 K = 1, NS
   19 HVCA(K) = 0.0

DO 20 J = 1, NCNODE(I)

IF (HVFLOW(I,J).GT.0.0) THEN
          FLOWIN = FLOWIN + HVFLOW(I,J)
         IB = ICMV(I,J)
HVTEMP = HVFLOW(I,J)
          HVTA = HVTA + HVTEMP*TBR(IB)
         DO 23 K = 1, NS
          IF (ACTIVS(K)) HVCA(K) = HVCA(K) + HVTEMP*HVCONC(IB,K)
   23
          CONTINUE
      ENDIF
   20 CONTINUE
      IF (FLOWIN.GT.O.O) THEN
         HVTA = HVTA / FLOWIN
DO 24 K = 1, NS
          IF (ACTIVS(K)) HVCA(K) = HVCA(K) / FLOWIN
   24
          CONTINUE
      ELSE
          DO 21 II = 1, NEXT
          IF (HVNODE(2,II).EQ.I) THEN
             HVTA = HVEXTT(II)
             DO 25 K = 1, \dot{N}S
             IF (ACTIVS(K)) HVCA(K) = HVEXCN(II,K)
   25
             CONTINUE
             GO TO 22
```

```
ENDIF
    21
            CONTINUE
            STOP 'MECH VENT. MODULE - YOU CAN NOT GET HERE FROM THERE'
    22
            CONTINUE
        ENDIF
calculate the temperature and concentrations in the ducts and fan cages
       DO 40 J = 1, NCNODE(I)

IB = ICMV (I,J)

IF (HVFLOW(I,J).LT.0.0) THEN

IF (NF(IB).EQ.0) THEN

FACTOR = -MIN(1.,HVFLOW(I,J)*HVDELT/(HVDVOL(IB)*ROHB(IB)))

TBR(IB) = TBR(IB)*(1.-FACTOR) + HVTA*FACTOR

DO 42 K = 1, NS

IF (ACTIVS(K)) HVCONC(IB,K) = HVCONC(IB,K)*(1.-FACTOR)

+ HVCA(K)*FACTOR
                                                       + HVCA(K)*FACTOR
    42
                CONTINUE
            ELSE
                TBR(IB) = HVTA
                DO 41 \text{ K} = 1, NS
                IF (ACTIVS(K)) HVCONC(IB,K) = HVCA(K)
    41
                CONTINUE
            ENDIF
        ENDIF
    40 CONTINUE
    30 CONTINUE
        RETURN
        END
        FUNCTION HVFRIC(RE,RR)
С
       CALCULATES FRICTION FACTOR FROM THE COLEBROOK EQUATION
        IF(RE .GT. 2300)GO TO 1
        HVFRIC=64./RE
        RETURN
1
        X=2.4*RE**0.0925
        I=0
2
        C=RR/3.7+2.51*X/RE
        G=X+2.*ALOG10(C)
        DG=1+2.18016/(RE*C)
        XN=X-G/DG
        IF(I .GT. 10)STOP
        IF(ABS(XN-X) .LT. .003)GO TO 5
        X=XN
        GO TO 2
5
        HVFRIC=1/XN**2
        RETURN
        END
        FUNCTION HVFAN(II, JJ, K, DP, DFF)
CCC
         THIS FUNCTION RETURNS THE MASS FLOW RATE THROUGH A FAN
```

```
С
               FAN NUMBER
        K =
CC
        DP =
               HEAD PRESSURE ACROSS THE FAN
               DERIVATIVE OF FAN FLOW (CALCULATED & RETURNED)
C
      FAST COMMON BLOCKS GO HERE
      LOGICAL ERRORL, ERRORH
      DATA ERRORL, ERRORH/ 2*.TRUE./
C
      ROH=ROHB(ICMV(II,JJ))
      IF (DP.LT.HMIN(K)) THEN
         IF (ERRORL) THEN
             WRITE(IOFILO, 700) DP
             ERRORL = .FALSE.
         ENDIF
         HVFAN = QMIN(K)
         DFF = DFMIN(K)*ROH
        ELSE IF(DP.GT.HMAX(K)) THEN
         IF (ERRORH) THEN
             WRITE(IOFILO, 700) DP
             ERRORH = .FALSE.
         ENDIF
         HVFAN = QMAX(K)
         DFF = DFMAX(K)*ROH
        ELSE
         F=HVBCO(K,1)
         DF=0.0D0
         XX=1.0D0
         DO 1 J = 2, NFC(K)
DF = DF + FLOAT(J-1)*HVBCO(K,J)*XX
             XX = XX*DP
             F = F + HVBCO(K,J)*XX
1
         CONTINUE
         HVFAN = F*ROH
         DFF = DF*ROH
      ENDIF
      RETURN
700
      FORMAT(/2X,10('*'),') Flow outside fan curve, DP = ',1PG12.3)
      END
      FUNCTION HVVIS(T)
      INCLUDE 'PRECIS.INC'
С
000000000
      FUNCTION CALCULATES ABSOLUTE VISCOSITY (PASCAL SECOND)
      BY INTERPOLATION FOR 200 TO 2000 DEG K. DATA FROM NASA TECH NOTE D-7488 BY POFERL, D. J. AND
      SVEHLA, R., 1974 EXCEPT FOR THE VALUE AT 200 DEG K
      WHICH IS FROM THE CRC HANDBOOK OF CHEMISTR & PHYSICS,
       66TH ED., 1985 PAGE F-42.
      T=ABSOLUTE TEMPERATURE IN DEGREES KELVIN
      LOGICAL ERROR
      DIMENSION V(19)
      DATA V/13.1,18.4,22.7,26.5,29.9,33.1,36.2,39.1,41.9
     +,44.5,47.0,49.4,51.7,54.0,56.3,58.5,60.7,62.9,65.1/
```

4. DESCRIPTION OF THE DATA FILE USED BY FAST

There are several new key words which are used to describe the mechanical ventilation. They are given here in the style of chapter 6 of reference [1]. The key words which apply to mechanical ventilation are

MVOPN - describe an opening between a compartment and the ventilation system

MVDCT - describe a piece of (circular) duct work

MVFAN - give the pressure - flow relationship for a fan

INELY - specify interior node elevations

An additional key word for diagnostic use

CNVG - specify convergence tolerances

and a fuel parameter is

O2.

Label	Parameter	Comments
MVOPN	(5)	Connect a compartment to a node in the mechanical ventilation system.
	Compartment Number	Specify the compartment number.
	Duct Work Node Number	Corresponding node in the mechanical ventilation system to which the compartment is to be connected.
	Orientation	V for vertical or H for horizontal.
	Height	Height of the duct opening above the floor of the compartment.
	Area	Area of the opening into the compartment.
MVDCT	(9)	Specify a piece of duct work.
	Node Number	First node number. This is a node in the mechanical ventilation scheme, not a compartment number (see MVOPN).

	Node Number	Second node number.			
	Length	Length of the duct.	m		
	Diameter	All duct work is assumed to be circular. Other shapes must be approximated by changing the flow coefficient. This is done implicitly by network models of mechanical ventilation and forced flow, but must be done explicitly here.	m		
	Absolute Roughness	Roughness of the duct.	m		
	Flow Coefficient	Flow coefficient to allow for an expansion or contraction at the end of the duct which is connected to node number one. To use a straight through connection (no expansion or contraction) set to zero.			
	Area	Area of the expanded joint.	m^2		
	Flow Coefficient	Coefficient for second node.			
	Area	Area at the second node.	m^2		
MVFAN	(9)	Specify fan curve with power law coefficients. There must be at least one coefficient.			
	First Node	First node in the mechanical ventilation system to which the fan is connected.			
	Second Node	Second node to which the fan is connected.			
	Minimum Pressure	Lowest pressure of the fan curve. Below this value, the flow is assumed to be constant.	Pa		
	Maximum Pressure	Highest pressure at which the fan will operate. Above this point, the flow is assumed to stop.	Pa		
	Coefficients	At least one, and a maximum of five coefficients to specify the flow as a function of pressure. See comments at the end of this section for more information.	-		

INELV	(2×n)	Specify interior elevations of the mechanical ventilation nodes. All nodes can be specified, but the exterior nodes, that is those connected to a compartment, will be set to the compartment elevation. The heights are absolute heights above the reference datum specified by TAMB. The heights are specified in pairs, the node number followed by the height.	(#,m)
O2	Production Rate of the Fuel	The mass ratio of oxygen to carbon as it becomes available from the fuel.	kg/kg
CNVG	(3)	Diagnostic parameters	
	Approximate Conduction	This is a logical switch. If set to zero, the usual heat transfer thru partitions is calculated. If set to any non zero value then the semi-infinite slab approximation is used.	0
	Convergence Factor	Modifies the convergence criterion used by the solver for the relative error at each time step.	1.0
	Pressure Damping	Used to damp pressure fluctuations.	1.0

The diagnostic parameters must be used with extreme caution. These parameters can not be set in the data editor for the main model. While running computations within the data editor, the speed enhancement for the conduction can be utilized. Normally, a linear parabolic equation is solved for the heat transfer through each partition. The solution is *via* a successive over-relaxation technique. When the walls are thick, or the simulation time will be very short, it is reasonable to assume that the thermal wave will not reach the outside boundary. In this case, there is an analytic solution to the conduction equation which can be written in terms of the "error function," ERFC [7]. The other two parameters modify the convergence criteria used by the numerical solver. The default values are unity, and should normally be left at those values.

Example 1:

```
MVDCT 1 3 20. .15 .19E-3 3.30 .01767 0. 0.
MVDCT 3 4 44. .2 .19E-3 0.0 0.0 0. 0.
MVFAN 4 5 0.0 140. 0.140 3.170E-04 -1.803E-05 1.898E-07 -8.104E-10
MVOPN 1 1 H 0. 1.
MVOPN 4 9 V 0. 2.5
INELV 3 0 4 0 5 0 7 0 8 0
```

Example 2: .19E-3 20. .15 1 3 3.30 .01767 MVDCT 0.0. 3 20. .15 .19E-3 2.94 MVDCT .01767 0.0. 3 MVDCT 4 44. .2 .19E-3 0.0 0.0 0.0. 40. 0. .2 0. .2 0. .2 0.0 140. 5 .19E-3 .03142 MVDCT 6 .51 0.0. 4 40. .19E-3 .51 .03142 MVDCT 0.0. 40. .19E-3 .51 MVDCT 9 8 .03142 0.0. 5 7 MVFAN 4 0.140 3.170E-04 -1.803E-05 1.898E-07 -8.104E-10 0.140 3.170E-04 -1.803E-05 8 0.0 140. 1.898E-07 -8.104E-10 MVFAN 1 2 H 0. 1. H 0. 1.5 MVOPN MVOPN 3 6 H O. 2.5 MVOPN 4 9 H O. 2.5 3 O 4 O MVOPN 5 0 7 0 8 0 INELV

This example describes a network which is shown in figure 2.

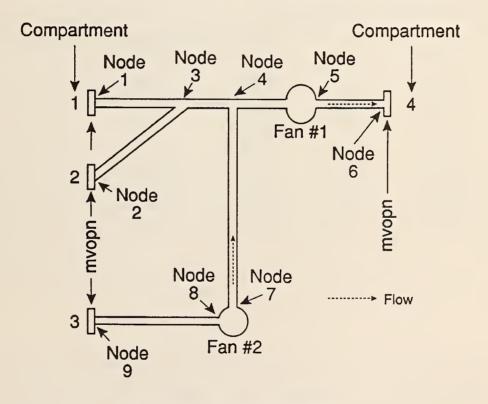


Figure 2. Node arrangement for example 2.

The fan coefficients are simple the coefficients of an interpolating polynomial for the flow speed as a function of the pressure across the fan housing. The fan described in the

Refinement of a Model for Fire Growth and Smoke Transport

previous example was for a pressure range of zero to 140 Pascals. An example of such a calculation is the following:

The following data (flow in kilograms per second)

```
FLOW .07 .07 .06 .06 .055 .05 .05 .045 .036 .031 .02 HEAD 0 35 60 70 80 90 100 110 120 130 140
```

produces the following coefficients

which correlates with the original data as

PRESSURE	FLOW	CALCULATED FLOW	PERCENT DIFFERENCE
0.00	0.070	0.070	0.08
35.00	0.070	0.070	-0.66
60.00	0.060	0.062	2.71
70.00	0.060	0.058	-2.79
80.00	0.055	0.055	0.17
90.00	0.050	0.052	3.61
100.00	0.050	0.048	-3.61
110.00	0.045	0.044	-2.57
120.00	0.036	0.038	6.06
130.00	0.031	0.030	-1.69
140.00	0.020	0.020	-0.72

5. EXAMPLE OF HYDROGEN CHLORIDE DEPOSITION AND MECHANICAL VENTILATION

An example of the interaction of mechanical ventilation with hydrogen chloride deposition (HCl) can be shown using the following data file:

```
VERSN
        18 SSU1
        180 30 0
TIMES
TAMB
        288. 101300.
                           0.
             0.0 0.0
HI/F
        0.0
WIDTH
        10.0 10.0 10.
DEPTH
       10.0 10.0 10.
              5.0 5.
HEIGH
        5.
HVENT
               1 1.0 2.1
                             0.0
HVENT
        2 4
                  1.0
                       2.1
                             0.0
        3 4
                      2.1
HVENT
               1 1.0
                             0.0
CEILI
        OFF WB GLASS
       OFF WB
FLOOR
               GLASS
WALLS
        OFF WB
               GLASS
LEBT
LFMAX
        16. 50. 10. 10000000. 300.
CHEMI
FMASS
        0.05 0.05 0.05
FTIME.
        120. 1800.
        .1 .1 .1 .10
        .1
HCL
CO
HCR
        0.
            0. 0.
MVDCT 1 2 5. .15 .19E-3 3.30 .01767 0. 0. MVDCT 3 4 5. .15 .19E-3 2.94 .01767 0. 0.
MVDCT 5 6 5. .15 .19E-3 3.30 .01767 0. 0.
MVDCT 7 8 5. .15 .19E-3 2.94 .01767 0. 0.
MVFAN
      2 3
            0.0 140.
                       0.140 3.170E-04 -1.803E-05 1.898E-07 -8.104E-10
      6 7 0.0 140.
MVFAN
                        0.140 3.170E-04 -1.803E-05 1.898E-07 -8.104E-10
       1 1 H 4.5 1.
MVOPN
MVOPN 2 4 H 4.5 1.
      1 5 H 4.5 1.
MVOPN
MVOPN
      3 8 H 4.5 1.
1NELV 2 4.4
               3 4.4 6 4.4 7 4.4
```

In this case, there are three compartments, each with a normal (HVENT) opening only to the outside. The three compartments are connected to each other by mechanical ventilation ducts. The compartment layout is shown in figure 3, with compartment #2 on the left, compartment #1 in the center and compartment #3 on the right hand side of the figure. The fire is in the center compartment (#1) and a pair of fans blows the fire gases into the other two compartments (#2 and #3). The wall lining for the second compartment is wall board, and for the third compartment glass. The two compartments are symmetric in that all openings to the outside are the same size and the fans have the same pressure curves, so flow will be the same to both sides. The fire is small, and the pyrolyzate contains 10% hydrogen chloride, to emphasize the effect of mechanical ventilation and deposition.

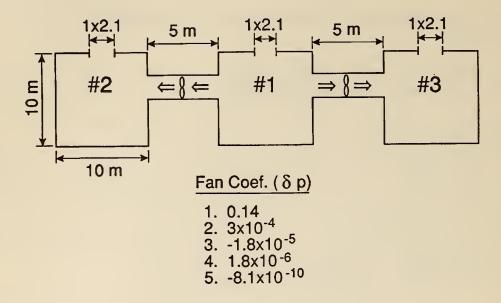


Figure 3. Plan diagram of the geometry used in the HCl deposition calculation.

Figure 4 shows the difference in the HCl concentration in the *lower* layer of the two compartments not containing the fire. If wall adsorption 34 were not important, then the concentrations of HCl in the two gas layers would be the same. As can be seen, the deposition onto the wall is influenced by the concentration in the environment, with the HCl concentration lower in the room which is lined with gypsum.

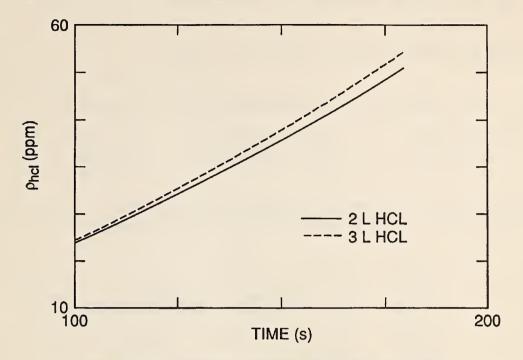


Figure 4. HCL concentration in the lower layer of compartments 2 and 3.

6. ERRATA for "Technical Reference Guide for FAST Version 18"

Page 13 has an incorrect power in the second line of the entrainment region

change intermittent: $\dot{m}_e/\dot{Q} = 0.026 \; (Z/\dot{Q}^{2/5})^{1.85} \qquad 0.08 \leq Z/\dot{Q}^{2/5} \leq 0.20$ to intermittent: $\dot{m}_e/\dot{Q} = 0.026 \; (Z/\dot{Q}^{2/5})^{0.909} \qquad 0.08 \leq Z/\dot{Q}^{2/5} \leq 0.20$

Page 40, section 5.5, the conversion coefficient from fuel (pyrolysate) to carbon dioxide was specific for methane. The form has been changed to reflect a general fuel.

OOSTOK = 13200000. / HCOMBAde1 QPYROL = MAX(0.,MIN(PYROL, OOSTOK*02MASS)) * HCOMBA change QPYROL = MAX (0., MIN(PYROL*HCOMBA, O2MASS*O2F))to NETO2 = - QPYROL / 1.32E+7change NETFUL = - NETFUELNETFUL = - NETFUELto NETO2 = - QPYROL * O2F (o2f = 1.32×10^7) NETCO2 = 3.67 * NETFUELchange /((1+HCRATT)*(1.+1.57*COCO2T+3.67*CCO2T)) FACTOR = (1.+HCOMBA*O2FI)-9.*HCRATT/(1+HCRATT) (02fi=7.578×10⁻⁸)to NETCO2 = FACTOR * NETFUEL / (1.+COCO2T+CCO2T)

Page 49, section 6.1

Parameter	Comments
(2)	
Version Number	in columns 8-10.
5.10	
(10)	•••
Label Number	
	(2) Version Number 5.10 (10) Label

Text

after Text and before Angle1, Angle2, insert

Color color number (0-15)

Angle1, ... Angle2

7. NOMENCLATURE

The variables used in the formulae are listed here. There are a few exceptions for local variables which are used only in a section for expository purposes. In general, most of these variables can be indexed by compartment (single i) or by the layer in a given compartment (u or ℓ). The variables shown in the implementation section correspond roughly to the mathematical variables shown here. Due to the limitations of character sets for computers, there can not be an exact correspondence, but the crosswalk should be clear. The first list is for the earlier discussion. The next list is for the numerical model as it is currently implemented.

Variables used in the mathematical description of the model:

A₀ - area of a mechanical ventilation duct (m²)

A_w - area of a boundary, such as the ceiling, floor (m²)

C_n - flow coefficient (nondimensional)

CO₂, CO, HCl, HCN, S(soot), H₂O - species production during pyrolysis

H, C, O - composition weight of the fuel - used only as a fraction H/C,...

HCl/C, HCN/C, HCN/f and HCl/f - ratio of species to carbon or fuel production (kg/kg)

fi - algebraic form of conservation of mass in a duct

F - friction factor (dimensionless)

f/C - fuel carbon production ratio (≥1)

G - conductance for mass flow

h_c - heat of combustion

k_c - transport coefficient for HCl (m/s)

k_e - equilibrium coefficient for HCl (m)

k_s - wall loss rate for HCl (s⁻¹)

 $\Delta m_O(actual)$ - the change of fuel during a time step

m_{HCl} - total mass of hydrogen chloride in a layer (kg)

d_{HCl,w} - mass density of hydrogen chloride on a wall surface (kg/m²)

 \dot{m} - time rate of change of a mass; this is the time equivalent of Δm

 Δm_f - change in the mass of fuel for an interval of time

```
\Delta m_C - change in available carbon (see comment on fuel) \Delta m_{xx} - change in species xx, where xx is one of CO<sub>2</sub>, CO, HCl, HCN, S(soot), H<sub>2</sub>O P - pressure (Pa) \Delta Q - heat released by a change in fuel (J) T_g - gas temperature (K) T_w - wall temperature (K)
```

I_w - wall temperature (K)

V - volume of a zone (layer)

 ρ_{HCl} - mass density of hydrogen chloride in the gas phase (kg/m³) ρ_g - mass density of a gas layer (kg/m³) ρ_{blHCl} - mass density of HCl in the boundary layer (kg/m³)

 $\left(\frac{xx}{yy}\right)$ - is used for the mass ratio of a species xx to yy.

This can refer to the properties of the fuel, which is reflected in the pyrolysis, or the production of species from burning.

8. REVISION HISTORY

This is an annotated list of changes for the various versions from 18.0 to the current version, 18.5.2.

Version 18.5.1 - March 3, 1990.

The input routine (and the size of the common block) have been changed so that the HCl data for wall absorption is now picked up from the thermophysical properties file. The routine "CHEMIE" has been changed to incorporate the complete chemistry scheme as shown in the revision document. A key word that has been added is O2 which is the oxygen/carbon ratio in the fuel. Both chlorine and oxygen content of the fuel are reflected in the actual amount of pyrolysate available for combustion. A new module has been added called "CF_rpt." It will read the dump file produced by FAST or FAST_in and generate a report. The codes are fetched with the option /r and are

```
1 configuration (B.1)
2 normal output (B.2)
4 flow
8 species (B.2)
16 fed type 1 (see the Hazard Technical Reference Manual) [8]
32 fed type 2 & 3 " " " "
```

The codes can be combined. For example, /r11 yields the usual output from FAST, whereas /r3 would show on the configuration information. The command is

```
CF_rpt/r11 xxx.dmp,
```

which would generate a list as shown in the Technical Reference Guide[1].

The "bug" noted below for monochrome CGA monitors has been fixed.

There is a bug in FAST_in in the section which sets the open/close parameters for vents. The problem arises if there are more vents than can be listed on the page (8), and one scrolls down the list and then back up. If one them attempts to set the open/close parameters, the vent retrieved is not the one pointed to by the inverse bar.

Version 18.5.0 - February 1, 1990.

Several changes were made to the routine that calculates the source terms for the solver. First, Hydrogen chloride deposition onto walls was added. The transfer coefficients are put

the in the thermophysical data; second, an error in the mass flow which occurs in certain cases was corrected. The problem arose when the natural stack effect was important, specifically if hot air entered near the floor in the summer time, or very cold air near the top in the winter; third, mechanical ventilation was added; finally, we have a place holder for smoke agglomeration and deposition. The overlay for this release is 185.

The relevant key words for the mechanical ventilation are

MVOPN, MVDCT, MVFAN AND INELV.

There is a known bug which will not be fixed until the next release. It occurs on monochrome monitors with cga or lower resolution. The problem arises when running the graphics mode of FAST, or FASTplot.

The wall absorption coefficients are wired into the code for gypsum. The correct data is in the THERMAL.TPF file but is not picked up. This too will be fixed in the next release. It will involve a change in the size of the dump files. The other coefficients, for boundary layer transfer,... are picked up correctly from the database.

Version 18.4.2 - October 3, 1989.

There was a bug in FAST_in which did not generate the correct value for the relative humidity in the output file. It was used correctly within each of the separate models (FAST and FAST in), and could be set separately in the data file.

Version 18.4.1 - September 14, 1989.

The factor for conversion from pyrolysate to CO₂ was changed. The value in the technical reference is correct only for methane. The change was in CHEMIE and is

```
NETCO2 = 3.67 * NETFUEL / ((1+HCRATT)*(1.+1.57*COCO2T+3.67*CCO2T))
```

becomes

```
FACTOR = (1.+HCOMBA/1.32E+7) - 9.*HCRATT/(1.+HCRATT)
NETCO2 = FACTOR * NETFUEL / ((1+HCRATT)*(1.+COCO2T+CCO2T))
```

PYROLS was changed to place a limit on the H/C ratio to 1/3, the value for methane. This is a mass ratio, $4 \times 1/12 \rightarrow 1/3$.

The default for the ignition temperature in vent flow was set to

pyrolysis temperature + 100 K.

This prevents spurious calculations when the layers are at ambient conditions.

This is an arbitrary choice. Any value above the highest ambient condition is sufficient, and can be set with the CHEMIE entry. Species information is included in the normal listing only if the "-print interval" switch is set. This is also the option to see the flow field.

The executable for the FAST module was split into two pieces, FAST.EXE and FAST.184, to conform with the Hazard I release format.

Any value above the highest ambient temperature is sufficient, and can be set with the "CHEMIE" entry. Species information is included in the normal listing only if the "-print interval" switch is set. This is also the option to see the flow field. The executable for the FAST module was split into two pieces, FAST.EXE and FAST.184, to conform with the Hazard I release format. The corresponding version of FASTplot is 4.1 and FAST in is 2.4.

Version 18.4.0 - July 1, 1989.

The outside boundary condition for the heat transfer thru walls was modified in CNDUCT to account for radiation from the walls:

after

```
QDOUTL = - QDOUTL
```

add

```
+ SIGM*EPW(NWW,NC)*(TWJ(NWW,NC,NTOT)**4-TWE(NWW,NC)**4).
```

Several changes were made to the routine that calculates the source terms for the solver. First, Hydrogen chloride deposition onto walls was added. The transfer coefficients are put in the thermophysical data. Second, an error in the mass flow which occurs in certain cases was corrected. The problem arose when the natural stack effect was important, specifically if hot air entered near the floor in the summer time, or very cold air near the top in the winter. The changes were made in DSOURC, the control program as follows:

```
. + (TU(J)-TU(I)) * (SSIN+SAIN)
. + (TL(J)-TL(I)) * (ASIN+AAIN)
```

became

```
. + (TU(J)-TU(I)) * INULU

. + (TL(J)-TU(I)) * INULL

. + (TL(J)-TU(I)) * INLLU

. + (TL(J)-TL(I)) * INLLL
```

Third, mechanical ventilation was added. Finally, a place holder for smoke agglomeration and deposition was inserted. The relevant key words for the mechanical ventilation are mvopn, mvdct, mvfan and inelv.

The routine (lenoco) which finds the size of the common block was made some what more general so that dump files from earlier runs would be accessible, and version 4.1 of FASTplot can read the dump files from version 18.3.

The input routines (NPUTP, NPUTPR, NPUTQ and NPUTQR) were combined into NPUTP and NPUTQ. The other two, which were used for restarts, are now eliminated, which does two things, first it makes updates easier, and second will allow (eventually) restarts from FAST in.

The species transport was updated to conform with the mass flow as calculated in the source routines. Previously, the same error which is described above for certain cases of stack effect would cause the same problems in the species transport.

The calculation of "target" was corrected from

```
60 ONTARGET(I) = SIGM * (P(I+N)-TAMB(I))**4
to
60 ONTARGET(I) = SIGM * (P(I+N)**4-TAMB(I)**4)
```

in the routine toxic.

The modules testga.exe and tequipt.exe have been replaced by list_fcg.exe.

Disk #4, which contained the build and system*.fnt files is no longer included. The Build module is in the process of begin revised extensively, and will be reissued when it is finished.

The executable for the FAST module was split into two pieces, FAST.EXE and FAST.184, to conform with the Hazard I release format.

Version 18.3.3 - June 30, 1989.

The parameter "inter" was not passed correctly between the code which reads the ASCII data file and the initialization routine, so it was not possible to set the interface at any point other than the top of the compartment. FASTplot was fixed so that when no data is present, the graphics routines will not quit in an unfriendly manner, as they sometimes did prior to 4.0. FAST_in now requires that an alternate installation procedure be done to enable the advanced features, which include the ability to do computations within the data editor itself. See Technical Note 1262 for details.

All of the routines which use the graphics mode now reset the lookup table (palette) to the values in use prior to executing a program upon termination.

```
Version 18.3.2 - February 1, 1989.
```

For FAST, the time for output was fixed so that output for restarts is calculated relative to the beginning of the restart rather than time 0. This allows for 50 intervals for each restart rather than 50 for the entire simulation. In FAST_in, the key prompt in the calculation screen does not show a "key" command, since this would be superfluous. Also, the length of the thermal names was put back to 8 characters. During optimization of the code, this was inadvertently truncated to 5 characters. The version number for FAST_in is 2.1 The parameter "TGIGNT" was added to the "CHEMI" line to specify the conditions for ignition of a gas. Below this temperature, a fuel/oxygen mixture will not burn, and above this limit, it will burn depending on the usual burning rate scheme.

Version 18.3.1 - November 14, 1988.

Added the key words "THRMF" and "DEFCG" to the input file to specify an alternate thermophysical data base, and configuration file from within the data file itself. Multiple layers in the thermophysical properties are now displayed. The limit on the oxygen index has been changed from

```
O2MASS = O2ENTR * O2INDEX
to
O2MASS = O2ENTR * 0.995 * (1.-EXP(-10.*O2INDEX))
```

which more closely represents what actually occurs in the kinetics process. The boundary conditions on the ceiling and floor to the ambient have been reversed. They are stated correctly in the journal article and the User's Guide, but were implemented for the outside the same way they were done on the interior walls in the model. This has been reversed. The ceiling now behaves as a floor on outside, and the floor behaves as a ceiling.

FAST now stops if it can not find the thermal properties which have been requested in the data file. FAST_in does not stop, but rather sets the corresponding values to "NONE." Two parameters have been added to the CHEMIE line. The sixth element is an ignition temperature and the seventh is the fraction of heat from the fire which is radiated rather than convected away. Default for the ignition temperature is the volatilization temperature and zero for the radiative fraction.

Relative humidity now sets the water content of the atmosphere by

```
DT = TAMB(I) - 273.

DP = ((36.6 + 3.54*DT + 0.1*DT**2)/760.) * (18./28.4)

O2N2(8) = RELHUM * DP.
```

These factors are fitted to a table of values in the Handbook of Chemistry and Physics. The corresponding versions are FASTplot v 3.6.4 and FAST in v 2.0.

Version 18.3.0 - October 16, 1988.

A type two fire limits burning (not pyrolysis) based on the available oxygen. FASTplot version 3.6.2 fixes a bug in the "clear" command when interacting with RAPID files. Entrainment into the upper layer via a plume has a limitation based minimum buoyancy. The source terms are reset for each pass of the source routine (DSOURC) so that the fire room can be moved. With FAST this must be done with a restart, but with FAST_in, the model can be stopped, the fire moved, and the model restarted. The base system has been expanded to four disks to contain all the modules. One of these disks contains only the program BUILD, which is used to generate the ".PIC" files for the real time display. If it is not needed, then BUILD.EXE and SYSTEMnn.FNT can be deleted. FAST in (v2.0) is official with this release.

Version 18.2.1 - July 30, 1988.

FASTplot (3.4) incorporates dashed/colored lines. The selection is through the DEFAULT key word. The appropriate setting is the "axes format."

Version 18.2.0 - May 16, 1988.

A bug in the opening/closing routine has been fixed. This has necessitated a modification in the common block, but does not affect the interaction of FAST and FASTplot. The corresponding version of FASTplot is 3.3 although 3.2 will work. FASTplot 3.3 works more smoothly now. Also, a provision is in place for substituting line types for colors in the plots, and changing devices, *i.e.* for pen plotters and laser printers. These are not implemented yet, but some of the commands to utilize these devices will appear in "default" and "help."

Version 18.1.0 - May 5, 1988.

The connection between the inside compartments and the outside ambient was changed so that each compartment could see a different outside. This allows the stack effect to work properly. Also a different wind speed vector is calculated for each opening to the outside world. Finally, a new key word('INTER') has been added to specify the initial position of the interface inside a compartment. This is applicable primarily for studying the effect of summer over winter in building flows. The corresponding version of FASTplot is 3.2.

The primary change in the inside-outside interaction was a change in the selection rules for flow. In order to get both summer and winter flows to behave in a reasonable way, the selection rules for vent flow have been modified. The selection rules for directing mass flow through vents in FAST is fairly simple. Upper layer goes to upper layer, and lower layer to lower layer. This follows the prescription of Tanaka, which is actually quite simple and elegant. We have improved greatly on the means of calculating the actual flow, but have kept

Refinement of a Model for Fire Growth and Smoke Transport

this prescription. However, the predictions for the stack effect have turned up some anomalies in this scheme. Thus the selection rules for flow have been modified. There are six combinations based on the temperature of the source and receiving compartments.

Version 18.0 - February 8, 1988.

Add the opening/closing parameter CVENT and vitiated combustion. This latter change require a change in "chemi". Corresponding changes were made in FASTplot (3.1) to accommodate the extra data.

9. REFERENCES

- [1] Jones, W. W. and Peacock, R. D., Technical Reference Guide for FAST Version 18, NIST Technical Note 1262, 1989.
- [2] Jones, W. W., A Multicompartment Model for the Spread of Fire, Smoke and Toxic Gases, Fire Safety Journal 9, 55 (1985).
- [3] Galloway, F. M. and Hirschler, M. M., A Model for the Spontaneous Removal of Airborne Hydrogen Chloride by Common Surfaces, Fire Safety Journal 14, 251-268 (1989).
- [4] Galloway, F. M. and Hirschler, M. M., Transport and Decay of Hydrogen Chloride: Use of a Model to Predict Hydrogen Chloride Concentrations in Fires Involving a Room-Corridor-Room Arrangement, Fire Safety Journal 16, 33-52 (1990).
- [5] Klote, J. H., A Computer Model of Smoke Movement by Air Conditioning Systems, NBSIR 87-3657 (1987).
- [6] 1989 ASHRAE Handbook Fundamentals, American Society of Heating, refrigeration and Air Conditioning Engineers, Inc., Atlanta, Georgia (1989).
- [7] Abramowitz, M and Stegun, I., Handbook of Mathematical Functions, National Bureau of Standards Applied Mathematics Series 55 (1964).
- [8] Hazard I Technical Reference Guide, NIST Special Publication 146 Volume II (1989).

10. ACKNOWLEDGMENTS

The procedures we followed to include the mechanical ventilation and hydrogen chloride ventilation is the paradigm for improving our models that will be used for the unified model at the Center for Fire Research. Several people contributed to the incorporation of the algorithms in the manner that we would like to see. For the mechanical ventilation, J. Klote, who was responsible for the SMACS model, was helpful with advice in using his algorithm. For the hydrogen chloride deposition model, N. Bryner did an independent review, and M. Galloway did the actual programming. Funding for this revision of the FAST model suite was provided in part by the Naval Research Laboratory and the Vinyl Institute.

	BIBLIOGRAPHIC DA
NIST-114A	U.S.
(REV. 3-89)	NATIONAL INSTITUTE OF

STANDARDS AND TECHNOLOGY 1. PUBLICATION OR REPORT NUMBER NIST/TN-1282

(ALLISTITUTE OF STANDARDS AND TECHNOLOGY	2. PERFORMING ORGANIZATION REPORT NUMBER
DIDLICODADUIO DATA CUEST	
BIBLIOGRAPHIC DATA SHEET	3. PUBLICATION DATE
	November 1990
4. TITLE AND SUBTITLE	1330
Refinement of a Model for Fire Growth and Smoke Transport	
5. AUTHOR(S) Walter W. Jones	
6. PERFORMING ORGANIZATION (IF JOINT OR OTHER THAN NIST, SEE INSTRUCTIONS)	7. CONTRACT/GRANT NUMBER
U.S. DEPARTMENT OF COMMERCE	7. CONTRACT/GRANT NOMBER
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY	8. TYPE OF REPORT AND PERIOD COVERED
GAITHERSBURG, MD 20899	Final
9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (STREET, CITY, STATE, ZIP)	1 1110 1
10. SUPPLEMENTARY NOTES	
DOCUMENT DESCRIBES A COMPUTER PROGRAM; SF-185, FIPS SOFTWARE SUMMARY, IS ATTAC	uen .
This document describes the changes which have occurred in FAS distribution disks in the change from 18.3, the release for Ha 18.5. Included are an errata section for the Technical Note I is distributed with the release disks, the addendum to the Technory, and the description of the implementation of the physical section is distributed.	azard I, and the current release .262, a revision history that chnical Note for the new key cal routines.
12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPAR	ATE KEY WORDS BY SEMICOLONS)
compartment fires; fire growth; mathematical models; numeric smoke; toxicity	al models; room fires;
13. AVAILABILITY	14. NUMBER OF PRINTED PAGES
X UNLIMITED	50
FOR OFFICIAL DISTRIBUTION. DO NOT RELEASE TO NATIONAL TECHNICAL INFORMATION SERVICE	
ORDER FROM SUPERINTENDENT OF DOCUMENTS, U.S. GOVERNMENT PRINTING OFFICE, WASHINGTON, DC 20402.	15. PRICE
ORDER FROM NATIONAL TECHNICAL INFORMATION SERVICE (NTIS), SPRINGFIELD, VA 22161.	





Periodical

Journal of Research of the National Institute of Standards and Technology—Reports NIST research and development in those disciplines of the physical and engineering sciences in which the Institute is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Institute's technical and scientific programs. Issued six times a year.

Nonperiodicals

Monographs—Major contributions to the technical literature on various subjects related to the Institute's scientific and technical activities.

Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies. Special Publications—Include proceedings of conferences sponsored by NIST, NIST annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NIST under the authority of the National Standard Data Act (Public Law 90-396). NOTE: The Journal of Physical and Chemical Reference Data (JPCRD) is published quarterly for NIST by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements are available from ACS, 1155 Sixteenth St., NW., Washington, DC 20056.

Building Science Series—Disseminates technical information developed at the Institute on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

Technical Notes—Studies or reports which are complete in themselves but restrictive in their treatment of a subject. Analogous to monographs but not so comprehensive in scope or definitive in treatment of the subject area. Often serve as a vehicle for final reports of work performed at NIST under the sponsorship of other government agencies.

Voluntary Product Standards—Developed under procedures published by the Department of Commerce in Part 10, Title 15, of the Code of Federal Regulations. The standards establish nationally recognized requirements for products, and provide all concerned interests with a basis for common understanding of the characteristics of the products. NIST administers this program as a supplement to the activities of the private sector standardizing organizations.

Consumer Information Series—Practical information, based on NIST research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

Order the above NIST publications from: Superintendent of Documents, Government Printing Office, Washington, DC 20402.

Order the following NIST publications—FIPS and NISTIRs—from the National Technical Information Service, Springfield, VA 22161.

Federal Information Processing Standards Publications (FIPS PUB)—Publications in this series collectively constitute the Federal Information Processing Standards Register. The Register serves as the official source of information in the Federal Government regarding standards issued by NIST pursuant to the Federal Property and Administrative Services Act of 1949 as amended, Public Law 89-306 (79 Stat. 1127), and as implemented by Executive Order 11717 (38 FR 12315, dated May 11, 1973) and Part 6 of Title 15 CFR (Code of Federal Regulations).

NIST Interagency Reports (NISTIR)—A special series of interim or final reports on work performed by NIST for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Service, Springfield, VA 22161, in paper copy or microfiche form.

U.S. Department of Commerce National Institute of Standards and Technology (formerly National Bureau of Standards) Gaithersburg, MD 20899

Official Business Penalty for Private Use \$300