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TITLE: FIRAC: A Computer Code to Predict Fire-Accident Effects in Nuclear Facilities

AUTHOR(S): J. Bolstad, F. R. Krause, P. K. Tang, R. W. Andrae, R. A. Martin, and W. S. Gregory

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Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

ABSTRACT

FIRAC is a medium-sized computer code designed to predict fire-induced flows, temperatures, and material transport within the ventilating systems and other airflow pathways in nuclear-related facilities. The code is designed to analyze the behavior of interconnected networks of rooms and typical ventilation system components. This code is one in a family of computer codes that is designed to provide improved methods of safety analysis for the nuclear industry. The structure of this code closely follows that of the previously developed TVENT and EVENT codes. Because a lumped-parameter formulation is used, this code is particularly suitable for calculating the effects of fires in the far field (that is, in regions removed from the fire compartment), where the fire may be represented parametrically. However, a fire compartment model to simulate conditions in the enclosure is included. This model provides transport source terms to the ventilation system that can affect its operation and in turn affect the fire. A basic material transport capability that features the effects of convection, deposition, entrainment, and filtration of material is included. The interrelated effects of filter plugging, heat transfer, gas dynamics, and material transport are taken into account. In this paper we will summarize the physical models used to describe the gas dynamics, material transport, and heat transfer processes. We also will illustrate how a typical facility is modeled using the code.

INTRODUCTION

FIRAC (1) is a computer code that is designed to predict the simultaneous gas dynamic, material transport, and heat transport transients that occur in a facility that is subjected to a fire. The code is directed toward nuclear fuel cycle facilities and the primary release pathway—the ventilation system. However, the code is applicable to other facilities and can be used to model other airflow pathways within a structure.

The models used in the code may be divided into three principal categories.

- Gas dynamics models
- Material transport models
- Heat transfer models

A brief summary of these models is given below. We have chosen to discuss the gas dynamics and convective material transport capabilities of the FIRAC code in detail. The code allows the user to couple to it any fire compartment model available provided that the output of the compartment model is in one of two forms.

- Pressure and temperature time history
- Energy and mass time history

We will illustrate the use of the code in modeling a typical nuclear facility.

MODELS OF PHYSICAL PHENOMENA

The lumped-parameter method is the basic formulation that describes the airflow system. No spatial distribution of parameters is considered in this approach, although an effect of spatial distribution can be approximated by noding. Network theory, using the lumped-parameter method, includes a number of system elements called branches joined at certain points called nodes. Ventilation system components that exhibit flow resistance and inertia (such as dampers, ducts, valves, and filters) and that exhibit flow potential (such as blowers) are located within the branches of the system.

The connection points of branches are nodes for components that have finite volumes, such as rooms, gloveboxes, and plenums, and for boundaries where the volume is practically infinite. Therefore, all internal nodes possess some finite volume where fluid mass and energy storage are taken into account.

Gas Dynamics (2)

Mass Equation. The continuity equation (conservation of mass) is applied at each internal node. The mass equation for such nodal points is

$$V \frac{d\rho}{dt} = \sum_k \dot{m}_k + \dot{M}_s \quad , \tag{1}$$

where $\dot{m}_k$ is the mass flow rate in branch k, and ρ is the density of the node. $\dot{M}_s$ is the user-specified mass source per unit time for the volume, and V is the volume of the node. The convention used here is that positive mass flows represent flow into the node.

Energy Equation. The energy equation used in the code is

$$\frac{dp}{dt} = \frac{R}{C_v V} \sum_k \dot{m}_k C_p T_k + \frac{v_k^2}{2} + \dot{M}_s C_p T_s + \dot{E}_s \quad , \qquad (2)$$

where the nodal pressure is p, and R, C_v, and C_p represent the gas constant, specific heat at constant volume and specific heat at constant pressure, respectively. T_k and v_k are the branch gas temperature and velocity. The temperature associated with mass addition is T_s, and the energy addition is E_s. A perfect gas law has been used to obtain this expression.

Momentum Equation. A momentum equation of incompressible form for a duct with constant area is used.

$$\frac{\ell}{A}\frac{d\dot{m}}{dt} = -\left(p_2 - p_1 - \frac{f}{D}\frac{1}{A^2}\frac{\dot{m}|\dot{m}|}{2\bar{\rho}} + \bar{\rho} g \Delta z\right) \quad , \qquad (3)$$

where ℓ and A are the duct length and cross-section area, ρ is the average density in the branch, g is the acceleration of gravity, and Δz is the elevation change across the branch. The values f and D represent the Moody friction factor and hydraulic diameter, respectively. For a branch with sudden area change, the following momentum equation is obtained.

$$I\frac{d\dot{m}}{dt} = p_i - p_j - K_{eff}\frac{1}{A^2}\frac{\dot{m}|\dot{m}|}{2\bar{\rho}} + \bar{\rho} g \Delta z \quad , \qquad (4)$$

where

$$I = \frac{\ell_i}{2A_i} + \frac{\ell}{A} + \frac{\ell_j}{2A_j} \quad , \text{ and} \qquad (5)$$

$$K_{eff} = \left(\frac{f\ell_i}{2D_i} + K_i\right)\left(\frac{A}{A_i}\right)^2 + \left(\frac{f\ell}{D} + K\right) + \left(\frac{f\ell_j}{2D_j} + K_j\right)\left(\frac{A}{A_j}\right)^2 \quad . \qquad (6)$$

I represents the inertia effect of the flow path between nodal points i and j. This includes the rooms as well as the duct. K_{eff} is the total effective resistance coefficient; the minor losses, such as turning, entrance, and exit, are represented by the K's.

An implicit numerical scheme is used to solve for the pressure and density corrections at each node. The iterative process continues until both the pressure and density corrections approach zero and the system is balanced.

Branches form the connection between any two nodes. Branch models are provided to represent

- ducts,
- dampers or valves,
- filters, and
- blowers or fans.

The individual components that are modeled within the network branches are discussed in more detail below.

Ducts. Ducts are modeled using the momentum equation discussed above. A distinguishing characteristic of the duct model is the nonlinear steady-state pressure drop relationship

$$\Delta p = R\rho v^2, \qquad (7)$$

where Δp is the pressure drop across the duct, ρ is the density, v is the gas velocity, and R is a constant resistance coefficient. The code will calculate the value of the resistance coefficient based on the initial values of pressure drop and flow. Alternately, a user-specified resistance coefficient may be used. The resistance coefficients are used to obtain both the steady-state and transient results.

Because a lumped-parameter formulation is used in this code, no spatial distribution of parameters along the length of the duct is calculated. However, the user may obtain more spatial detail by dividing the duct into a number of smaller sections. For example, a 100-ft-long duct could be treated as 10 10-ft-long ducts in series.

The heat transfer effects along the length of the duct will be calculated if requested by the user. Otherwise, heat transfer effects are neglected.

Filters. Filters are modeled as elements that exhibit only resistance to flow (that is, no inertia, buoyancy, or heat transfer). In general, the pressure drop across a clean filter consists of a sum of linear and quadratic dependences on the flow rate. The equation is of the form

$$\Delta p_o = aQ + b\rho Q^2 \quad , \qquad (8)$$

where Δp_o is the filter pressure drop, Q is the volumetric flow rate, ρ is the gas density, and a and b are constants. In general, use of only the linear part of the curve (b = 0) is applicable to fire situations. In this case, the code will calculate the value of the resistance coefficient, a, based on initial values of pressures and flow rates. If necessary, the complete equation may be specified; this option requires additional user information.

A filter plugging model is provided when there is material accumulation on the filter. The net result is that a filter with material accumulated on it is modeled by a relation of the form

$$\frac{\Delta p}{\Delta p_o} = 1 + \alpha M_a \quad , \qquad (9)$$

where Δp_o is the pressure drop for a clean filter (at the same flow rate), Δp is the pressure drop for the dirty filter, M_a is the material mass on the filter, and α is the filter plugging factor dependent on filter and material properties and has units of the reciprocal of mass. The resistance for dirty filters usually is estimated as 2 to 5 times that for clean filters.

Dampers and Valves. Dampers and valves are modeled as elements that exhibit only resistance to flow. The pressure drop across these elements is modeled as a quadratic dependence on the flow rate,

$$\Delta p = RQ^2 \quad . \qquad (10)$$

The resistance coefficient, R, may be calculated by the code or specified by the user.

Blowers and Fans. The blower model essentially depends on the performance curve of the blower obtained at standard conditions. The model then adjusts these data to predict the blower performance at off-design conditions. The blower head/flow characteristic curve is specified as a number of points on the curve obtained from the manufacturer's data and measured at standard conditions ($\rho = 0.075$ lb/ft^3). The curve then is approximated by a number of straight-line segments as shown in Fig. 1. All the segments should have a negative slope.

During a fire transient, the gas density at the fan may vary a great deal, and the curve must be modified to take into account the density variation from standard conditions. Similarity analysis as well as experimental measurements show that it is possible to correlate the blower performance at any density, ρ, if the performance at a given density ($\rho = \rho^0$) is measured.

In the solution procedure for the gas dynamics it is necessary to have an expression for the flow rate as a function of the differential pressure. Therefore, the solution is of the form

$$Q = g\left(\frac{\rho^0}{\rho}\right)\Delta p \quad , \tag{11}$$

where Q is the volumetric flow rate of the blower, Δp is the static pressure difference across the blower, and ρ^0 is the standard density from the manufacturer's literature.

Rooms, Cells, or Plenums. Components that have a finite volume (such as rooms, gloveboxes, plenums, cells, and so on) are modeled using capacitance or room nodes. The capacitance of the node is represented by its volume. Duct volume should be taken into account by including its volume in an adjacent room(s). Mass and energy storage at these nodes is taken into account by using the equations for conservation of mass and energy. The conservation equations are applied to the room nodes using a lumped-parameter formulation assuming a homogeneous mixture and thermodynamic equilibrium. Therefore, spatial details within the nodes are not predicted.

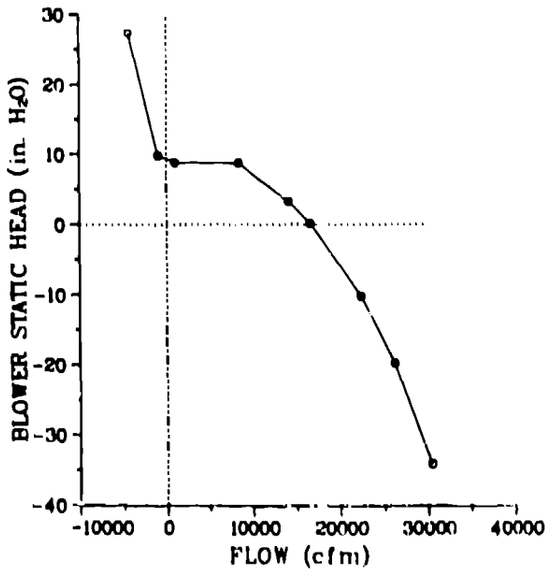

Fig. 1 Blower curve used

An ideal gas (air) equation of state is assumed in the conservation equations. In the room nodes, the user may specify various combinations of pressure and temperature transient values along with various combinations of energy and mass sources. If the quantities are not specified, they are calculated by the code.

Leakage. Leakage paths from the system to the atmosphere may be approximated in the model by using a boundary node and a fictitious duct. The initial specified duct flow rate is the desired leak rate. During the course of a transient, the leak rate will vary depending on the calculated system pressure response.

Material Transport Models (3)

The object of the material transport portion of the code is to estimate the movement of material (aerosol or gas) in an interconnected network of ventilation system components representing a given fuel cycle facility. Using this capability, the code can calculate material concentrations and material mass flow rates at any location in the network. Furthermore, the code will perform these transport calculations for various gas-dynamic transients. The code solves the entire network for transient flow and in so doing takes into account system interactions.

A generalized treatment of material transport under fire-induced accident conditions could become very complex. Several different types of materials could be transported. Also, more than one phase could be involved including solids, liquids, and gases with phase transitions. Chemical reactions could occur during transport, leading to the formation of new species. Further, for each type of material there will be a size distribution that varies with time and position depending on the relative importance of effects such as homogeneous nucleation, coagulation (material interaction), diffusion (both by Brownian motion and by turbulence), and gravitational sedimentation. We know of no codes that can handle transient flow induced material transport in a network system subject to the possibility of all of these complications. The transport portion of the code also does not include this level of generality. However, this version of the code does provide a simple material transport capability.

The material transport components of this code consist of the following.

(1) Material characteristics
(2) Transport initiation
(3) Convective transport
(4) Aerosol depletion
(5) Filtration

Material characteristics and transport initiation are areas that must be considered by the user as he begins to set up the code to solve a given problem. Calculations of convective transport, aerosol depletion, and filtration are performed automatically by the code. Items 2—5 are actually separate subroutines or modules within the code. Item 3, convective transport, is a key subroutine that calls on items 2, 4, and 5 as needed during the course of the calculation. We also will specify the required user specifications and provide appropriate references for the theory in each case.

Material Characteristics. The limitations of the material transport models with regard to the physical and chemical characteristics of the material are as follows. The pneumatically transportable contaminant

material can consist of any number of aerosol or gaseous species. However, no phase transitions or chemical reactions are allowed. For example, condensation and gas-to-particle conversion are not permitted. If the contaminant is an aerosol (solid particles or liquid droplets suspended in air), a size distribution can be simulated. In this case, within each size range, the material will be treated as monodisperse (equal-sized), homogeneous (uniform density), spherical particles or droplets during a given code run. Both the size and density of each specie must be specified by the user. If the contaminant is a gas, it is assumed to be inert.

Convective Transport. The code includes a simple material transport model with the capability of predicting airborne material distribution in a flow network and its release to the environment. Accidental release to the environment from a fire is a major concern in nuclear facilities because the airborne material could be radioactive or chemically toxic. The model is based on the assumptions that the particle size is small and its mass fraction is small relative to the gas mass in the same volume. This allows us to assume that the material and the gas form a homogeneous mixture and that they are in dynamic equilibrium. In this case, the gas-dynamic aspect of the problem is not affected by the presence of the airborne material, and the particulate or material velocity is the same as the gas velocity at any location and time. Accordingly, the only relation needed to describe the motion of the material is the continuity equation.

The continuity equation for any phase or component in a mixture is

$$\frac{d}{dt}\int_V \rho_p' dV = -\int_S \rho_p' \vec{u}_p \cdot d\vec{S} + \dot{M}_p \quad . \tag{12}$$

The time-derivative term on the left-hand side represents the change of the particulate density inside a control volume V. The first term on the right-hand side is the particulate flow through the boundary S of the volume V, and the last term is the particulate source. ρ_p and u_p are the mixture density and particulate velocity, respectively. M_p is an arbitrary material source term. Assuming that u_p is uniform over the control volume and using the same representation we used in the gas dynamics for the gas continuity equation, Eq. (12) becomes

$$V \frac{d\rho_p'}{dt} = \sum_i \rho_{pi}' u_{pi} A_i + \dot{M}_p \quad . \tag{13}$$

Here we drop the vector notion for the velocity but add subscript i to indicate the flow path connecting to that volume. A_i is the flow area and u_{pi} is the flow velocity normal to the area. The positiveness of the flux term is referred to as the flow into the volume. Introducing Y_p (defined as the mass fraction of the particulate) into Eq. (13),

$$V \frac{d}{dt}[Y_p \rho] = \sum_i Y_{pi} \rho_i u_{pi} A_i + \dot{M}_p \quad , \tag{14}$$

or

$$V \frac{dY_p}{dt} = \frac{1}{\rho}\left[\sum_i Y_{pi} \rho_i u_{pi} A_i + \dot{M}_p - Y_p V \frac{d\rho}{dt}\right] \quad . \tag{15}$$

The last term in Eq. (15) is the gas density change and is determined by the gas continuity equation.

Under the dynamic equilibrium condition, the particulate velocity is almost identical to the gas velocity everywhere and at any instance. Namely,

$$u_{pi} = u_i \quad . \tag{16}$$

u_i represents the gas velocity in the pathway i. Substituting that into Eq. (15) and recalling the gas mass flow in branch i,

$$\dot{m}_i = \rho_i u_i A_i \quad , \tag{17}$$

we obtain

$$V \frac{dY_p}{dt} = \frac{1}{\rho}\left[\sum_i Y_p \dot{m}_i + \dot{M}_p - Y_p V \frac{d\rho}{dt}\right] \quad . \tag{18}$$

Equation (18) is a differential equation for the unknown Y_p. Once the gas-dynamic quantities (ρ, m_i) are known, Eq. (18) can be integrated to obtain Y_p at a new time. The advantage of using Y_p instead of ρ_p as an unknown is that Y_p is not subject to the effect of compressibility as is ρ_p. Once Y_p is calculated, the particulate density can be obtained through

$$\rho_p' = Y_p \rho \quad . \tag{19}$$

The quantity mass fraction (or molar fraction) has been used extensively in fluid flow with chemical reaction.

Finally, we must emphasize again that the assumptions we have made about the dilute condition of particulates enable us to solve the gas-dynamic problem independently. The validity of the assumptions depends on the individual case, but we do believe this simple model provides a framework to establish a more enhanced combustion product transport scheme.

Material Depletion. Once the user has chosen to exercise the material transport option, he can calculate aerosol losses caused by gravitational sedimentation in rectangular or round horizontal ducts. Aerosol depletion may be calculated throughout the network during transient flow. The theory is based on quasi-steady-state settling with the terminal settling velocity corrected by the Cunningham slip factor. The flow in ducts and rooms is assumed to be well-mixed so that the aerosol concentration is uniform within the volume. The user must supply the aerosol diameter, density, and duct height to this model. The aerosol may consist of solid particles or liquid droplets.

Duct Heat Transfer

The purpose of the duct heat transfer model is to predict how the combustion gas in the system heats up or cools down as it flows throughout the ducts in the ventilating system. The model predicts the temperature of the gas leaving any section of the duct if the inlet temperature and gas properties are known. An ancilliary result of the calculation yields the duct wall temperature. A duct component is the only one for which a heat transfer calculation is performed. Furthermore, the calculation is performed in a given duct only if that branch has been flagged in the user specifications. Experience in using the code has shown that duct heat transfer calculations can increase the computer running time by a factor of 2. Therefore, we advise that duct heat transfer calculations be performed only where needed. The main region of interest and concern is generally those ducts downstream from

the fire compartment and especially between the fire compartment and any filters downstream from the fire compartment.

The overall model is composed of five distinct sub-models of heat transfer processes along with a numerical solution procedure to evaluate them. The heat transfer processes modeled are the following.

- Forced convection heat transfer between the combustion gas and the inside duct walls
- Radiation heat transfer between the combustion gas and the inside duct walls
- Heat conduction through the duct wall
- Natural convection heat transfer from the outside duct walls to the surroundings
- Radiation heat transfer from the outside duct walls to the atmosphere

FACILITY ANALYSIS EXAMPLE (4)

Facility Description

As an example fire accident, we have selected a slug-press fire in a pit enclosure in a large, 2474.9-m^3 (87 400-ft^3) process canyon. For illustrative purposes we chose to model a fuel fabrication plant (or a part of one) using the facility shown in Fig. 2. We located the process canyon at node 10 in Fig. 2. The initial steady-state volumetric flow rate through the process canyon is 56.6 m^3/s (2000 ft^3/min). The ventilation system inlet and outlet, burned-out glove ports, and all other leak paths must be considered as potential flow paths for aerosol-laden air in the case of a fire because the fire could produce a positive gauge pressure in a room under certain conditions.

Each facility (fuel fabrication plant, reprocessing plant, and so on) has unique parameters for each accident type. For instance, in fires, this requires selecting the combination of combustible materials along with the radioactive materials at risk that could become airborne from the accident-generated stresses. Materials that are at risk generally include open containers of finely divided powders (for spills) and liquids (for spills and boiling) and contaminated noncombustible surfaces, contaminated combustible material (liquids and solids), liquid and powders in containers that could exceed design pressures and fail when heated in fires, and radioactive metals, such as plutonium or uranium, that are combustible in themselves.

We selected the slug-press enclosure for the example fire because it contains combustible hydraulic fluid, large numbers of combustible rubber gloves set in glove ports, and surface contamination that can become airborne during the fire.

Fire Accident Description

Although FIRAC will accept arbitrary parameterization of the fire accident from compartment fire models, we have chosen to define these parameters without using a compartment fire model.

The following are considered as combustibles in the hypothetical example accident.

- 1 pt of acetone used in cleaning a hydraulic fluid spill
- 2 pt of hydraulic fluid
- 34.3 kg of other combustibles (rubber gloves, other elastomers, and plastics) calculated as 1,3 butadiene rubber

The radioactive source terms are a result of contamination on the rubber combustibles and on a mixed-oxide storage container that overpressurizes and spills at 230 s, resulting in 940 g of airborne material.

In defining an accident scenario, we recognize that accidents probably only occur if abnormal conditions exist in the room or process area of concern. These abnormalities could be spilled combustibles, inappropriately used solvents, failed and shorted electrical equipment, leaked explosive gases, degraded ion exchange resins, weakened process equipment, and accidentally arranged critical masses.

The fire example was constructed from two abnormalities, a leaky slug press and an accidental spill during cleanup with a flammable solvent. The solvent was spilled and ignited by hot equipment, which in turn caused the leaked slug-press fluid to burn and melt the rubber gloves, adding to the burning material. The accident data shown in Table I result from this hypothetical scenario. The combustible materials were

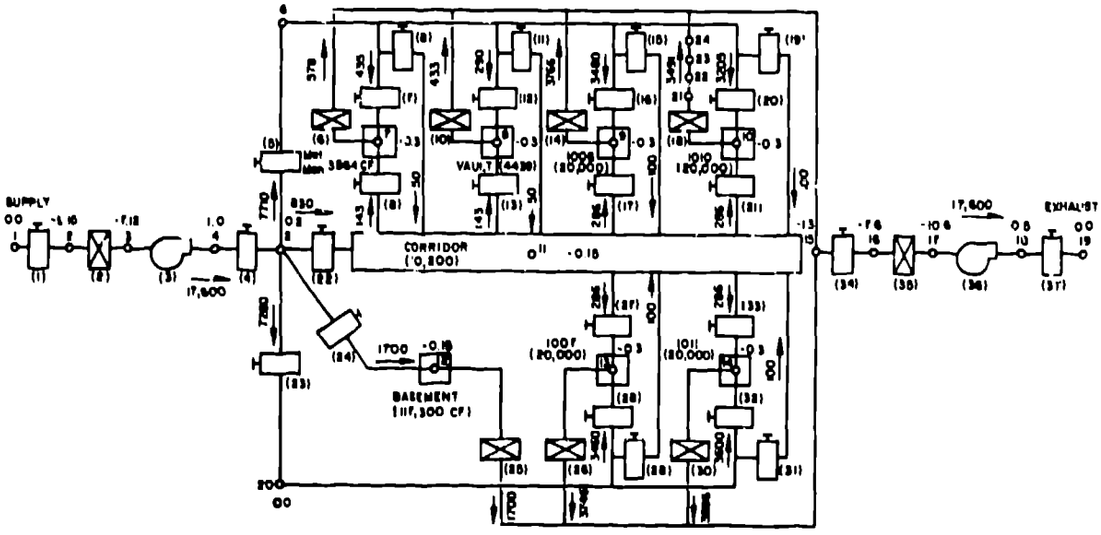

Fig. 2 FIRAC representation of a fuel processing facility

Table 1. Summary of source terms.

Individual Combustibles

Material	Acetone	Hydraulic Fluid as Dodecane	Other combustibles as 1,3 Butadiene Polymer	FIRAC Combined Source term
Amount (g)	374.0	710.0	34,300.0	
Burning Time (s)	37.4	71.0	230.0	230.0
q_t (kcal/s)	73.5	102.2	1225.0	
(kW)	308.0	428.0	5122.0	
q_c (kcal/s)	44.1	48.0	503.0	
(kW)	185.0	201.0	2098.0	2190.0
q_r (kcal/s)	29.4	54.2	722.0	
(kW)	123.0	227.0	3024.0	
Smoke Amount (g)	0.01	1.0	1300.0	1300.0
Size Distribution VMD (μm)		1.3	1.0	1.0
σg	2.0	1.5	1.5	
Gas Volume Flowrate (L/s)	510.0	605.0	348.0	
Gas Temperature (°C)	1100.0	900.0	695.0	
Radioactive Particles Given Off (g MOX/s)	5×10^{-6}	5×10^{-6}	1.043	1.043
Equipment Failure at 230 s				940.0 g MOX
MOX Size Distribution	g = 2.46 mean AED = 13 μm			

assumed to burn completely over the same time interval. The fire source terms are shown schematically in Fig. 3.

Using the facility described above, we can calculate the effect of a fire in the process canyon as described above. We will use the FIRAC computer code to show what the analyst can determine in this example. We have added three nodes in the exhaust duct from node number 10 to better calculate the spatial temperature variation leaving the process canyon. The revised detail noding is shown in Fig. 4.

Calculative Results. The initial pressure in the process canyon is 0.76 cm w.g. (-0.3 in. w.g.). During the transient, this pressure is expected to increase because of two factors.

1. Volumetric expansion of the gas in the fire compartment (and possibly reverse flow in the intake ducts) because of heating from the fire.
2. A general decrease in the fire compartment exhaust flow rate, which has two causes.
   - Degradation in the blower performance because of higher temperatures (lower densities) at the exhaust blower inlet
   - Higher resistance to flow in the exhaust duct because of filter plugging

The FIRAC-predicted pressure transient experienced in the process canyon is shown in Fig. 5 and is a consequence of the above factors (as are the other results). The process canyon generally experiences positive pressure for 325 s. During the period of positive pressure, unfiltered leakage from the canyon and reverse flow in the intake ducts is a possibility.

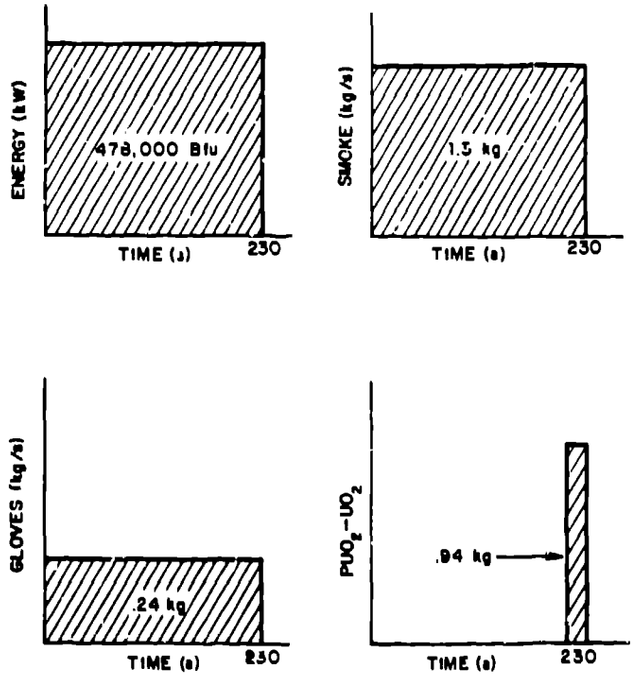

Fig. 3 MOX plant accident source terms for slug-press scenario

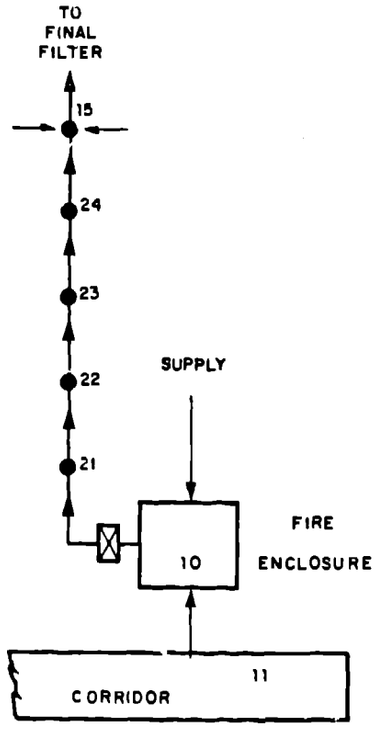

Fig. 4 System schematic (near fire enclosure)

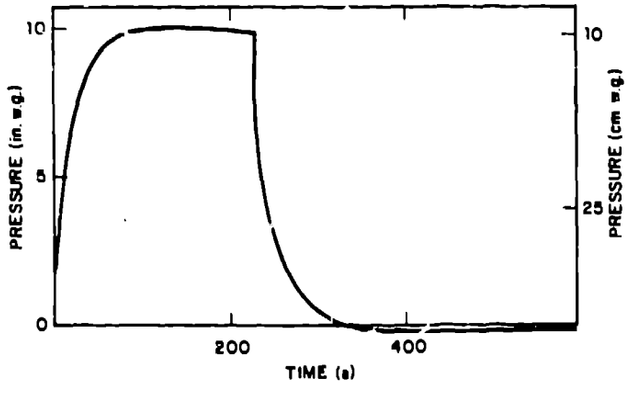

Fig. 5 Process canyon average pressures

The resulting reverse flow in the intake ducts is shown in Fig. 6. The supply duct experiences a flow reversal for approximately 4 min, whereas the corridor flow rate remains negative because of filter plugging by particulate material. These negative flows could contaminate the facility.

Two of the principal results of the calculation are the gas temperature and the differential pressure that occur at various locations, especially the filters. The temperature at the process canyon exhaust filter is shown in Fig. 7. The maximum temperature reached is 461°F, and therefore, the filter is not in jeopardy because of high temperatures. The differential pressure across this filter is shown in Fig. 8. The peak differential pressure achieved is 10.7 cm w.g. (4.2 in. w.g.), which is well below the filter's breaking point.

The particulate species are injected and mixed with the combustion gas in the process canyon, are further diluted by the intake air, and are swept constantly into the exhaust system. In the exhaust system, they are swept toward the filters and diluted by merging airstreams. Figure 9 shows the distribution of each species at the end of the calculation (10 min). The largest fraction of each species remains airborne at this time, and almost none escape through the exhaust filters because all exhaust from the system must pass through double filtration.

SUMMARY

We have discussed a computer code called FIRAC that is designed to predict simultaneous gas dynamic, material transport, and heat transport transients that occur in a facility that is subjected to fire. The code is directed toward nuclear fuel cycle facilities and the primary release pathway—the ventilation system. We have described the gas-dynamic and material convection models in considerable detail. The heat transfer models that are used in the code are listed for review. Finally, we have illustrated the application of the FIRAC computer code with a hypothetical fire in a fuel fabrication facility. Temperature, pressure, flow, and material distribution data within the facility at selected locations are provided.

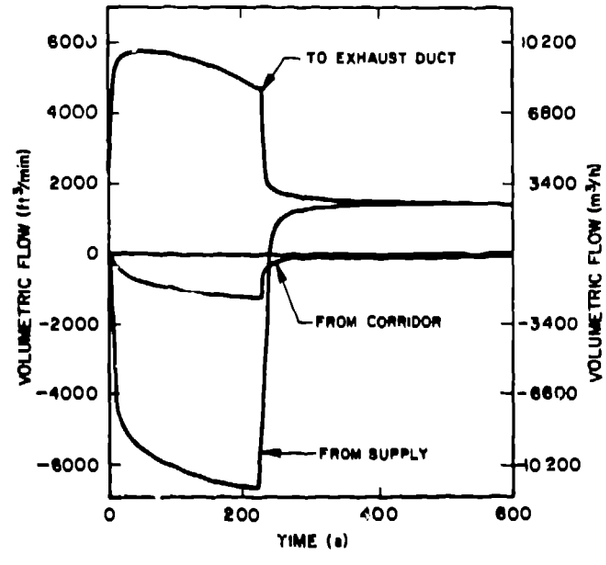

Fig. 6 Flow rates into and out of the process canyon

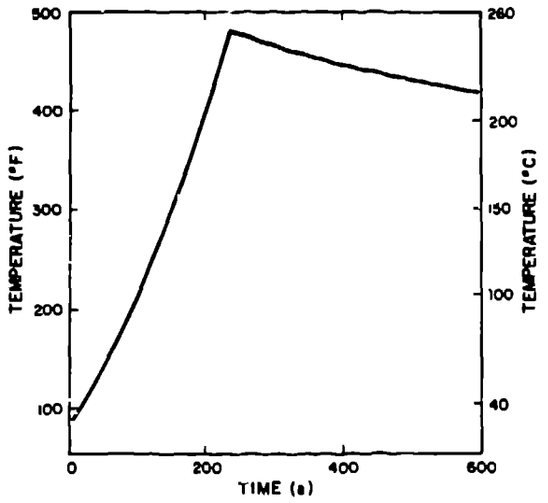

Fig. 7 Process canyon exhaust filter temperature

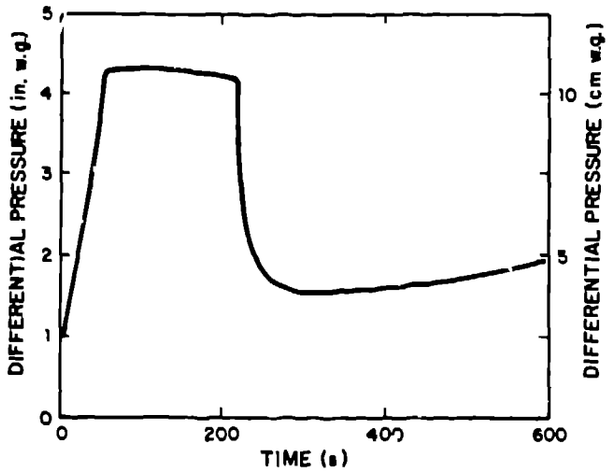

Fig. 8 Process canyon exhaust filter differential pressure

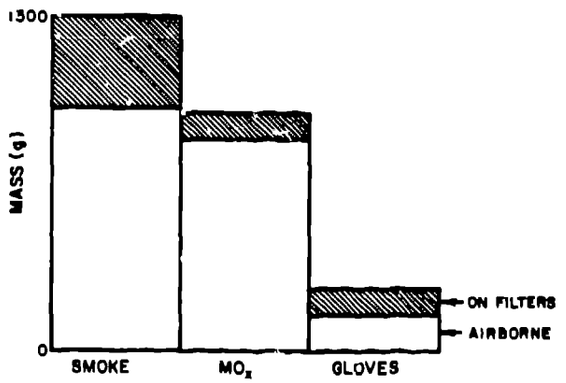

Fig. 9 Material distribution 10 min after accident

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