

## USE OF REAL DATA IN MODEL DEVELOPMENT FOR ACCIDENT ANALYSIS

**Clint Shaffer,\*\* Patrick McClure,\* Bruce Letellier,\* and Mark Leonard\*\***

\* Los Alamos National Laboratory

\*\* Innovative Technology Solutions

(505) 872-1089 • CJShaffer@itsc.com

### ABSTRACT

This work supported the accident analysis at the Device Assembly Facility (DAF) located at the Nevada Test Site by predicting facility leak path factors (LPFs) for a comprehensive selection of accident scenarios. DAF is the nation's most modern joint high explosive and plutonium facility, where its unique design and capability make it ideally suited for many operations in support of the nation's Stockpile Stewardship and Management Program. The MELCOR 1.8.4 severe accident computer code was chosen to perform these accident simulations because the code contained models for both the thermal-hydraulic processes and the aerosol transport processes and solved the models simultaneously in a fully integrated calculation.

Validation of the data used in the model and of model results was an important part of the model development phase for this effort. As a part of the effort to model the facility accurately, actual flow and pressure measurements were made for the critical areas of the facility. (For this facility, these were the explosive confinement cells). The data from these measurements were reduced into an equivalent set of flow-resistance parameters that could be represented in the model. This allowed for modeling of the flow distribution during real accident situations as accurately as possible. The technique used for these measurements, the reduction of the data, and its input into the computer model are discussed in the paper.

The assembly cells at DAF use a gravel roof concept to mitigate the consequences of an explosion. Following a sufficiently large explosion, the gravel bed overlying the cell is designed to lift and vent explosive gases and while filtering the plutonium aerosol from the gas flows. A realistic simulation of the lifting of the gravel roof was essential to adequately predict plutonium releases to the environment; including simulating the explosion, the dynamically changing free volume of the cell, and gas flow through the gravel bed. A 1982 full-scale test of the gravel roof concept was used as a benchmark to validate these models. The pertinent test data included the pressure and temperature within the cell immediately following the explosion, and aerosol transport and release data. The MELCOR model used for the DAF study very accurately predicted the appropriate response from the 1982 test. The method developed for modeling a gravel-roof device assembly cell could be adapted to other facilities employing the gravel-roof assembly cell concept. The results are discussed in the paper.

The entire model is described. Explosive venting into the remainder of the facility was also simulated including the operating ventilation systems. The models for important components of the facility, such as, the blast valves, the fire dampers, ventilation fans, were based on operational data. In addition to explosive scenarios, postulated fire scenarios were simulated, based on the results of the accepted CFAST fire code.

These analyses were more realistic, yet conservative, than typical safety analyses of this type. Analyses performed using realistic and validated models and with attention paid to detail and thoroughness led to a greater understanding and acceptance of how a facility would respond to postulated accidents. Further, realistic simulations substantially reduced the need for excessively conservative assumptions. This paper provides an illustration of the potential of state-of-the-art analytical tools to perform realistic safety analyses and how they can be enhanced by use of real data and benchmarking.

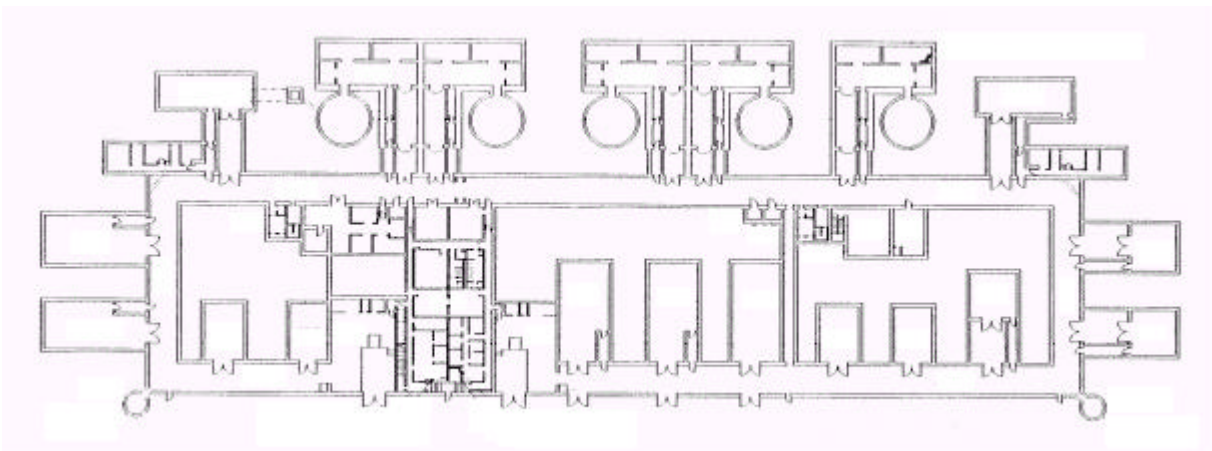
## INTRODUCTION

Severe postulated explosion and fire accidents at the Device Assembly Facility (DAF) located at the Nevada Test Site were performed in support of the DAF safety analysis report (SAR). These analyses were performed in a realistic and comprehensive manner resulting in a much more complete accident knowledge base than is usually created for a DOE facility. The models were benchmarked to the extent reasonably possibly using full-scale test data, as well as system and component performance data. Use of real facility data led to more realistic simulations that in turn tended to reduce the overall level of conservatism. The knowledge base, resulting from a comprehensive selection of over 100 accident simulations, provided extensive information regarding facility contamination and personnel hazards, as well as, the risk to the public. The relative importance to confinement of various systems functioning as intended was determined. Many future safety questions that may come up during the operation of the facility could well be answered from information in the knowledge base alone. Additional simulations using existing analytical models with relatively minor modifications might well answer other safety questions. Further, the analytical models can be upgraded to match facility upgrades.

## THE FACILITY

The Device Assembly Facility (DAF), located in the east central portion of the Nevada Test Site, is the nation's most modern joint high explosive and plutonium facility. The DAF unique design and capability make the facility ideally suited for many operations in support of the nation's Stockpile Stewardship and Management Program, such as assembly, disassembly, modification, staging, transportation, radiography, maintenance, repair, retrofit, and surveillance of nuclear weapons and weapons components. In the unlikely event of an accidental explosion in the presence of plutonium, a plutonium release to the environment could potentially put the public at risk.

The DAF consists of a group of 30 individual steel-reinforced concrete buildings connected by corridors in a rectangular plan as shown in Fig. 1. The DAF is completely covered with earth except for one wall that was left exposed to allow access. The buildings include assembly cells, radiography bays, assembly bays, high bays, bunkers and vaults, a testing laboratory, decontamination rooms, shipping/receiving docks, an administration building, and security facilities. The DAF meets the DOE criteria for moderate-hazard facilities. Among these criteria is the requirement to prevent fatalities and severe injury to personnel in normally occupied areas. Design features to ensure this level of protection include interlocking blast doors to mitigate the propagation of an explosion, blast-actuated valves to prevent migration of contamination, special ventilation features such as zoned air-pressure systems and high-efficiency particulate air filters, and the gravel roof design in the assembly cells.



**Fig. 1. Floor Plan of the DAF Complex.**

The gravel-roof design employed a confinement system based on a suspension system supporting more than 20 ft of gravel. In the unlikely event of an explosive detonation, the roof is designed to expand upward, then collapse back into the cell thereby trapping virtually all-radioactive particles in the gravel matrix. Assembly cells, because of their gravel roof feature, are the only facilities at the DAF where special nuclear material and uncased conventional high explosives may be collocated.

## **ACCIDENT SCENARIOS**

Severe accident analyses were performed for postulated explosions and fires in typical buildings of the DAF facility. This paper focuses on the postulated explosion scenarios for an assembly cell. The primary result of these analyses was conservative estimates of the leak path factors (LPFs) for the respirable portion of an explosion-generated plutonium aerosol. These LPFs subsequently were used in other analyses to estimate potential radiological dosages to the nearest public. In addition to these LPFs, considerable other knowledge was gleaned from the analyses regarding the transport of plutonium through and from the facility, the important transport pathways, internal contamination, the effect of isolation equipment failures, etc.

Three sizes of explosion scenarios were simulated in the analyses, i.e., 55 lbm, 85 lbm, and 423 lbm of high explosives located in the round room. The 55- and 85-lbm explosions were assumed to not produce pressures high enough to lift the gravel roof, whereas the 423-lbm explosion most certainly would lift the roof, thereby venting the explosive gasses through the bed of gravel. Following the simulation of a base scenario for each size of explosion, other scenarios were run to simulate alternate facility configurations, such as the positions of the blast doors at the time of the explosion. Still other calculations simulated postulated failures of facility systems and components to perform their designed functions, such as a blast valve failing to close.

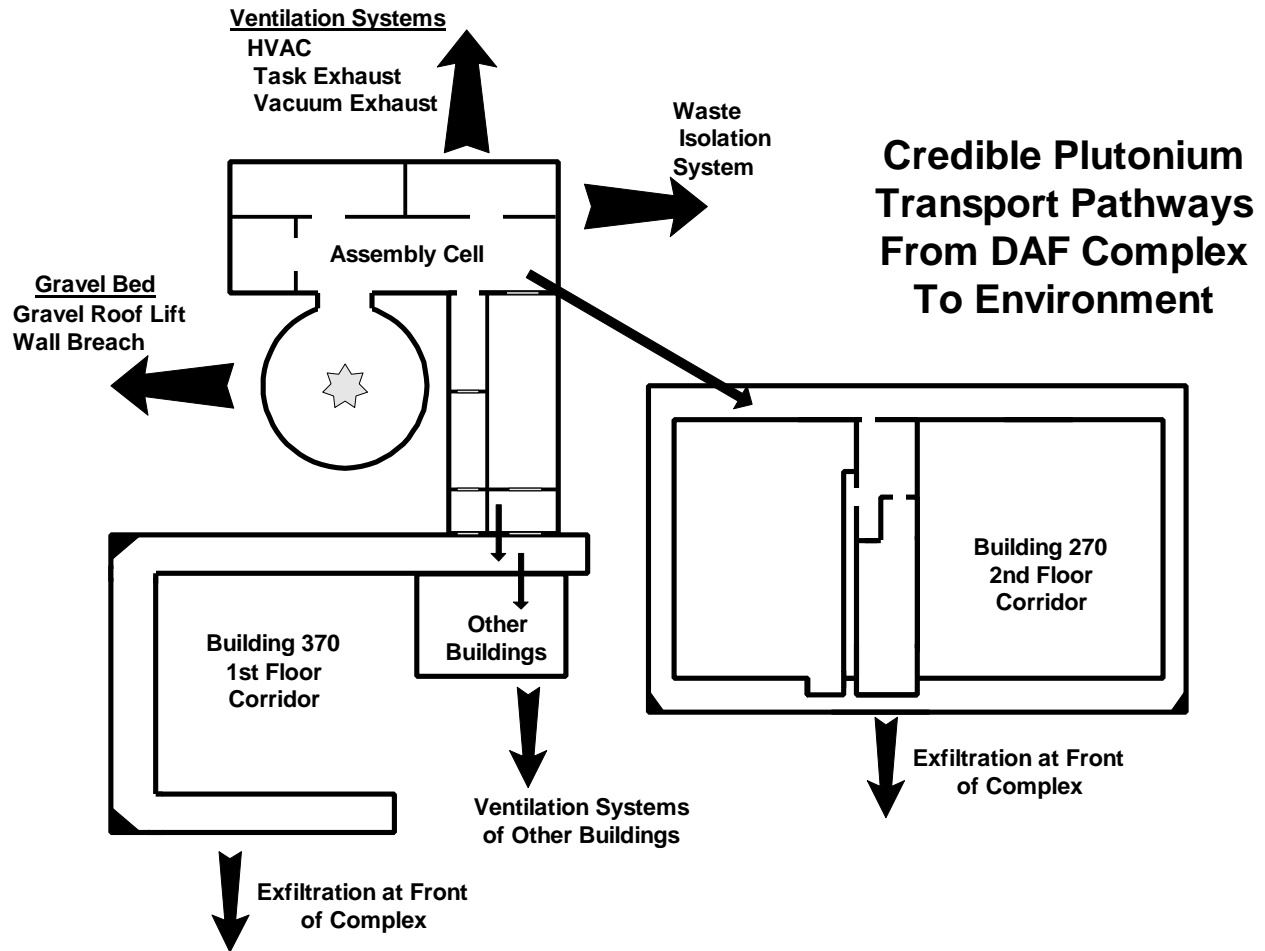
## **LEAKAGE PATHWAY IDENTIFICATION**

The important pathways through which plutonium could escape the confinement of the assembly cell and be transported to the environment were identified. These pathways, shown in Fig. 2, included the assembly cell gravel roof, an assembly cell wall breach, the assembly cell ventilation systems, and the waste isolation system and pathways leading into and through the remainder of the facility. The facility pathways included wiring conduits between the cell and the service level and the blast and entry doors from the cell to the other buildings and from the other buildings to the environment.

## **THE COMPUTER CODE**

The MELCOR 1.8.4 code [NUREG/CR-6119] was chosen to perform these accident simulations because this code contained models for both the thermal-hydraulic and the aerosol transport processes and solved the models simultaneously in a fully integrated calculation. Further, the extreme flexibility of the input capability of MELCOR made it possible to model the variety systems and system components at DAF. The MELCOR code, which was developed at Sandia National Laboratories for the U. S. Nuclear Regulatory Commission, is a fully integrated computer code that models the progression of severe accidents in light-water-reactor nuclear power plants. MELCOR was adapted to simulate the DAF facility through user input by activating only the applicable code models, specifically the thermal-hydraulic models and the radionuclide transport models.

The thermal-hydraulic behavior is modeled with a lumped-sum approach using control volumes connected by flow paths. Noncondensable gases are modeled as ideal gases with temperature-dependent specific heat capacities. The transfer of heat between control volume atmospheres and their surrounding surfaces are modeled using heat structures. Radionuclides may deposit directly on surfaces such as heat



**Fig. 2. Illustration of Credible Plutonium Transport Pathway from DAF to Environment.**

structures, and aerosols may agglomerate and settle. The particle coagulation processes modeled include Brownian diffusion, gravitational settling, and turbulent impaction. The aerosol deposition processes modeled include gravity, diffusion, thermophoresis, and diffusiophoresis.

### **GRAVEL ROOF LIFT MODEL**

The gravel roof was designed to confine large-scale explosions inside the DAF assembly cell by relieving the explosive pressures directly to the outside, thereby limiting structural damage to the cell. In effect, a large-scale explosion would lift the gravel roof of the round room to a height where the explosive gases can vent through the gravel to the outside. The gravel bed would also filter most of the plutonium aerosols from the vented flows. Of the explosions simulated in this study, only a 423-lbm explosion was sufficiently large to lift the gravel roof.

Detonation of high explosives generates heat and gas combustion products that both can lead to pressurization and/or expansion of the confinement volume. The amounts of each depend on the availability of oxygen to drive combustion. Oxygen can be provided in the chemical composition of the explosive, and it can be drawn from air present in the confinement volume. For this analysis, pure HMX was detonated in the round room with an excess of oxygen. The heat of combustion was computed from

the assumed stoichiometry by taking the difference of the combined heats of formation for the reactants and for the products. Combustion products added to the round room included nitrogen, carbon dioxide, and vapor. Oxygen was removed from the round room.

The functionality of the gravel roof design was tested in 1982 by performing a full-scale test of a 423-lbm explosion [SAND84-0618]. The gravel roof was shown to function as designed to relieve pressures and to retain most of the simulated plutonium aerosols within the gravel. The internal geometry of the round room roof extension following the explosion could not actually be determined; however the exterior rise of the gravel bed was measured as a function of time. Other important data such as the round room pressure also were measured. The MELCOR model of the gravel roof was benchmarked against the full-scale test.

The operation of the gravel roof is shown in the schematic series shown in Fig. 3, i.e., its initial configuration before the explosion, the fully extended height of the gravel bed, and its final position. The height of the gravel bed indicated that the maximum round room volume would be approximately twice its normal operational volume. Following the explosion, the gravel bed would drop back into the round room, effectively filling the entire room with gravel and likely some gravel would spill out into the staging area.

An examination of the full-scale test results suggested that the operation of the gravel roof might be simulated using a simple piston model. Therefore, a simple cylindrical piston model was developed for implementation into MELCOR. The experimental bed height was simply multiplied by the cross-sectional area of the round room to obtain the time-dependent volume. The piston model round-room volume expanded to about twice its initial volume in about 1.4 s and then collapsed to zero at about 3 s as shown in Fig. 4.

For the objectives of this study, the important aspects of the gravel roof model were those thermal-hydraulic aspects that most affected the transport of plutonium aerosols from the assembly cell to the environment. Perhaps the single most important thermal-hydraulic aspect was the airflow rates from the round room, both the upward airflow through the gravel and the inward airflow to the staging area. Of course, the prediction of airflow rate depended heavily on the pressure differential driving the flows. Of secondary importance, but still important, were the temperatures of the air within the cell. Normally, the most important aerosol deposition mechanism for heavy plutonium particles would be gravitational settling. However, at higher temperatures such as those immediately following the explosion in the round room, the diffusion of submicron particles to surfaces was important as well.

Therefore, any valid model of the gravel roof and round room must have the features of simulating the explosive masses and energies of the explosion, the variable volume of the round room, and the flow resistance for each pathway from the round room, especially the flow through the gravel bed. As discussed, the variable volume can be reasonably approximated from the variation in the height of the gravel bed measured during the full-scale test. The flow characteristics for the gravel bed could not actually be measured; however, some reasonable approximations were deduced from the round-room pressure history of the test.

A MELCOR input model was developed that simulated this variable free volume in the round room by altering the volume of a fictitious pool of water. In this model, the control volume representing the round room included a water pool, as well as an atmospheric free volume. Obviously, the total volume of this control volume was substantially larger than the operational free volume of the round room. Initially following the explosion, water was removed from the control volume, so its free volume expanded. Then, when the maximum free volume was achieved, water was forced back into the control volume until almost all of the free volume was gone. The geometry of the control volume was arranged so that the

## Explosive Movement of Assembly Cell Gravel Roof

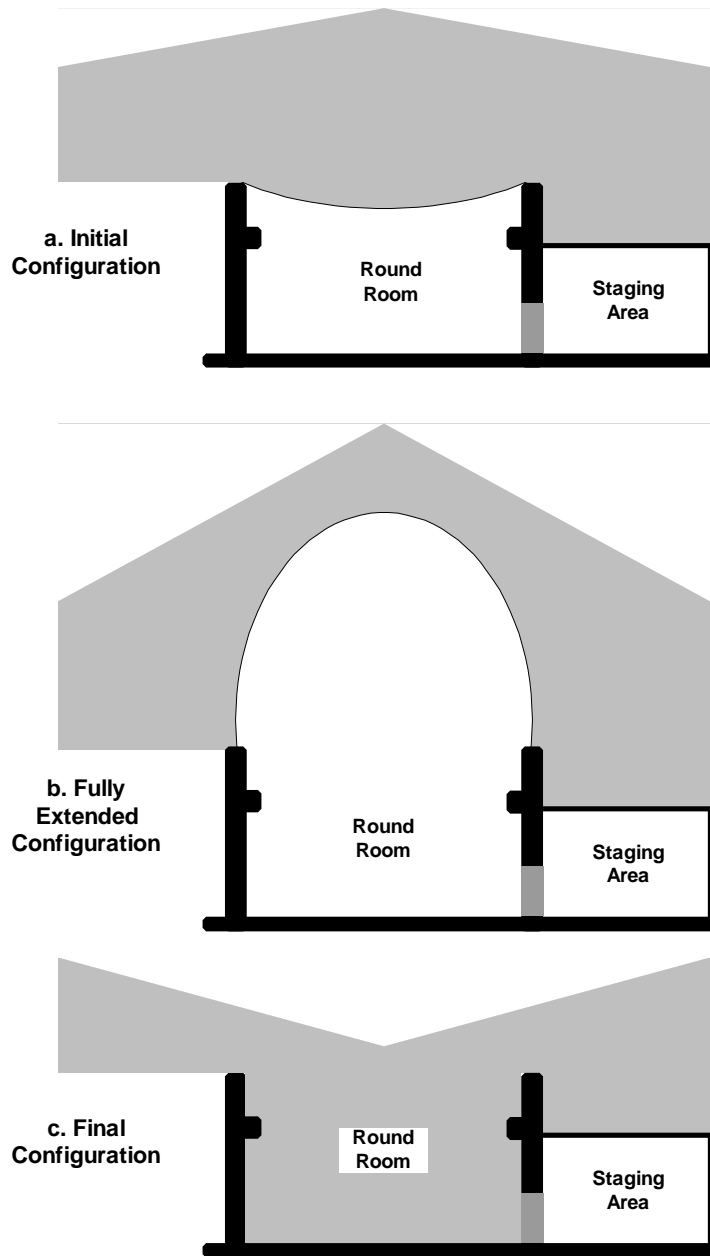
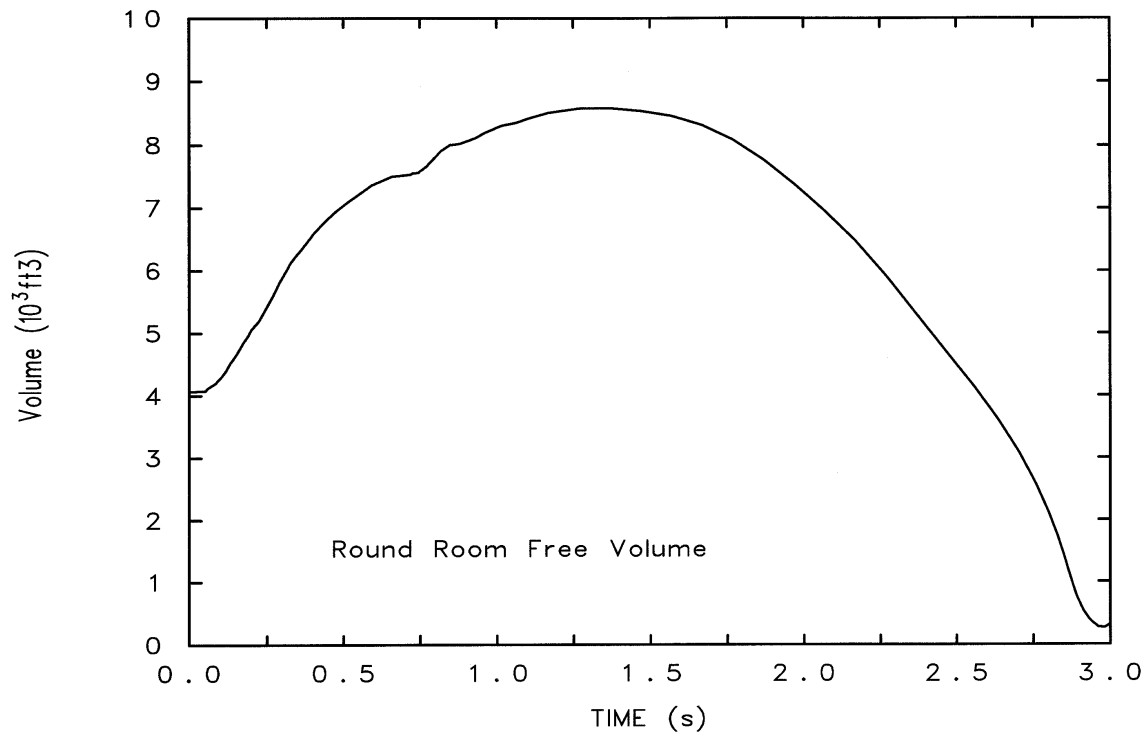


Fig. 3. Schematic of Gravel Roof Response to Explosion.



**Fig. 4. As-Modeled Round Room Free Volume.**

pool did not overflow into the staging area. Although this somewhat fictitious geometry did not exactly mimic the actual geometry of the expanding and collapsing gravel bed, the model accomplished the dynamic free volume changes needed to correctly simulate the round-room thermal-hydraulics and the aerosol transport from the round room. In other words, the goal of correctly simulating the internal pressure and temperature responses and the airflow from the cell to the outside and the staging area were adequately achieved.

The water pool was prevented from interacting thermal-hydraulically with the free volume by means of a MELCOR code modification that effectively turned off the pool's free surface in terms of mass and energy transfer. Other aspects of the fictitious pool also were considered. Heat transfer from the air to the floor was handled by moving the floor surface area above the maximum pool height. Aerosol deposition that normally would deposit onto the floor actually deposited into the fictitious pool at the same rates; however, the round room floor surface had to be deactivated as a deposition surface to avoid double accounting the round room floor deposition. Thus, the variable volume model did not affect the aerosol deposition process. All aspects considered, the MELCOR input variable volume model worked very well and accomplished all its modeling goals.

Because the explosion was simulated using the MELCOR code, its flow equation was necessarily used to simulate the gravel bed flow. The basic form of the MELCOR flow equation is

$$\Delta P = \frac{1}{2} \cdot K \cdot \rho \cdot V^2 = \frac{1}{2} \cdot \frac{K}{A^2} \cdot \frac{m^2}{\rho} \quad ,$$

where

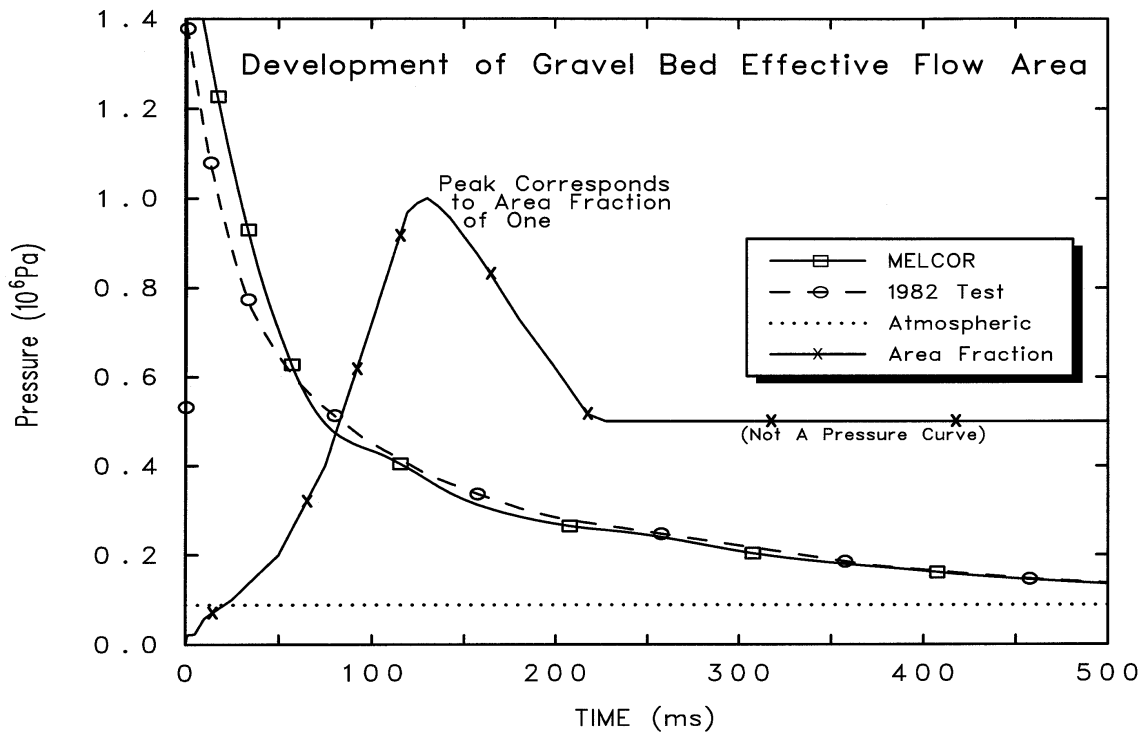
$V_p$  = the pressure differential,  
 $K$  = a constant known as the loss coefficient,  
 $\rho$  = the density of the fluid,  
 $A$  = the cross-sectional area of flow,  
 $V$  = the velocity of flow, and  
 $m$  = the mass flow rate.

This equation is valid for both incompressible flows and subsonic compressible flows of the type generally used in these types of analyses, i.e., flows moving at less than about half the speed of sound (~500 ft/s). Although the explosive flow through the gravel bed was extremely dynamic, as demonstrated by the full-scale test, the MELCOR simulation of the test indicated that peak flow velocities through the gravel were on the order of 300 ft/s. Therefore, the MELCOR equation for flow was reasonably appropriate for the gravel bed explosive flow.

The MELCOR flow equation required the specification of two flow parameters, i.e., the form loss coefficient and the flow area. Note that the value of one of these two parameters depended on the value selected for the other one and that one of the parameters needed to be time-dependent. In MELCOR, the flow area can be modeled in a time-dependent manner, but the loss coefficient cannot. Therefore, a reasonable value for the loss coefficient was estimated, and the time-dependent area was deduced from the full-scale test using its measured pressure in the round room. That is, having specified the variable volume and the gravel bed form loss coefficient, the time-dependent area was adjusted until the MELCOR predicted pressure reasonably well simulated the experimental pressure. Knowing what fixed value to use for the gravel bed form loss coefficient would be extremely difficult to do precisely, especially because it would actually be time-dependent. The objective here was to obtain a coefficient that would allow the time-dependent area to be reasonably sized. A loss coefficient appropriate to a steady-state fluidized gravel bed was selected as an estimate for the loss coefficient of the DAF gravel roof model. Treating the gravel roof as though it was a steady-state fluidized bed with a flow area equivalent to the round room floor area resulted in a loss coefficient of 240.

With the loss coefficient fixed at 240, the effective gravel bed flow was adjusted until the experimental pressure was reasonably approximated with MELCOR simulating the full-scale test. This simulation required certain models, such as the blast valves and other air leakage pathways from the cell, to be deactivated to correctly approximate the geometry of the full-scale test facility. The deduction of the effective time-dependent area is shown in Fig. 5. In this figure, the MELCOR-predicted pressures and the experimental pressures are compared directly along with the time-dependent area expressed as a fraction of the total round room floor area.

Initially, the flow area increased very rapidly to allow enough of the explosive gases to escape; otherwise, the MELCOR-predicted pressure could not drop fast enough. In reviewing this model, one should keep in mind the dynamics of the explosion. The cycling of the gravel from its initial state to its final collapsed state took place in only 3 s. The bed reached its maximum altitude in about **1¼ s**. Therefore, the explosion had to be vented in substantially less time than the peak bed height time. As shown in the figure, the area fraction peaked at a value of one at about 0.13 s and then rapidly dropped back down again. Note that the figure indicates a constant flow area after about 0.22 s. This was done because the area deduction process did not seem to work beyond this point; i.e., the remaining depressurization was not sensitive enough to the area to further develop the area. Instead, the area was held constant at this value until 3 s, when it was reduced to a small value that represented long-term leakage through the collapsed gravel bed.

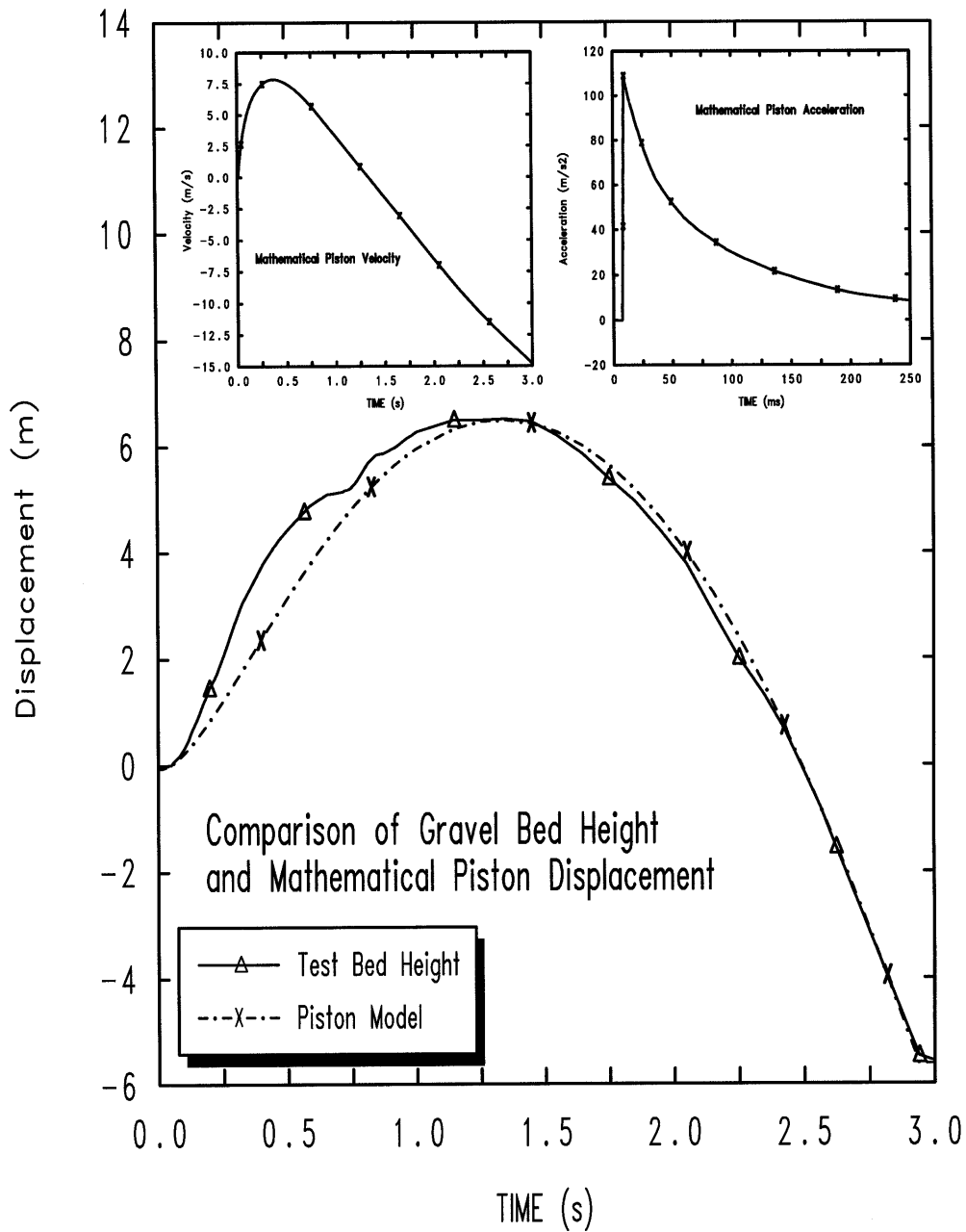


**Fig. 5. Development of the Gravel Bed Effective Flow Area.**

It should be remembered that these flow characteristics apply only when the time-dependent area, the loss coefficient of 240, and the MELCOR flow equation are used simultaneously. This gravel roof flow model was tested by successfully simulating the full-scale test, including the experimental aerosol transport.

After the complete collapse of the gravel bed back into the round room, air could still leak from the cell by way of the gravel filling the round room. The gravel roof flow pathway was kept partially open from 3 s to the end of the calculation as a means of simulating this leakage. Because leakage through the gravel was highly filtered by the gravel, it was conservative to underestimate the magnitude of the leakage.

The applicability of the simple piston model was verified further by comparing the piston dynamics, as predicted by Newton's Second Law ( $F = ma$ ), with the experimentally measured gravel bed height from the full-scale test. The force on the piston would be the round room pressure times the round room area less the force of gravity. The equations for piston displacement, velocity, and acceleration were programmed into the MELCOR input model using its control logic. Note that these equations were solved along with the rest of the model for additional information only and in no way affected the simulation of the gravel roof. The full-scale test pressure was used to drive the piston solution. The piston mass was estimated to be 1.7 million pounds based on a gravel bed depth, round room diameter, and the density of commercial grade gravel. The piston dynamics, i.e., displacement, velocity, and acceleration, derived from the solution of Newton's Second Law and the full-scale test pressure are shown in Fig. 6. The mathematically generated displacement is compared directly in the figure with the experimental gravel bed height, and these two curves compare rather well, resulting in additional reason to believe that the motion of the gravel bed can be modeled adequately as a simple piston. If future



**Fig. 6. Motion of Mathematical Piston Model.**

analyses were to attempt to estimate the gravel bed motion for other sizes of large explosions, other than the 423-lbm explosion, this finding should be useful.

The gravel bed filtration MELCOR input model was based on the filtration efficiency deduced from the data for the full-scale test. The test report stated that

- the total aerosol release fraction was 0.004 +/- 0.0015 and
- the respirable release fraction was 0.003 +/- 0.0011

Based on this information, a maximum of 0.004 of the respirable aerosol was released into the environment, resulting in a minimum respirable filtration efficiency of 99.6%. Further, it can be reasonably assumed that the nonrespirable mass released was nominally 1/3 that of the respirable release mass.

The gravel roof input model used in the 423-lbm explosion simulations was benchmarked against the 1982 full-scale test to ensure that both the thermal-hydraulic and aerosol transport models agreed with known experimental data. The MELCOR DAF model performed well in simulating the full-scale test. The test data indicated that the predicted respirable aerosol mass released from the gravel should range from 2.2 to 6.1 g. The MELCOR simulation predicted a respirable mass release of 5.7 g, well within the range for a successful simulation.

### **ASSEMBLY CELL BLAST DOORS**

When the blast and entry doors were closed, air infiltration around the doors occurred through gaps around the door perimeters with the largest gaps located at the bottom of the doors. The arrangement of the doors is shown in Fig. 7, which shows the nodalization of the assembly cell schematically. Either the personnel airlock or the equipment airlock, each of which has two unsealed blast doors and one sealed entry door accesses the cell. These leakage flows needed to be modeled correctly to determine such events as the time when the blast valves reopened correctly. Note that aerosol concentrations would be higher earlier in the scenario and the aerosol transport to the environment also would be higher if the blast valves opened earlier. Further, air also infiltrates through the conduits from the second floor into the cell. Estimating effective leak areas for the doors and conduits proved difficult to do because of the shapes of the seals, etc. Therefore, small-scale tests were conducted to measure effective leak areas. The tests were conducted by sealing off the ventilation except for the heating, ventilating, and air conditioning (HVAC) exhaust line and measuring the pressure differential between the first-floor corridor and the interior of the cell while measuring the HVAC airflow from the cell simultaneously. With these data, an effective flow resistance was calculated. The flow resistance then can be used to specify the area and loss coefficient used to model the flow, i.e.; the flow resistance in its simplest form is expressed as the area divided by the square of the loss coefficient. The measurements were made for a number of different door configurations, i.e., some doors were open and others were closed. Enough tests were conducted to deduce the effective flow resistance for each door and the conduits analytically.

### **COMPONENTS PERFORMANCE DATA**

Key components of the assembly cell ventilation and blast protection systems were modeled using manufacture performance data. These components included fans, airflow dampers, and valves. A schematic of the model for the main cell ventilation system is shown in Fig. 8. The ventilation systems were assumed to operate in their alarm mode following an explosion, i.e., signal would be received from either the fire alarm system or the radiation sensor alarm system. In the alarm mode, the entire HVAC system would be de-energized except for two exhaust fans.

The HVAC relief/exhaust and task exhaust fans were modeled using their respective fan performance curves, i.e., the static pressures across the fans as a function of the airflow rate through the fan. The performance curves were imposed on the respective fan flow pathway as a pressure addition. The performance of this model provided realistic flow rates through the fans.

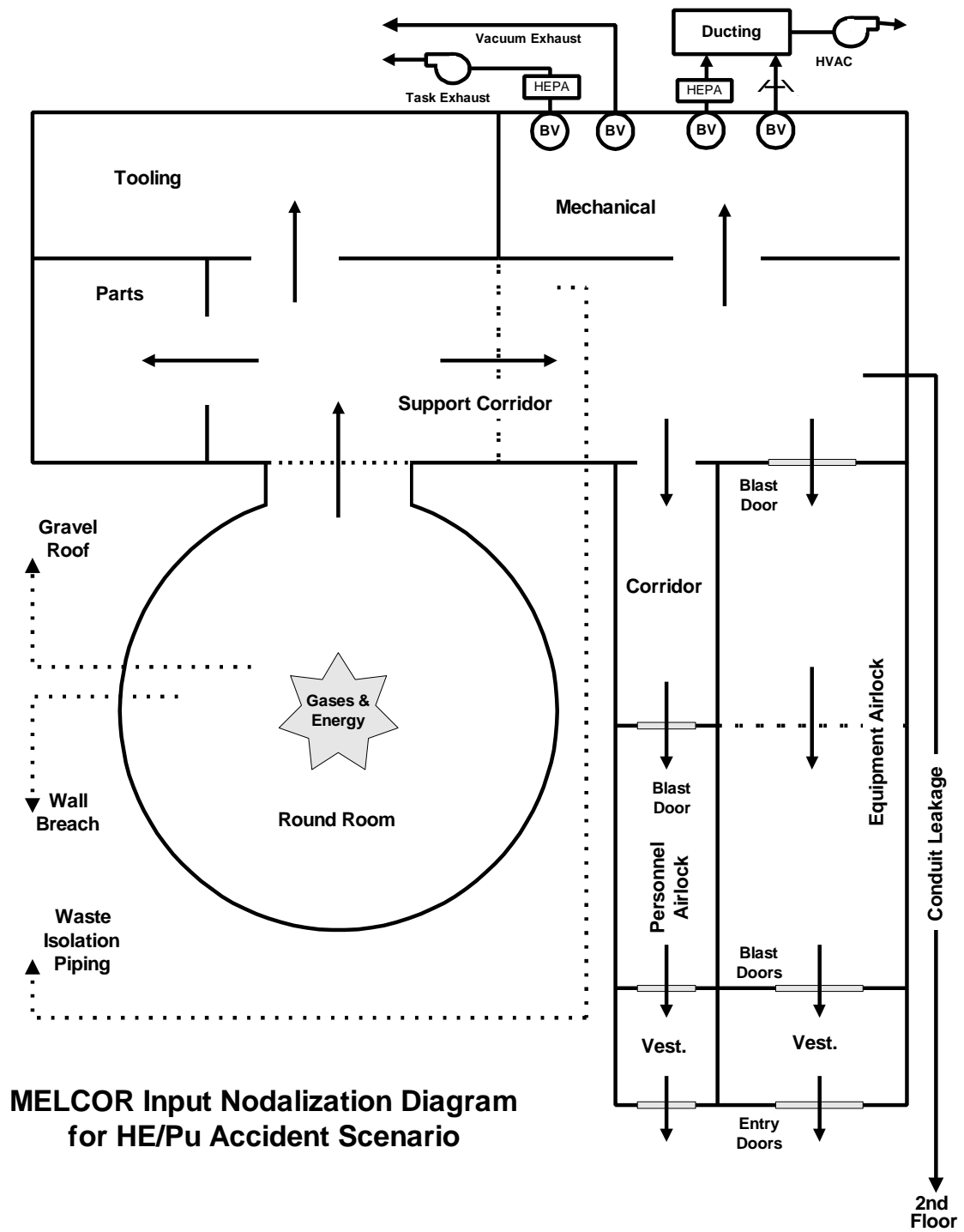
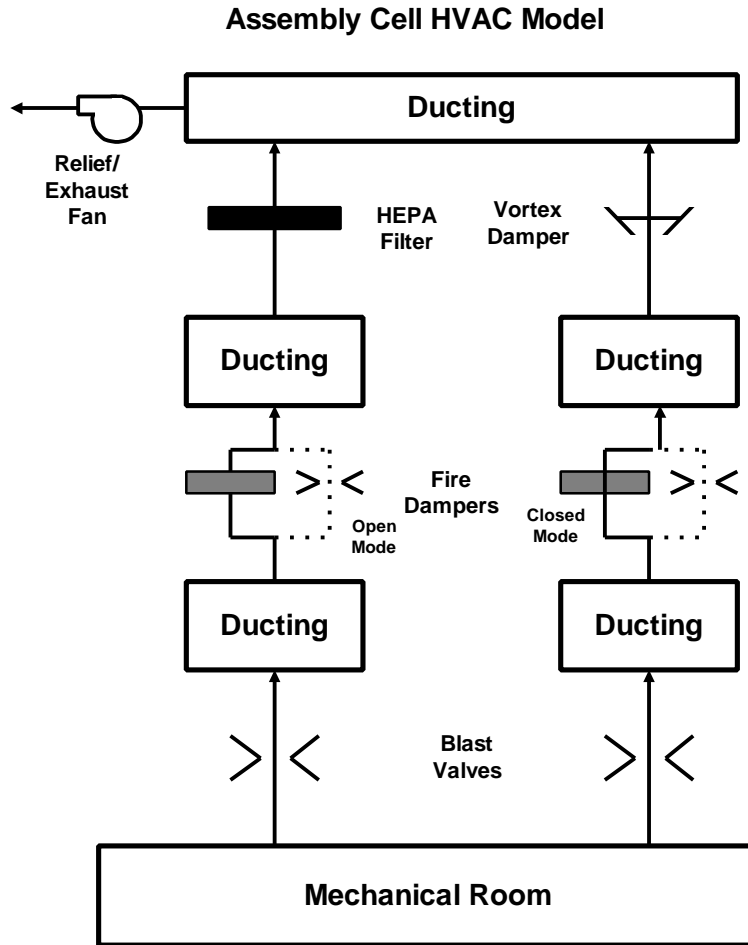


Fig. 7. MELCOR Assembly Cell Nodalization Diagram.



**Fig. 8. MELCOR Model of the Assembly Cell HVAV System.**

An important model in these analyses was the fire damper leakage model. The data used in the MELCOR fire damper leakage model were data obtained for Class IV Fire/Smoke Dampers (the most leaky classification). These data provided the minimum leakage flow per unit area as a function of pressure differential across the damper when the damper was closed. To achieve realistic flows, a safety factor of 1.2, based strictly on engineering judgment, was applied to the minimum leakage flows. The MELCOR input model first determined the pressure differential across the fire damper from the control volume pressures, then looked up the correct minimum leakage flow, then applied the safety factor, and then forced the closed damper flow pathway to transfer the correct airflow through the pathway. The open mode of the fire damper provided little resistance to flow, so the pathway was simply modeled by applying a loss coefficient to the flow.

Twin flow pathways were required for the fire dampers, i.e., a path for the open configuration and one for the closed configuration. A valve model was used to select the appropriate pathway. Initially, the open pathway was active, but a control logic signal that the fire damper fuse had melted caused the valve model to switch to the closed pathway. The fuses were modeled with lump mass heat structures that were heated by the gas flows in their respective upstream duct control volumes. The thermal properties of the fuses were those available for typical fusible metals. In practice, the fuses, as modeled, readily melted

when the air temperatures exceeded the melting temperature of the fuse. However, the heating of the air and surfaces in the relatively long piping lengths between the blast valves and the fire dampers effectively delayed the melting of the fuses.

A model similar to the fire dampers was used for a closed vortex damper on the supply side of the HVAC system, which also leaks. This leakage was important because this airflow would bypass the HEPA filters.

The DAF assembly cell has ventilation equipment inside the cell, as well as outside it. An explosion would most certainly destroy the equipment inside the cell. Blast valves activated by blast overpressure protect the ventilation system hardware outside the cell by closing almost immediately following a blast. Because the valves are of a nonlatching design, the valves would reopen when the cell static pressure differential with the outside atmosphere dropped below 0.5 psi. The resistance to airflow through the blast valves was modeled using manufacture's data.

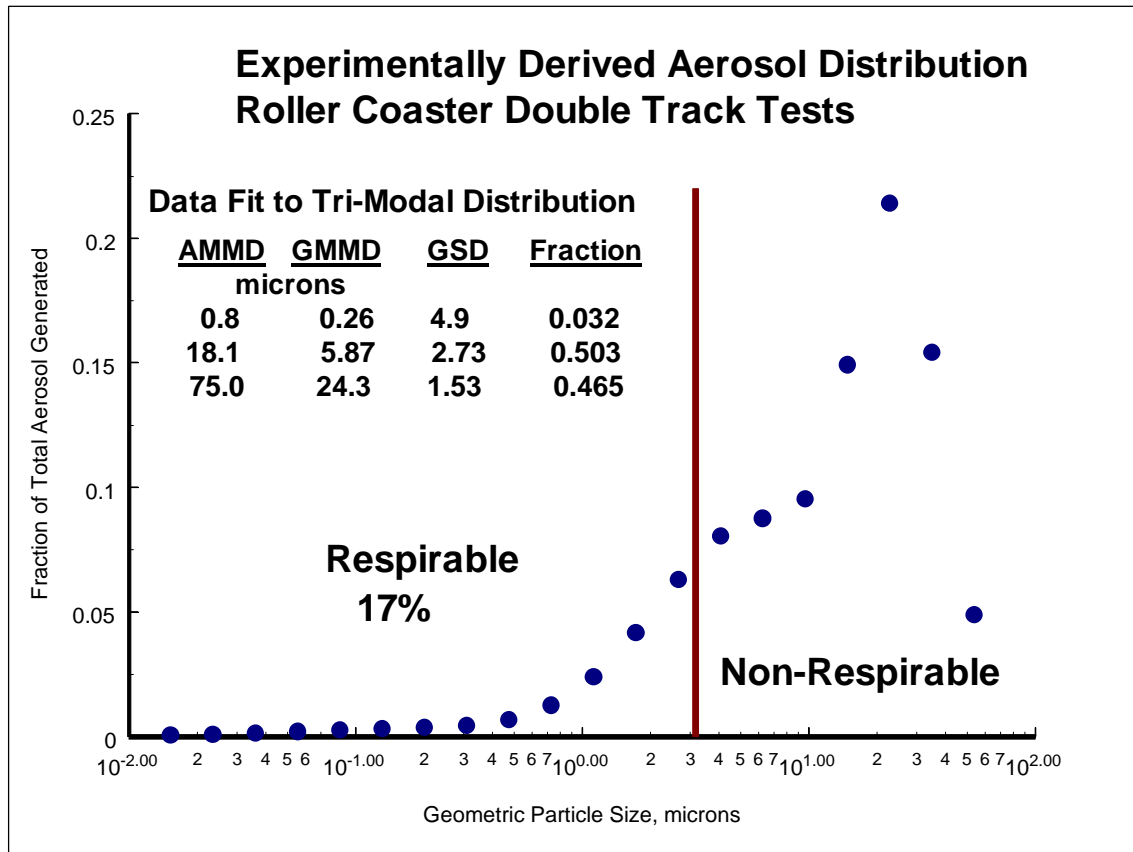
Besides filtering aerosols from the air stream, the high-efficiency particulate air (HEPA) filters also provide a significant resistance to flow. The flow through an intact HEPA filter was modeled using a flow form loss coefficient enhanced to account for the pressure drop across the filter. This enhanced loss was based on experimental data [ERDA-7621] that concluded the head loss across a 1-in.-deep, 2-ft by 2-ft HEPA filter at 1000 ft<sup>3</sup>/min would be 1 in. WC. The HEPA filters in this study were assumed to survive the 0.5-psi pressure differential associated with the reopening of the blast valves.

## **AEROSOL TRANSPORT**

The thermal-hydraulic models provided the means to transport the aerosol from one location to another, but the aerosol transport models determined the deposition of aerosol particles within the facility. If aerosol deposition did not occur, the aerosol would transport with the movement of air in the same manner that an inert gas would transport. Because all of the transport processes depend on the particle characteristics, representing the simulated aerosol adequately was extremely important to the transport analyses.

An explosive-generated aerosol size distribution derived from data taken during the Roller Coaster Double Tracks experiments [SAND96-XXXX] was used for the DAF explosion analyses. The data from the Roller Coaster Double Tracks test was found to more accurately fit a tri-modal distribution than a single lognormal distribution, which is usually assumed in these types of analyses. The tri-modal distribution was simply the sum of three single distributions; each applied to a fraction of the total aerosol mass. The Roller Coaster Double Tracks distribution is shown in Fig. 9 as the distribution was applied to the MELCOR input model. The MELCOR numerical aerosol transport model subdivided the size spectrum into as many as 20 discrete sections where the particles in that size section were represented as a single size.

Approximately 17% of the tri-modal distribution were smaller than the 3.2 μm geometric diameter (10 μm aerodynamic diameter) generally designated as the boundary between respirable and non-respirable aerosol particles. Although the primary interest in these calculations was the respirable sized particles, the entire tri-modal size distribution was modeled and the entire size spectrum was tracked throughout the calculations. This provided a realistic shape to the distribution on the respirable side. Note that the respirable side of this distribution taken alone cannot be represented adequately as a lognormal distribution. The added knowledge gained by tracking the nonrespirable as well as the respirable particles provided further insights into the severe accident behavior of DAF.



**Fig. 9. Explosion Generated Aerosol Size Distribution.**

In the MELCOR input model, the aerosol was introduced into each calculation as a burst release into the round room following the explosion ( $< 0.1$  s). Further, it was assumed that the entire mass of plutonium in the round room was converted to an aerosol with the tri-modal distribution. Thus, 17% of the total mass was formed into the transportable respirable mass.

Gravitational settling dominated the aerosol deposition process, especially for the heavier particle ( $>0.3 \mu\text{m}$ ). Approximated 98% of the aerosol mass consisted of particles where gravitational settling clearly governed their deposition. The diffusion process dominated the deposition process for the lightest particles and the temperature dependence of the diffusion process increased in importance during the high-temperature period associated with the explosion. Inertial impaction was not modeled.

HEPA filters will typically filter more than 99.99% of particles larger than about  $0.3 \mu\text{m}$  and more than 99.95% of particles smaller than  $0.3 \mu\text{m}$  when the filter is relatively new and clean. To avoid undue operational requirements regarding HEPA filter replacements at DAF, an administrative decision was made to perform the severe accident analyses using a very conservative HEPA filter efficiency of 99%. That is, if the 99% filtration environmental source terms were acceptable, then special operational controls to ensure clean HEPA filters would not be needed.

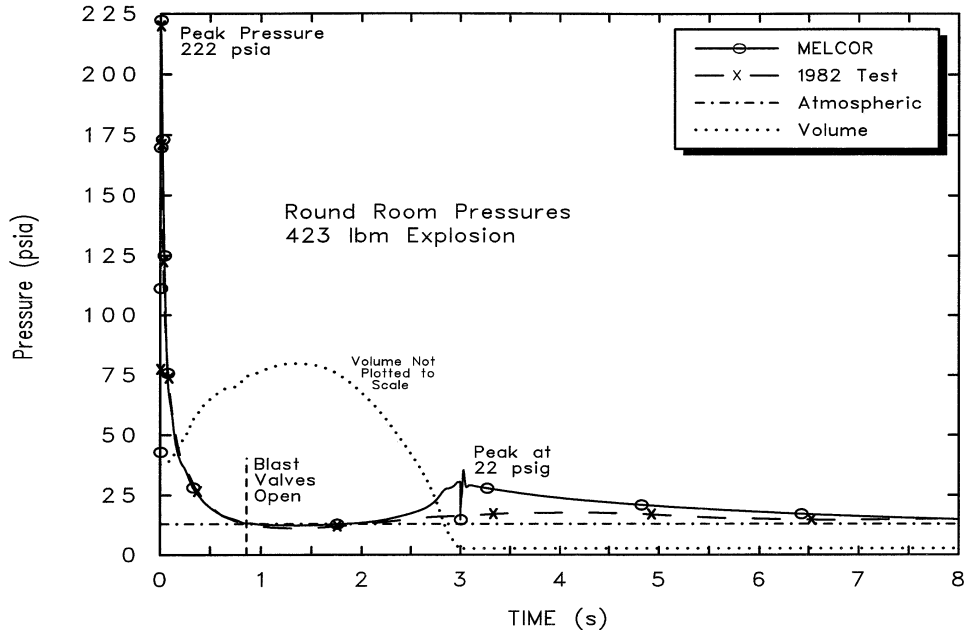
A substantial mass of nonradioactive or inert material would almost certainly be aerosolized along with the plutonium following a detonation in a round room. The round rooms are lined with gypsum wallboard that could be fragmented easily. Aerosol coagulation could have an important effect on the transport of plutonium when the plutonium particles agglomerate with the gypsum particles. The agglomerated particles would be both larger and lighter than the original plutonium particles. It was expected that the net effect of plutonium aerosol agglomeration with inert aerosols would lead to enhanced deposition, but this needed calculational verification. Enhanced deposition would mean that it was conservative to neglect the inert aerosol from the calculation model. Therefore, a two-component aerosol transport was used in a few alternate calculations. The inert aerosol model was used simply to verify a calculational trend to defend the assumption that it was conservative to neglect inert aerosol from the accident calculations. Further, no credit was taken for enhanced deposition because of the almost certain presence of substantial quantities of inert aerosols.

## **THERMAL-HYDRAULIC EXAMINATION**

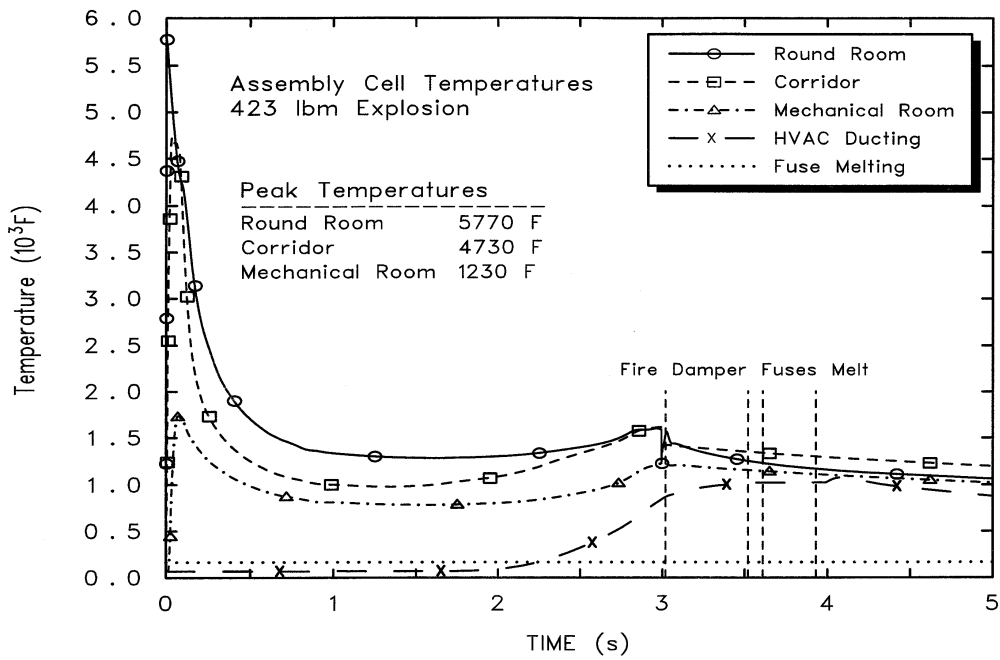
Understanding the thermal-hydraulic responses to the explosion was necessary to establish the credibility of the aerosol transport results and to ensure that the predictions were conservative with respect to the potential risk to the public. Examples of the type of available thermal-hydraulic information are included to show the level of detail considered in this study. The thermal-hydraulic response to the 423-lbm explosion is shown in the pressure and temperature results in Figs. 10 and 11.

The round-room pressure for the MELCOR simulation is compared with the measured pressure from the 1982 full-scale test in Fig. 10. Immediately after the explosion, the peak round room pressure of the simulation was 222 psia, comparing reasonably well with the corresponding test pressure of ~280 psia, when the uncertainties associated with both the analytical models and the experimental measurements are considered. The MELCOR input models that simulated the explosion were not developed to predict the initial first few thousandths of a second transient accurately. Because of an explosive venting of gases through the gavel following the lift of the gravel roof, the round-room pressure dropped rapidly to a pressure that was slightly subatmospheric. At 0.85 s, the pressure dropped below the 0.5-psi differential pressure needed to keep the blast valves closed. Thus, the blast valves were predicted to reopen at 0.85 s, allowing airflow between the cell mechanical room and the ventilation equipment exterior to the cell. The round-room volume is also shown in Fig. 10 for direct comparison with the pressure. The round-room pressure reaches its minimum value at roughly the same time that the gravel roof reaches its maximum, then the pressure increased again, as it did in the 1982 full-scale test, when the gravel collapsed back into the round room. The second pressurization of the assembly cell was caused by the rapid reduction of gas volume in the round room. The second pressure peak corresponds roughly with the time the gravel hits the round room floor at 3 s. Because HEPA filters will likely fail with any pressure differential greater than about 2 psi, the airflow associated with the depressurization of the second peak through the exterior ventilation equipment would most likely blow out the filters. The HVAC exhaust and task exhaust HEPA filters were conservatively not modeled in the 423-lbm explosion scenarios.

Temperatures for the 423-lbm simulation are shown in Fig. 11 for the round room, staging corridor, and the mechanical room atmospheres and for airflow in the HVAC ducting. Generally speaking, the further from the explosion, the cooler was the air. The air in the HVAC ducting, which was isolated until the blast valves reopened at 0.85 s, increased in temperature as the assembly cell pressurized the second time, driving hot gases into the ventilation piping. The figure shows the duct air temperatures exceeding the 165°F melt temperature of the fusible links that hold the fire dampers closed, at about 2.2 s. Then, it took another 1 to 2 s for the fusible link to actually melt so that the fire dampers would slam closed. The figure shows the times where each of the four fire dampers was predicted to close. Although only one duct temperature is shown in the figure, a separate duct connected the assembly cell to each of the fire dampers, i.e., four ducts, four fire dampers, four fusible links, and four temperatures.



**Fig. 10. Pressures in the Round Room.**



**Fig. 11. Temperatures in the Assembly Cell.**

## **AEROSOL TRANSPORT KNOWLEDGE BASE**

The simulations verified that the vast majority of the plutonium would be contained within the facility. However, some small quantity of plutonium aerosol would escape the confinement of the facility even when all systems and system components functioned as designed and as intended. Simulations were performed for the three sizes of postulated explosions where all systems were modeled to function as designed. Other simulations examined the effect of system and system component failures, as well as, alternate configurations. The simulations tracked the transport of both respirable- and nonrespirable-sized particles, although only the respirable particles were of interest from a public risk perspective.

Performing a relatively complete facility analysis, including such aspects as tracking the nonrespirable particles, provided a global view of the facility response to an accident that, among other things, provides a quality assurance type of “sanity check.” In other words, do the results make sense?

The knowledge gained by comparing the results of these simulations and examining their details enhanced the understanding of how the facility would respond to a variety of accident scenarios. For example, the important pathways where plutonium could escape the confinement of the assembly cell and transport to the environment were identified. The masses released to the environment were obtained for each pathway for each simulation. For DAF, the majority of the masses released to the environment were released through the assembly cell ventilation systems, and the masses released by first passing through the facility were trivial by comparison. In the 423-lbm scenario, only about 20% of the released mass entered the environment by means of venting through the gravel roof.

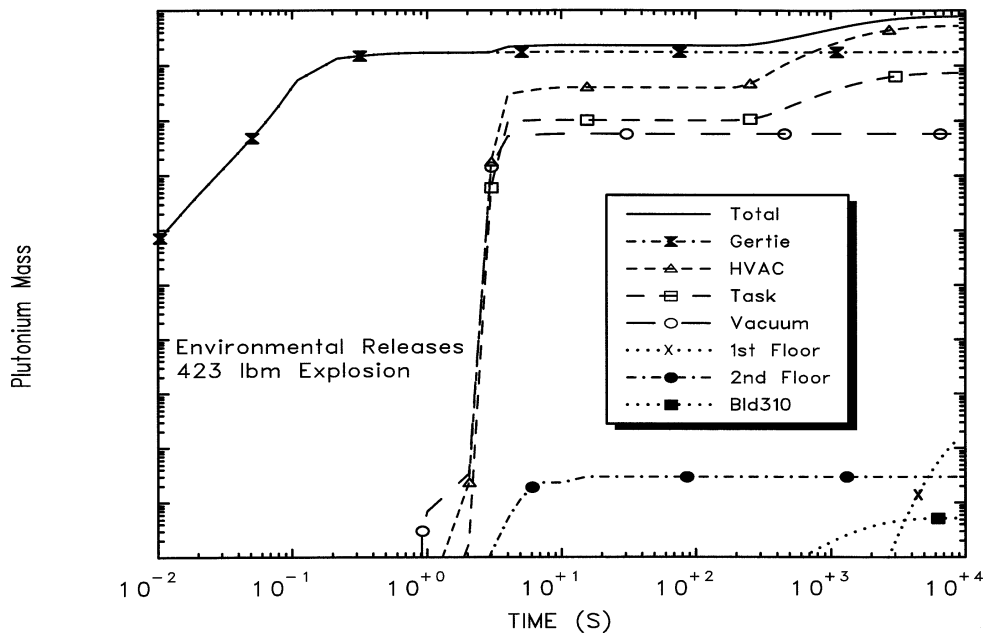
The time-dependence results, such as the releases of respirable masses to the environment, were determined. Figure 12 shows the time-dependent releases for each pathway of the 423-lbm scenario.

The possibility of a failure of a system or a system component to function as designed inherently increases the risk to the public, and many of these postulated failures dramatically increased the predicted releases of respirable aerosol to the environment. Alternate scenarios were simulated to determine the impact of various equipment failures on the environmental releases and the importance of systems relative to confining an accident. These results helped identify equipment needing safety classification.

Several alternate scenarios assumed that one or more of the blast valves failed to close because of blast pressure following the explosion. In selected scenarios, the additional failures of fire dampers or the waste isolation valve were postulated. Absolutely worst-case scenarios were postulated, where everything failed to function as designed, to demonstrate some kind of upper limit on the possible releases to the environment. In the worst cases, nearly half of the total initial respirable mass stayed within the facility.

One scenario was simulated for each of the 55- and 85-lbm explosion scenarios, where the ventilation exhaust HEPA filters were postulated to fail by some mechanism other than the failure of a blast valve to close. One very possible mechanism for HEPA filter failure would be the potential overloading of the filter by aerosol accumulation, not only the plutonium aerosol but all other inert aerosol as well. The potential increase in plutonium release to the environment was substantial.

The ventilation system fire dampers were designed to close whenever the airflow through the piping was sufficient to melt the fire damper’s fusible link, which was designed to melt when heated to a temperature of 165°F. When the blast valves functioned as designed in the 55- and the 85-lbm scenarios, the predicted airflow temperatures in the ventilation piping were insufficient to melt the fusible links and the fire dampers remained open. In the 55- and 85-lbm scenarios, the forced closure of the fire dampers in the



**Fig. 12. Environmental Release by Pathway for the 423-lbm Scenario.**

pipng to the task and HVAC exhaust HEPA filters forced more flow through the unfiltered supply side of the HVAC system. This in turn increased the masses released to the environment by factors of about 9 and 4, respectively.

The waste isolation system consists of a sump located in the assembly cell staging area and piping leading to a waste storage tank located underground and towards on side of the front parking lot. The storage tank is vented to the atmosphere to prevent any buildup of pressure within the tank. An isolation valve in the piping located near the sump normally prevents flow from the cell to the storage tank. If this isolation valve were open or to otherwise fail following an explosion, the explosion would vent directly to the storage tank and then to the atmosphere. The failure of the waste isolation valve provided an immediate and direct path to the environment. A significant amount respirable aerosol was predicted released directly into the front parking lot within the first couple of minutes in the 55- and 85-lbm scenarios. Besides the enhancement to the environmental source term, these immediate releases to the front parking lot would affect the risk to evacuating personnel. Both respirable and nonrespirable aerosol would likely be present along the evacuation route.

Accident progression trends were identified. For example, the result that the 55-lbm scenario released slightly more aerosol than did the 85-lbm scenario seemed counterintuitive, but a detailed review of the aerosol transport process revealed the reasons for the difference. The primary reason for the difference was the higher temperatures of the larger explosion resulted in a higher aerosol deposition rate for the smaller respirable particles because of the temperature dependence of the diffusive deposition process. Further, the LPFs for the three basic explosions examined was comparable.

The assembly cell would of course be heavily contaminated following an explosion in that cell and most of the original mass of plutonium would remain within the assembly cell. Plutonium escaping the cell by way of either the first-floor corridor or the second-floor service corridor would spread contamination to

other buildings connected to these corridors. For example, only trace amounts of plutonium entering the first-floor corridor from the assembly cell were predicted to transport to the front of the building where the aerosol could escape to the environment. The first-floor corridor model with its operating ventilation system is shown in Fig. 13.

In addition to the final aerosol deposition, the knowledge base includes information regarding airborne aerosol concentrations that is pertinent to personnel hazard issues. Figure 14 shows the concentrations at various locations within the first floor corridor as a function of time.

Alternate scenarios were run to determine the sensitivity of aerosol transport into the first floor corridor on the configuration of cell doors, i.e., whether or not each of the four blast doors or the two entry doors was open or closed. The operational requirement was that at least one of the two blast doors in each of the personnel and the equipment airlocks be closed during an operation. These alternate scenarios provided additional information pertinent primarily to both personnel hazards and to facility contamination.

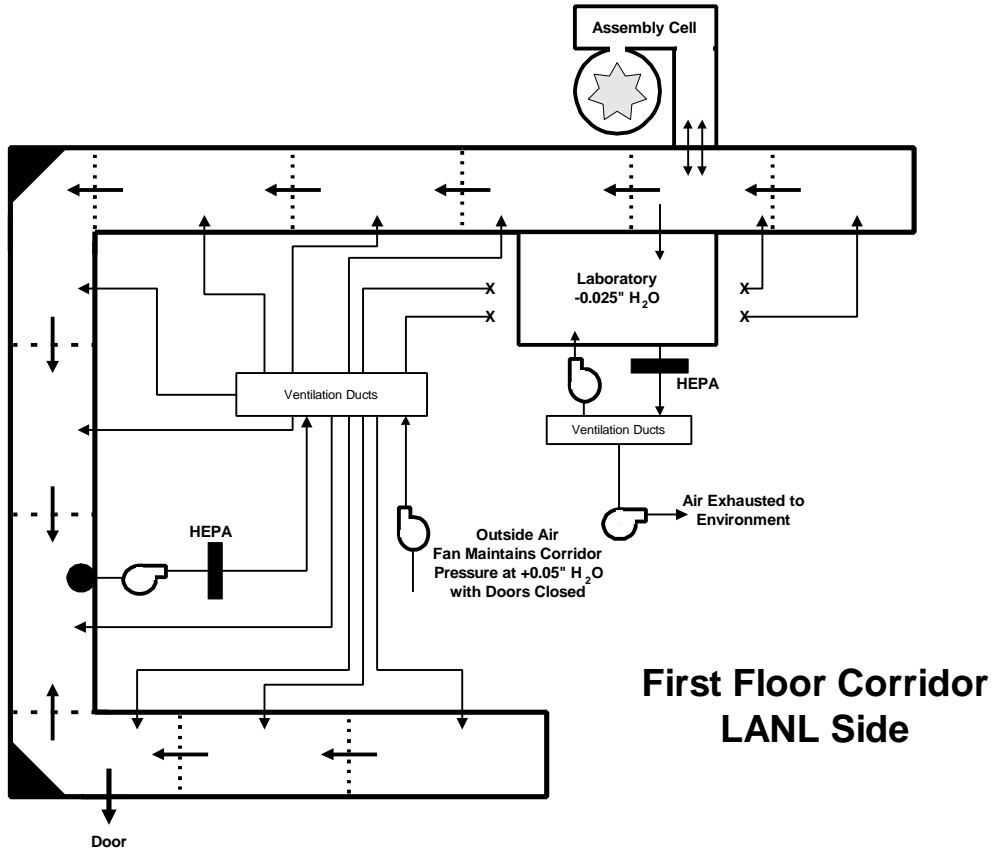
## REFERENCES

NUREG/CR-6119. R. O. Gauntt et al, "MELCOR Computer Code Manuals," Volumes 1 and 2, US Nuclear Regulatory Commission report NUREG/CR-6119, SAND97-2398 (July 1997).

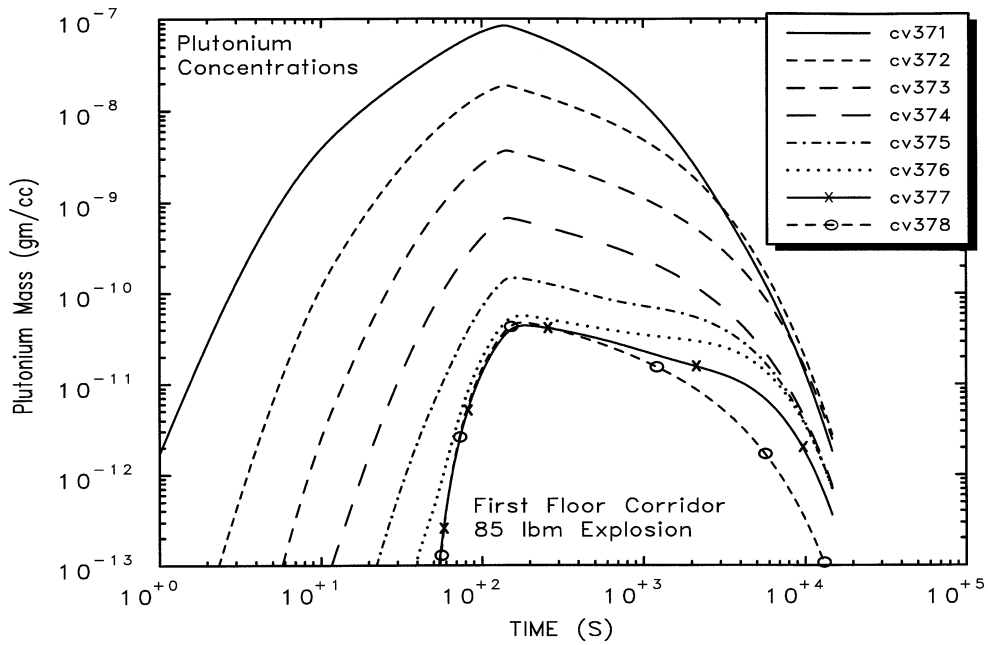
SAND84-0618. R. E. Luna, R. P. Sandoval, J. M. Taylor, N. R. Grandjean, L. L. Keller, and G. F. Newton, "Gravel Gertie Confinement Verification Program – Final Report," Sandia National Laboratories report SAND84-0618 (March 1984).

ERDA-7621. C. A. Buchsted et al, "Nuclear Air Cleaning Handbook," Energy Research and Development Administration report ERDA-7621 (March 1976).

SAND96-XXXX. R. O. Griffith, J. E. Brockmann, D. Carlson, N. Grandjean, R. Luna, K. Murata, J. Sprung, E. Tadios, D. C. Williams, and M. L. Young, "Preliminary Assessment of the Radiological Consequences of an Accident Involving High Explosives and Plutonium in a Pantex Assembly Cell," Sandia National Laboratories report SAND96-XXXX (Draft for Review) (September 1996).



**Fig. 13. First Floor Corridor Model.**



**Fig. 14. Concentrations of Airborne Plutonium Aerosol in First Floor Corridor.**