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Source Term Evaluation for Postulated UF_6 Release Accidents in Gaseous Diffusion Plants— Summer Ventilation Mode (Non-Seismic Cases)

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**SOURCE TERM EVALUATION
FOR POSTULATED UF₆ RELEASE ACCIDENTS
IN GASEOUS DIFFUSION PLANTS
- Summer Ventilation Mode (Non-Seismic Cases)**

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U.S. DEPARTMENT OF ENERGY
under contract DOE-84OR21400

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SOURCE TERM EVALUATION FOR POSTULATED UF_6 RELEASE ACCIDENTS IN GASEOUS DIFFUSION PLANTS

ABSTRACT

Computer models have been developed to simulate the transient behavior of aerosols and vapors as a result of a postulated accident involving the release of uranium hexafluoride (UF_6) into the process building of a gaseous diffusion plant. For the current study, gaseous UF_6 is assumed to get released in the cell housing atmosphere through B-line break at 58.97 kg/s for 10 min and 30 min duration at the Paducah and Portsmouth Gaseous Diffusion Plants. The released UF_6 undergoes an exothermic chemical reaction with moisture (H_2O) in the air to form hydrogen fluoride (HF) and radioactive uranyl fluoride (UO_2F_2) while it disperses throughout the process building. As part of a facility-wide safety evaluation, this study evaluated source terms consisting of UO_2F_2 as well as HF during a postulated UF_6 release accident in a process building. UO_2F_2 mainly remains as airborne-solid particles (aerosols), and HF is in a vapor form. Some UO_2F_2 aerosols are removed from the air flow due to gravitational settling. The HF and the remaining UO_2F_2 are mixed with air and exhausted through the building ventilation system. The MELCOR computer code was selected for simulating aerosols and vapor transport in the process building. To evaluate spatial effects in conjunction with plant-specific nuances related to ventilation flow distribution effects, the entire process building was included in MELCOR modeling. In specific, the process was discretized into about 50 control volumes interconnected by about 200 flow paths. To characterize leakage flow through the cell housing wall, 3-D CFD tool (CFDS-FLOW3D) was used. Results indicated that substantial amount of UO_2F_2 particles get settled onto the cell housing floor, and the surfaces of equipment and piping in the cell housing. About 57% of UO_2F_2 was predicted to be released into the environment. Since HF was treated as vapor, close to 100% was estimated to get released into the environment. Also predicted in the results, was that substantial amount of UO_2F_2 and HF were dispersed from the unit where initial UF_6 was released, to other neighboring units. This study also provides spatial variations of source term release from various locations of the process building.

1. INTRODUCTION

The gaseous diffusion process is currently employed at two plants in the United States: the Paducah Gaseous Diffusion Plant and the Portsmouth Gaseous Diffusion Plant. As part of a facility-wide safety evaluation, a postulated design basis accident involving large line-rupture induced releases of uranium hexafluoride (UF_6) into the process building of a gaseous diffusion plant (GDP) is evaluated. When UF_6 is released into the atmosphere, it undergoes an exothermic chemical reaction with moisture (H_2O) in the air to form hydrogen fluoride (HF) and aerosolized uranyl fluoride (UO_2F_2). The objective of this study is to evaluate the above-mentioned accident-related source term magnitude of UO_2F_2 as well as HF. An ancillary objective is to evaluate the spatial and temporal distribution of UO_2F_2 and HF within the process building to address the issues related to impact on in-plant personnel.

The process building for US GDPs is a two-story structure. The ground floor (also called the operating floor) contains an area control room, maintenance shops, power transformers, and other auxiliary service equipment. The second floor (called as the cell floor) contains many axial-flow compressors that pump gaseous UF_6 through large cylindrical steel vessels, referred to as converters. Each compressor is driven by a large electric motor. A compressor, a converter, and interconnecting piping comprise one stage. The stages are connected in series. Groups of eight are physically set apart from other similar groups and enclosed within an uninsulated, sheet metal housing (called cell housing). Such a housed group of stages comprises a "cell". The cells are interconnected by piping which is also enclosed in an uninsulated, sheet metal housing. Ten connected cells comprise a "unit". There are six and eight units in the Paducah and Portsmouth process buildings, respectively, that are currently under consideration. The ventilation system in the process building is reconfigured between summer and winter months. This leads to significantly different airflow patterns during summer versus winter. For this paper, assessments are presented only for the summer ventilation pattern, as shown in Figure 1. During summer, the ventilation system works as a once-through system in which air is drawn into the operating floor, and then forced to the cell floor by large blowers. About 57% of air delivered to the cell floor passes through the electric motors, which drive stage compressors. This air flow is drawn by a powered exhaust system, which discharges directly to the atmosphere at roof level. The remaining air is exhausted through openings in the roof, centrally located over each cell housing.

A lumped parameter model was developed in the past to evaluate the transient behavior occurring as a result of the postulated accidental release of UF_6 in various process buildings of GDPs [Williams, 1986]. The model included treatment of UF_6 in solid, liquid, and vapor phases, whereas both HF and H_2O could exist in liquid and vapor phases. Self-association (polymerization) of HF also was included. The model solves mass and energy balance equations for a compartment with a single volume representation, assuming that all the atmospheric materials are uniformly mixed in the volume. For aerosol transport, it specifies gravitational settling at a constant deposition velocity of 1 cm/s based on global experimental observations. This model only considers aerosol deposition by gravitational settling, and neglects other mechanisms. Also by assuming a simple geometry for the entire process building, spatial effects of aerosol distribution and potential additional equipment and piping surfaces for aerosol deposition are also neglected.

A study was performed to verify the degree of conservatism in previous evaluations using a more systematic and mechanistic approach. The MELCOR computer code was selected for simulating aerosols and vapor transport in process building [Summers, 1991]. This code has been developed by the US Nuclear Regulatory Commission (NRC), and widely used for simulating postulated severe accidents in nuclear facilities. This code is written in a highly modularized fashion, and each module is designed to allow the user to change selected important parameters for maximizing capability for sensitivity studies. The MELCOR model was first used to develop a single volume representation of the process building and its results were compared with those from the previous model developed by Williams; hereafter referred to the cascade-summer (CSCDSM) model for convenience. MELCOR predicted results were found to be comparable with those from previously developed models [Kim, 1996]. Thereafter, a study was extended to examine the effect of finer nodalization by specifying the cell housing as a separate volume to observe spatial effects from multi-volume calculations on aerosol/vapor transport (e.g., three control volumes for single unit of the process building). This study revealed that much less amount of aerosols were predicted to be released into the environment as compared to that of a single volume representation. This study, however, neglected much of spatial effects of air flow distribution and mixing behavior in presence of ventilation flow distribution effects. Therefore, the current study was extended to include much finer nodalized system of the entire process building, in contrast with the previous study in which we modeled only a single unit of the process building.

Specifically, the process building was modeled with about 50 control volumes interconnected by about 200 flow paths. Also about 800 control functions were used to simulate chemical reaction-related phenomenology throughout the volumes, and for tracking of aerosols and vapor transport. The pipe break was assumed to occur in the fifth cell housing of unit 4. The volume of this affected unit 4 was thereafter, finely nodalized to capture temporal and spatial effects of aerosol and vapor dispersion in the immediate vicinity of the UF_6 source. Each cell housing in unit 4 was represented by an individual control volume, and the cell floor volume outside the cell housing was divided into several control volumes. However, surrounding units were modeled to have two control volumes, one for the cell housing, and the other for the rest of the cell floor volume. Leakage through walls and joints of the cell housing was estimated to be $9 \text{ m}^3/\text{s}$ of air per cell housing, based on actual plant test data [Riepe, 1974]

This paper describes MELCOR modeling of multi-volume representation of the entire process building where gaseous UF_6 is assumed to be released. Also described are the results of MELCOR simulations for such an accident in the Paducah and Portsmouth GDPs.

In the postulated accident scenario, 58.97 kg/s (130 lb/s) of UF_6 vapor is released over a 10 min and 30 min periods from the process piping inside the cell housing, generating $30,958 \text{ kg}$ of UO_2F_2 and $8,031 \text{ kg}$ of HF for 10 min release case, and $92,873 \text{ kg}$ of UO_2F_2 and $24,160 \text{ kg}$ of HF for 30 min release case. UO_2F_2 is assumed to remain mainly as airborne-solid particles (aerosols), whereas HF is in vapor form. Bonding between HF and water molecules in the air as well as the polymerization of HF into $(\text{HF})_n$ are neglected in the current study for the sake of conservatism. Some UO_2F_2 aerosols are removed from the air flow due to gravitational settling. The HF and the remaining UO_2F_2 get mixed with air and then get exhausted through the building ventilation system.

2. MELCOR AEROSOL TRANSPORT MODEL WITH MULTI-VOLUME BUILDING REPRESENTATION

The X-333 process building of the Portsmouth GDP that contains 640 stages (80 cells, 8 units), is 443.8 m ($1,456 \text{ ft}$) long, 295.7 m (970 ft) wide, and 25 m (82 ft) high [Portsmouth GDP FSAR, 1985]. A similar process building (C-337 building) in the Paducah GDP consists of 6 units. Each unit is identical in terms of equipment and its

layout. Figure 2 illustrates two cell housings which are interconnected to each other by inter-cell piping ducting. Cell bypass housing passes next to the cell housings. The approximate dimensions of cell housing are also shown in the same figure. In the Paducah GDP, there are 10 cells per unit and 6 units in the C-337 building, which yields 60 cells in the building. In the Portsmouth GDP, because of 8 units instead of 6, 80 cells are enclosed in the X-333 process building. The capacity of air supply blower is $47.67 \text{ m}^3/\text{s}$ ($1.01 \times 10^5 \text{ cfm}$) per each cell. If the transformer cooling is allowed in the operating floor (or ground floor) which is the case for the current study, about $26.43 \text{ m}^3/\text{s}$ ($5.6 \times 10^4 \text{ cfm}$) of air is exhausted through motor exhaust for each cell. If the transformer cooling line is closed, motor exhaust will increase to $35.4 \text{ m}^3/\text{s}$ ($7.5 \times 10^4 \text{ cfm}$) per cell. The remaining air is exhausted through a roof opening that is located above each cell housing. Figure 2 also includes information regarding cell housing geometry description and its volume.

2.1 MELCOR Nodalization of the Process Building

Figure 3 shows schematics of MELCOR nodalization of the C-337 process building of the Paducah GDP. This figure shows the nodalization of the cell floor area outside cell housings. As shown in the figure, the cell floor area of each unit is lumped into a single control volume except for the unit 4 where UF_6 gas is sourced into. Because mass and energy sources exist in the unit 4, this unit is nodalized finely to capture a spatial variation of UF_6 chemical reaction and aerosol/vapor transport. In specific, the cell floor area outside cell housings of the unit 4 is divided into three (3) story control volumes, as seen in Figure 3. Figure 4 shows more explicit view of how the unit 4 volume is nodalized for the current study using MELCOR. The first floor consists of twenty control volumes. Each cell at this level has two control volumes; one for cell housing, and the other for cell floor volume outside cell housing. The cell floor volume above the cell housings of the unit is divided equally into two stories. The second story volume was nodalized into ten control volumes, one corresponding to each cell. The third story volume is treated as a large single control volume. Figure 5 illustrates nodalized control volumes of the entire C-337 building. Also shown are flow paths interconnecting these control volumes. The environment, outside the process building is distinguished into seven control volumes. As a reservoir of released source term (radioactive and/or non-radioactive material released into the environment), one control volume is assigned to each unit of the building. These control volumes (cv-901 through 906) are not interconnected because the source term magnitude from individual unit needs to be distinguished. One control volume (cv-999) provides fresh air to the process building, and is not connected to any control volumes other than the process building volumes to provide air. Also flow paths connecting the

process building control volumes and control volumes representing the environment are not shown in the figure. As described above, each unit is divided into two control volumes (e.g., cv-101 for the cell floor volume outside cell housing, and cv-102 for cell housing of unit 1). The unit 4 includes ten control volumes for ten cell housings (cv-401 through 410), ten control volumes for each cell floor volume next to cell housings (cv-411 through 420), ten additional control volumes for each cell above cell housings (cv-421 through 430), and one large control volume beneath the process building roof (cv-431). Each cell floor volume has a single air blower shown as squares with cross-hatch in the figure, and also lumped motor exhaust shown as small circles in the same figure. Each control volume contacting the building roof has an opening to the environment, and is not shown in the figure. Configuration shown in Figures 3 and 5 is MELCOR nodalization of 6 unit process building, C-337, in Paducah. For the X-333 building, 8 unit process building of the Portsmouth GDP, control volumes for additional two units (e.g., units 7 & 8) are added to the Paducah's 6 unit model, as seen in Figure 6. Also two additional environmental control volumes are included to represent the reservoir control volume for source term released from these two additional units. Table 1 lists information about each of the control volumes modeled in MELCOR. Input data for flow paths are also listed in Table 2.

2.2 Modeling of Cell Housing Wall Leakage

The cell housing wall is constructed of steel with 3/8-inch transite siding bolted in place. The tops of the housings are 20-gauge ribbed steel with removable hatches for ease of equipment removal. The bell ends of the compressors are connected to the housings with heavy, reinforced plastic shroud bolted to the ends of the compressor with a metal ring. Although the housing seams are tightly closed, the cell housing was not designed to provide 100 percent secondary confinement in the event of a rupture inside the housing. Atmosphere in the housing will heat up due to heat convection/radiation from equipment surfaces such as compressors. A significant temperature difference between inside and outside the housing develops buoyancy force that convects air naturally through cracks, untightened seams, and other leak paths. The quantity of this leakage was calculated on the basis of an energy balance for the cell using temperature and pressure data collected in various locations in the cell housing (see Appendix A). During normal operation at the Paducah GDP, the maximum air flow magnitude was estimated to be $9 \text{ m}^3/\text{s}$ (19,000 cfm) housing [Riepe, 1974]. Leakage paths and their size in MELCOR modeling have been characterized to have this amount of air flow during steady state normal operating condition. To be specific, three flow paths are assumed to represent leakage through cell housing wall during steady state. When UF_6 is released into the housing volume, a door

(7'x3') installed at the cell housing floor is expected to swing open to the outside. No restraint is installed to restrict the door open. Therefore, during the transient, it is assumed the door to stay open throughout the calculations. Figure 7 illustrates leak flow paths between inside and outside cell housing. For each cell housing, therefore, four flow paths are modeled to represent leakage including the access door. Two horizontal flow paths represent leakage-in and -out paths at the lower and higher elevations, respectively. Also at the floor level, a door is modeled as an additional horizontal flow path. Also modeled is a vertical flow path representing leakage at the top of the cell housing. To obtain an appropriate size of these flow paths, results obtained from MELCOR calculations with specified flow paths were compared and adjusted per guidance obtained from localized three-dimensional simulations using the Computational Fluid Dynamics (CFD) tool, CFDS-FLOW3D¹.

A single cell was discretized into approximately 50,000 control volumes with CFDS-FLOW3D [Wendel, 1996]. Aerosols were sourced into the cell housing control volume uniformly as tracer particles. Because of limitation of the code, aerosol deposition due to gravitation and other effects were not considered. A steady state calculation was established, and then a transient calculation was performed. During the steady state calculations, the solution was calibrated to the measured through-cell circulation air flow rate ($9 \text{ m}^3/\text{s}$), cell internal air temperature (360 K), and roof exhaust temperature (330 K) by adjusting leakage area, equipment temperature, and heat convection from the cell housing exterior wall to the process building atmosphere. Results showed that about 50% of the aerosols released are exhausted through the roof vent. The remaining 50% of the aerosols exit through the motor exhaust, or are passed out of the computational domain to an adjacent cell. Subsequently, a transient solution was obtained starting from the steady state flow field and zero initial conditions assumed for the aerosol concentration. A 26.5 kg/s aerosol mass source and a heat-of-reaction source of $9.635 \times 10^6 \text{ W}$ were assumed for a 5 min period. The transient case was run to 521 s. At this time 70% of the aerosol was predicted to escape through the roof vent. To produce compatible results as CFDS-FLOW3D, MELCOR input for specifying these leakage flow paths was calibrated to match the transient results obtained from CFDS-FLOW3D.

2.3 Sensible Energy and Chemical Reaction of Gaseous UF_6 Released into Cell Housing

¹ CFDS-FLOW3D is a commercially available computational fluid dynamics program developed by AEA Technology Engineering Software, Inc.

As gaseous UF_6 is sourced, the control volume is subjected to not only exothermic energy generated from UF_6 reaction with moisture, but also sensible energy carried by UF_6 gas. The magnitude of the sensible energy of UF_6 gas is determined based on temperature of UF_6 (T_U) at its release through a broken pipe. The enthalpy of gaseous UF_6 is based on $H_v = 0$ at $T = 0$ K, as [Williams, 1986]

$$H_v = \left[43.2614 + 9.21307 \times 10^{-2} T_U + 6.26265 \times 10^{-6} T_U^2 + \frac{2951.71}{T_U} \right] + \left[3.0939 \times 10^{-3} T_U (Z|_{p,T} - Z|_{14.7,T}) \right] \quad (1)$$

where H_v is given in Btu/lb, and T_U is given in R. The compressibility factor in Eq. (1), is defined as

$$Z = \frac{T_U^3}{T_U^3 + 4.8923 \times 10^5 p} \quad (2)$$

where p is pressure in psia.

We assume that gaseous UF_6 instantaneously mixes with air in control volume, and undergoes an instantaneous chemical reaction.

However, this chemical reaction is limited in magnitude by availability of moisture content in the air. For MELCOR modeling of the UF_6 chemical reaction process limited by moisture content, a set of control functions has been built to: (1) monitor moisture content in each control volume atmosphere, (2) calculate UF_6 reaction rate limited by the moisture content, and (3) determine the rate of moisture consumption in the control volume. Such an amount of moisture consumption is utilized as input into the Control Volume Hydrodynamics (CVH) package of MELCOR as a mass sink in corresponding control volumes. Since each control volume is interconnected unless the interconnecting flow paths are blocked by any physical means such as valve or blind flange, the air moisture content will be updated by air being circulated into the control volume. Any unreacted UF_6 is subjected to convection to neighboring control volumes, and to a chemical reaction with moisture present.

2.4 Aerosol Model

Aerosol agglomeration and deposition processes are modeled in the radionuclide (RN) package of the MELCOR code. The code allows specification of aerosol size distribution

and a particular type of aerosol material. This multi-sectional, multi-component aerosol dynamics model evaluates the size distribution of each type of aerosol mass, or component, as a function of time. This size distribution is described by the mass in each size bin, or section. Each section may have a different chemical composition as described by the masses of various components of that section. Aerosols can directly be deposited onto the heat structure and water pool surfaces through a number of processes, including gravitational settling, diffusion to surfaces, thermophoresis (a Brownian process causing migration of particles toward lower temperature), and diffusiophoresis (deposition induced by condensation of water vapor onto structural surfaces). Aerosols can also settle from one control volume to another through "flow-through" areas (i.e., gravitational settling and Brownian diffusion kernels are applied to "flow-through" areas along with heat structure and pool surfaces). Such areas will ordinarily correspond to open flow paths between the control volumes, through which aerosols and radionuclide vapors are also advected.

The MELCOR calculation of changes in aerosol distribution and location considers the following general processes:

1. aerosol phenomenological sources from other packages, such as release from fuel rods or during core-concrete interactions, and/or arbitrary user-specified sources;
2. condensation and evaporation of water and fission products to and from aerosol particles;
3. particle agglomeration (or coagulation), whereby two particles collide and form one larger particle;
4. particle deposition onto surfaces or settling through flow paths into lower control volumes;
5. advection of aerosols between control volumes by bulk fluid flows; and
6. removal of aerosol particles by engineering safety features (ESFs), such as filter trapping, pool scrubbing, and spray washout.

For our case of UF_6 release accident calculations, the effect of gravitational settling dominates deposition magnitude over other deposition processes (i.e., it was noted to be 1 or 2 orders of magnitude larger than from processes such as thermophoresis and diffusiophoresis).

Aerosols in the current study need to be characterized and specified in MELCOR input for the aerosol transport calculations with consideration of aerosol growth by agglomeration, condensation, etc. Aerosol size is assumed to be a log-normal distribution between $0.4 \mu\text{m}$

and 2.5 μm diameter. This aerosol size range is based on guidance from the uranium particle size distribution measurements taken on Sequoyah Nuclear Fuel air filters [NUREG-1189, Vol.1]. According to the measurements, most of the uranium particles fell in the size range between 0.4 μm and 2.5 μm diameter with a peak between 1.27 μm and 1.59 μm . An experiment was also performed by Pickrell to study UO_2F_2 particle formation following UF_6 release in a small bell jar and in a Plexiglas cube [Pickrell, 1982]. The conclusion drawn from the series of tests is that particles produced in high relative humidity start out as spheroids in the 0.3 to 0.6 μm diameter range and age to be between 1 to 2 μm diameter. Another experiment was conducted at the Portsmouth GDP [Lux, 1982], where UF_6 samples were released within a 34 m^3 (1,200 ft^3) chamber. An average particle size appears to be in the range of 1.1 ~ 1.4 μm . This appears to further corroborate the data obtained from the Sequoyah measurements.

In the current model, the aerosol size range is binned into five sections, and in each section, one aerosol component is assumed to represent aerosols in that section since we have a single component aerosol (UO_2F_2) in the current study.

Other important parameters in determining the aerosol transport/ settling involve a dynamic shape factor and an agglomeration shape factor. The MELCOR code was assessed against the LWR Aerosol Containment Experiments (LACE) to investigate MELCOR's capability of simulating aerosol transport phenomena [Kmetyk, 1991]. Aerosols used in the experiments were CsOH and MnO . This study shows that MELCOR predicted aerosol behavior most closely to data collected from the experiments with a dynamic shape factor of 1.85 and an agglomeration shape factor of 2.25. For the current study, we decided to use these numbers for the shape factors. Also 6,375 kg/m^3 for aerosol particle density is used for the current study, which builds upon similar past work [Williams, 1986].

For the deposition surface of aerosol settling, the surfaces of equipment and piping are included in addition to floor surfaces. The gravitational settling model of MELCOR calculates aerosol mass settled on heat structure (floor, equipment, wall, etc.) surface based on settling velocity calculated accounting for various atmospheric condition. However, the model does not track individual particle paths for settling. As a consequence, the model does not acknowledge the relative altitude of heat structures for aerosol settling calculation; that is, aerosol traveling (settling) length for settling is not factored in the calculation. Therefore, to account for the aerosol traveling length, equipment/piping surface area was

increased to twice assuming that they are distributed uniformly throughout at the different elevations in cell housing control volumes.

3. RESULTS and DISCUSSION

One of the depleted UF_6 piping lines (B-line) was assumed to break in the fifth cell housing of the unit 4 (cv-405). As a result of the break, 58.97 kg/s (130 lb/s) of UF_6 gas was assumed to be released at 426.5K (290 F) into the atmosphere of cv-405. The appropriate accident management actions should be taken to rapidly isolate the broken process piping system. In the current study, however, such an action was assessed as being successful within a time span ranging from 10 min to 30 min since the pipe break. Assessments further indicate the release to continue at a fairly constant rate for a duration of the transient. For the current study, therefore, two scenarios were selected as bounding calculations; that is, 10 min release for case 1, and 30 min release for case 2. MELCOR input was prepared for both the Paducah GDP and the Portsmouth GDP, and for both scenarios, cases 1 & 2. For both cases, the steady state calculations were performed for the first 500s, and then followed by the transient simulation until 3,500s for case 1 (10 min release case) and 5,000s for case 2 (30 min release case), respectively.

3.1 Case 1 (10 Min Release Case)

Figures 8 through 22 show the results calculated by MELCOR for case 1 (10 min release case) of the Paducah GDP. Air mass flow rate through the leakage flow paths of the cell housing (cv-405) is shown in Figure 8. This is the control volume where UF_6 gets sourced into at 500s. A steady state is established for the first 500s, and air flow rate through the leaks, as seen in the figure, is summed to be about 9 m³/s (19,000 cfm). Upon cessation of UF_6 release at 1,100s, flow oscillates initially, and then begins to damp off and finally approaches an equilibrium of about 9 m³/s. Figure 9 shows the mass reaction rate of UF_6 with moisture in various control volumes. UF_6 is released at the rate of 58.97 kg/s (130 lb/s). However, its chemical reaction with moisture is limited by the availability of moisture content in the air. Once the moisture is consumed, unreacted UF_6 migrates to the neighboring control volumes where it undergoes a chemical reaction. Even though the moisture is consumed quickly, it is replenished by the air circulated into the cell housing control volume, and undergoes further reaction with UF_6 . The oscillatory behavior in the reaction rate as seen in the figure is due to the explicit numerical coupling between hydrodynamics calculations and the reaction rate calculations that are defined through

MELCOR Control Functions (CFs). The processes defined through CFs are designed to be coupled explicitly with those simulated by built-in models in MELCOR. Therefore, CF processes are always one time-step behind. Also seen in Figure 9, is the UF_6 reaction in its neighboring control volumes; mainly control volumes in immediate vicinity of the cv-405. These volumes are the cell housing control volumes (cv-404 and 406) interconnected to cv-405, and control volumes outside the cell housing cv-405. Note that the UF_6 reaction ceases upon the end of its release. Figure 10 shows pressure variation at the bottom of the control volumes surrounding the cell housing cv-405. The pressure difference between the control volumes shown in the figure is mainly due to the static head since cv-425 represents the control volume for the process building area above the cell housing cv-405. Also the pressure difference is noticed between cv-405 and cv-415 (control volume outside the cell housing at the same elevation as cv-405), resulting from the lower density head inside the cell housing due to higher air temperature caused by hot equipment surfaces. Note that the pressure in the cell housing, cv-405, oscillates somewhat during the period of the UF_6 release.

The mass source term distribution is shown in Figures 11 through 18. Figure 11 shows UF_6 , UO_2F_2 and HF mass released into the environment. The total amount of UF_6 released for this scenario is 35,380 kg. Results indicated that 100% of UF_6 is eventually reacted with moisture, resulting in UO_2F_2 and HF. The total amount of UO_2F_2 and HF is 30,958 kg, and 8,031 kg, respectively. As seen in Figure 11, no UF_6 was released into the environment, and 17,580 kg of UO_2F_2 and 7,961 kg of HF were estimated to be released into the environment. These source term magnitude represents 57% of UO_2F_2 and 99.1% of HF available in the process building volume. Most of the remaining 43% of UO_2F_2 particles was settled down on the floor and equipment surfaces in various control volumes. The variation of UO_2F_2 release at different locations into the environment are shown in Figure 12. As expected, a significant portion was predicted to be released from unit 4 where gaseous UF_6 was sourced into. Also seen in the same figure, substantial UO_2F_2 mass was also released from the units 3 and 5. This clearly indicates significant dispersion of UO_2F_2 into the neighboring units. Similar behavior of HF dispersion and release is also shown in Figure 13. Figure 14 shows an integrated atmospheric source term from various units of the process building. The atmospheric mass includes air and moisture other than UF_6 , UO_2F_2 and HF. The total source term including UF_6 , UO_2F_2 , HF and atmospheric mass is shown in Figure 15. Figures 16 through 18 show fractional mass source term from various units of the process building. Since the major released component is air, the

fraction of released UO_2F_2 and HF is not significant in comparison with the magnitude of air released.

Figures 19 through 21 show the enthalpy of materials released into the environment. Figure 19 shows the enthalpy of total material (atmosphere, UF_6 , UO_2F_2 and HF) released from various units of the process building. Figures 20 and 21 show the integrated enthalpy of UO_2F_2 and HF released into the environment, respectively. Figure 22 shows the temperature of materials released into the environment from various locations of the process building.

The summary of the results for the case 1 (10 min release case) for the Paducah GDP is listed in Tables 3 and 4.

Similar plots for the Portsmouth GDP for the case 1 (10 min release case) are shown in Figures 23 through 38. Behavior looks similar and the results are summarized in Tables 5 and 6. Since the units 7 and 8 are too far from the unit 4 where UO_2F_2 and HF start to disperse, an addition of these two units to the 6-unit model of the Paducah GDP does not affect much in overall source term magnitude and its distribution of release into the environment.

3.2 Case 2 (30 Min Release Case)

Behavior of aerosol transport and source term calculation results are similar as the case 1. The results for the Paducah GDP are shown in Figures 39 through 69, and for the Portsmouth GDP are shown in Figures 54 through 72. Results are summarized in Tables 7 through 10.

4. SUMMARY and CONCLUSION

The MELCOR computer code was used for simulating aerosols and vapor transport for postulated UF_6 release accident as a result of a large break in B-line piping in cell housing in the process building of both the Paducah and Portsmouth GDPs. The released UF_6 undergoes a chemical reaction with moisture in the air while it is dispersed, producing UO_2F_2 aerosol and HF vapor. To evaluate spatial effects in conjunction with plant-specific nuances related to ventilation flow distribution effects, the entire process building was included in MELCOR modeling. Specifically, the entire process building (C-337 of the

Paducah GDP and X-333 of the Portsmouth GDP) was discretized into about 40 control volumes interconnected by about 200 flow paths. To characterize leakage flow through cell housing wall, 3-D CFD tool (CFDS-FLOW3D) was used for guidance and modeling of turbulent mixing effects. Results indicated that substantial amount of UO_2F_2 particles get settled onto cell housing floor, and surfaces of equipment and piping in cell housing. About 57% of UO_2F_2 was predicted to be released into the environment. Since HF was treated as vapor, close to 100% was estimated to get released into the environment. Also predicted in the results, was that substantial amount of UO_2F_2 and HF were dispersed from the unit where initial UF_6 was released, to other neighboring units. This study also provides spatial variations of source term release from various locations of the process building.

5. REFERENCES

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Table 1 Input Data of MELCOR Control Volumes

Units	Description	CVH ID	From Elev (m)	To Elev (m)	Volume (m ³)
Unit 1	Cell Housing	101	8.8392	14.5999	13,490
	Floor Volume	102	8.8392	24.9936	229,907
Unit 2	Cell Housing	201	8.8392	14.5999	13,490
	Floor Volume	202	8.8392	24.9936	229,907
Unit 3	Cell Housing	301	8.8392	14.5999	13,490
	Floor Volume	302	8.8392	24.9936	229,907
Unit 4	Cell Housing	401-410	8.8392	14.5999	1,349
	Low-Floor	411-420	8.8392	14.5999	5,043
	Mid-Floor	421-430	14.5999	19.7815	7,374
	High-Floor	431	19.7815	24.9936	74,178
Unit 5	Cell Housing	501	8.8392	14.5999	13,490
	Floor Volume	502	8.8392	24.9936	229,907
Unit 6	Cell Housing	601	8.8392	14.5999	13,490
	Floor Volume	602	8.8392	24.9936	229,907
Unit 7*	Cell Housing	701	8.8392	14.5999	13,490
	Floor Volume	702	8.8392	24.9936	229,907
Unit 8*	Cell Housing	801	8.8392	14.5999	13,490
	Floor Volume	802	8.8392	24.9936	229,907
Process Building Outside		901-908	0.0	100.0	10 ⁶
Air Intake Volume		999	0.0	100.0	10 ⁹

(*) Units 7 & 8 are only for the Portsmouth GDP.

Table 2 Input Data for MELCOR Flow Paths

	FL #	from CVH	to CVH	description	category	Altitude of from-CVH (m)	Altitude of to- CVH (m)	Flow Area (m ²)	Length (m)	Hyd Diameter (m)	Velocity (m/s)
Between Cell Housing & Floor Volume	101	101	102	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	102	101	102	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	103	101	102	door	3	9.906	9.906	19.5096	1	4.9840	
	104	101	102	leak-out@top	4	14.5999	14.5999	33.4451	1	6.5256	
	105	201	202	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	106	201	202	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	107	201	202	door	3	9.906	9.906	19.5096	1	4.9840	
	108	201	202	leak-out@top	4	14.5999	14.5999	33.4451	1	6.5256	
	109	301	302	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	110	301	302	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	111	301	302	door	3	9.906	9.906	19.5096	1	4.9840	
	112	301	302	leak-out@top	4	14.5999	14.5999	33.4451	1	6.5256	
	113	401	411	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	114	401	421	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	115	401	411	door	3-a	9.906	9.906	1.95096	1	1.5761	
	116	401	411	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	117	402	412	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	118	402	422	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	119	402	412	door	3-a	9.906	9.906	1.95096	1	1.5761	
	120	402	412	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	121	403	413	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	122	403	423	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	123	403	413	door	3-a	9.906	9.906	1.95096	1	1.5761	
	124	403	413	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	125	404	414	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	126	404	424	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	127	404	414	door	3-a	9.906	9.906	1.95096	1	1.5761	
	128	404	414	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	129	405	415	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	130	405	425	leak-out@ wall	2-a	13.1597	14.5999	1.5	1	1.3820	
	131	405	415	door	3-a	9.906	9.906	1.95096	1	1.5761	
	132	405	415	leak-out@top	4-a	13.1597	13.1597	2.55	1	1.8019	
	133	406	416	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	134	406	426	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	135	406	416	door	3-a	9.906	9.906	1.95096	1	1.5761	
	136	406	416	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	137	407	417	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	138	407	427	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	139	407	417	door	3-a	9.906	9.906	1.95096	1	1.5761	
	140	407	417	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	141	408	418	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	142	408	428	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	143	408	418	door	3-a	9.906	9.906	1.95096	1	1.5761	
	144	408	418	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	145	409	419	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	146	409	429	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	147	409	419	door	3-a	9.906	9.906	1.95096	1	1.5761	
	148	409	419	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	149	410	420	leak-in @ wall	1-a	10.2793	10.2793	4.05	1	2.2708	
	150	410	430	leak-out@ wall	2-a	13.1597	14.5999	0.405	1	0.7181	
	151	410	420	door	3-a	9.906	9.906	1.95096	1	1.5761	
	152	410	420	leak-out@top	4-a	13.1597	13.1597	3.645	1	2.1543	
	153	501	502	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	154	501	502	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	155	501	502	door	3	9.906	9.906	19.5096	1	4.9840	
	156	501	502	leak-out@top	4	14.5999	14.5999	33.4451	1	6.5256	
	157	601	602	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	158	601	602	leak-out wall	2	13.1597	14.5999	40.5	1	7.1810	
	159	601	602	door	3	9.906	9.906	19.5096	1	4.9840	
	160	601	602	leak-out@top	4	14.5999	14.5999	33.4451	1	6.5256	
	161	101	201		5	11.1557	11.1557	73.1519	264.9	9.6509	
Between Cell Housings	162	201	301		5	11.1557	11.1557	73.1519	264.9	9.6509	
	163	301	401		5-a	11.1557	11.1557	7.31519	26.49	3.0519	
	164	401	402		5-a	11.1557	11.1557	7.31519	26.49	3.0519	
	165	402	403		5-a	11.1557	11.1557	7.31519	26.49	3.0519	
	166	403	404		5-a	11.1557	11.1557	7.31519	26.49	3.0519	

	167	404	405	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	168	405	406	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	169	406	407	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	170	407	408	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	171	408	409	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	172	409	410	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	173	410	501	5-a	11.1557	11.1557	7.31519	26.49	3.0519
	174	501	601	5	11.1557	11.1557	73.1519	264.9	9.6509
Between Floor Volumes	175	102	202	6	16.9164	16.9164	2388.07	111.6	55.1415
	176	202	302	6	16.9164	16.9164	2388.07	111.6	55.1415
	177	302	411	6-a	11.7196	11.7196	321.324	88.7	20.2268
	178	302	420	6-a	11.7196	11.7196	321.324	88.7	20.2268
	179	302	421	6-b	17.1907	17.1907	289.021	88.7	19.1832
	180	302	430	6-b	17.1907	17.1907	289.021	88.7	19.1832
	181	302	431	6-c	22.3876	22.3876	581.443	147.8	27.2088
	182	411	412	6-a	11.7196	11.7196	321.324	29.57	20.2268
	183	411	421	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	184	411	420	6-d	11.7196	11.7196	170.319	55.78	14.7261
	185	412	413	6-a	11.7196	11.7196	321.324	29.57	20.2268
	186	412	422	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	187	412	419	6-d	11.7196	11.7196	170.319	55.78	14.7261
	188	413	414	6-a	11.7196	11.7196	321.324	29.57	20.2268
	189	413	423	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	190	413	418	6-d	11.7196	11.7196	170.319	55.78	14.7261
	191	414	415	6-a	11.7196	11.7196	321.324	29.57	20.2268
	192	414	424	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	193	414	417	6-d	11.7196	11.7196	170.319	55.78	14.7261
	194	415	416	6-d	11.7196	11.7196	170.319	55.78	14.7261
	195	415	425	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	196	416	417	6-a	11.7196	11.7196	321.324	29.57	20.2268
	197	416	426	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	198	417	418	6-a	11.7196	11.7196	321.324	29.57	20.2268
	199	417	427	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	200	418	419	6-a	11.7196	11.7196	321.324	29.57	20.2268
	201	418	428	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	202	419	420	6-a	11.7196	11.7196	321.324	29.57	20.2268
	203	419	429	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	204	420	430	6-c	11.7196	17.1907	1259.32	5.471	40.0427
	205	421	430	6-f	17.1907	17.1907	153.197	55.78	13.9663
	206	422	429	6-f	17.1907	17.1907	153.197	55.78	13.9663
	207	423	428	6-f	17.1907	17.1907	153.197	55.78	13.9663
	208	424	427	6-f	17.1907	17.1907	153.197	55.78	13.9663
	209	425	426	6-f	17.1907	17.1907	153.197	55.78	13.9663
	210	421	422	6-b	17.1907	17.1907	289.021	29.57	19.1832
	211	422	423	6-b	17.1907	17.1907	289.021	29.57	19.1832
	212	423	424	6-b	17.1907	17.1907	289.021	29.57	19.1832
	213	424	425	6-b	17.1907	17.1907	289.021	29.57	19.1832
	214	426	427	6-b	17.1907	17.1907	289.021	29.57	19.1832
	215	427	428	6-b	17.1907	17.1907	289.021	29.57	19.1832
	216	428	429	6-b	17.1907	17.1907	289.021	29.57	19.1832
	217	429	430	6-b	17.1907	17.1907	289.021	29.57	19.1832
	218	421	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	219	422	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	220	423	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	221	424	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	222	425	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	223	426	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	224	427	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	225	428	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	226	429	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	227	430	431	6-g	17.1907	22.3876	1649.12	5.471	45.8228
	228	416	502	7-a	11.71955	11.71955	170.319	83.67	14.7261
	229	417	502	7-a	11.71955	11.71955	170.319	83.67	14.7261
	230	418	502	7-a	11.71955	11.71955	170.319	83.67	14.7261
	231	419	502	7-a	11.71955	11.71955	170.319	83.67	14.7261
	232	420	502	7-a	11.71955	11.71955	170.319	83.67	14.7261
	233	426	502	7-b	17.1907	17.1907	153.197	110.9	13.9663
	234	427	502	7-b	17.1907	17.1907	153.197	110.9	13.9663
	235	428	502	7-b	17.1907	17.1907	153.197	110.9	13.9663
	236	429	502	7-b	17.1907	17.1907	153.197	110.9	13.9663
	237	430	502	7-b	17.1907	17.1907	153.197	110.9	13.9663

	238	431	502	7-c	22.3876	22.3876	770.491	111.6	31.3212		
	239	502	202	8	16.9164	16.9164	1802.13	147.8	47.9014		
	240	502	602	6	16.9164	16.9164	2388.07	111.6	55.1415		
	241	602	102	8	16.9164	16.9164	1802.13	147.8	47.9014		
Air Supply	901	999	102	11	8.8392	8.8392	22.3	1	5.3285	21.3767	
	902	999	202	11	8.8392	8.8392	22.3	1	5.3285	21.3767	
	903	999	302	11	8.8392	8.8392	22.3	1	5.3285	21.3767	
	904	999	411	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	905	999	412	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	906	999	413	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	907	999	414	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	908	999	415	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	909	999	416	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	910	999	417	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	911	999	418	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	912	999	419	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	913	999	420	11-a	8.8392	8.8392	2.23	1	1.6850	21.3767	
	914	999	502	11	8.8392	8.8392	22.3	1	5.3285	21.3767	
	915	999	602	11	8.8392	8.8392	22.3	1	5.3285	21.3767	
Motor Exhaust	916	102	901	12	8.8392	24.9936	24.07	1	5.5360	11.1757	
	917	202	902	12	8.8392	24.9936	24.07	1	5.5360	11.1757	
	918	302	903	12	8.8392	24.9936	24.07	1	5.5360	11.1757	
	919	411	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	920	412	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	921	413	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	922	414	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	923	415	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	924	416	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	925	417	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	926	418	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	927	419	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	928	420	904	12-a	8.8392	24.9936	2.407	1	1.7506	11.1757	
	929	502	905	12	8.8392	24.9936	24.07	1	5.5360	11.1757	
	930	602	906	12	8.8392	24.9936	24.07	1	5.5360	11.1757	
Roof Exhaust	931	102	901	13	24.9936	24.9936	29.714	1	6.1509		
	932	202	902	13	24.9936	24.9936	29.714	1	6.1509		
	933	302	903	13	24.9936	24.9936	29.714	1	6.1509		
	934	431	904	13	24.9936	24.9936	29.714	1	6.1509		
	935	502	905	13	24.9936	24.9936	29.714	1	6.1509		
	936	602	906	13	24.9936	24.9936	29.714	1	6.1509		
Portsmouth GDP additional data											
	266	701	702	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	267	701	702	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	268	701	702	door	3	9.906	9.906	19.5096	1	4.9840	
	269	601	701		5	11.1557	11.1557	73.1519	264.9	9.6509	
	270	602	702		6	16.9164	16.9164	2388.07	111.6	55.1415	
	271	702	802		8	16.9164	16.9164	1802.13	147.8	47.9014	
	272	801	802	leak-in @ wall	1	10.2793	10.2793	40.5	1	7.1810	
	273	801	802	leak-out@ wall	2	13.1597	14.5999	40.5	1	7.1810	
	274	801	802	door	3	9.906	9.906	19.5096	1	4.9840	
	275	801	101		5	11.1557	11.1557	73.1519	264.9	9.6509	
	276	802	102		6	16.9164	16.9164	2388.07	111.6	55.1415	
	277	702	907	motor exhaust	12	8.8392	24.9936	24.07	1	5.5360	11.1757
	278	702	907	roof exhaust	13	24.9936	24.9936	29.714	1	6.1509	
	279	802	908	motor exhaust	12	8.8392	24.9936	24.07	1	5.5360	11.1757
	280	802	908	roof exhaust	13	24.9936	24.9936	29.714	1	6.1509	

* Flow Path Categorization :

- 1 cell housing leakage-in @ low-elevation (unit level)
- 1-a cell housing leakage-in @ low-elevation (cell level)
- 2 cell housing leakage-out @ high-elevation (unit level)
- 2-a cell housing leakage-out @ high-elevation (cell level)
- 3 cell housing door @ mid-elevation (unit level)
- 3-a cell housing door @ mid-elevation (cell level)
- 4 cell housing hatch (unit level)
- 4-a cell housing hatch (cell level)
- 5 between cell housings (unit level)
- 5-a between cell housings (cell level)

- 6 between unit floor volumes (E&W, unit level)
- 6-a between unit & cell floor volumes @ low-elevation(N&S), or
 between cell floor volumes @ low-elevation (N&S)
- 6-b between unit & cell floor volumes @ mid-elevation(N&S), or
 between cell floor volumes @ mid-elevation (N&S)
- 6-c between unit & cell floor volumes @ high-elevation(N&S), or
 between cell floor volumes @ high-elevation (N&S)
- 6-d between cell floor volumes @ low-elevation (E&W)
- 6-e between low- & mid-cell floor volumes
- 6-f between cell floor volumes @ mid-elevation (E&W)
- 6-g between mid- and high-cell floor volumes
- 7
- 7-a between unit 4&5 cell floor volume @ low-elevation (E&W)
- 7-b between unit 4&5 cell floor volume @ mid-elevation (E&W)
- 7-c between unit 4&5 cell floor volume @ high-elevation (E&W)
- 8 between unit floor volumes (N&S, unit level)
- 9 between cell housing & bypass housing (unit level)
- 9-a between cell housing & bypass housing (cell level)
- 10 between bypass housings (unit level)
- 10-a between bypass housings (cell level)
- 11 air supply (unit level)
- 11-a air supply (cell level)
- 12 motor exhaust (unit level)
- 12-a motor exhaust (cell level)
- 13 roof exhaust

Table 3 UO₂F₂ and HF Mass Source Term for 10 min Release Case for the Paducah GDP (in terms of mass) (total UO₂F₂ mass = 30,958 kg, total HF mass = 8,031 kg)

mass (kg)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	total
UF ₆	0	0	0	0	0	0	0
UO ₂ F ₂	49.6	835.9	4,358	7,620	4,557	159.3	17,580
HF	21.7	381.4	2,048	3,320	2,102	87.7	7,961

Table 4 UO₂F₂ and HF Mass Source Term for 10 min Release Case for the Paducah GDP (in terms of mass fraction to total available mass)

fraction (%)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	total
UF ₆	0	0	0	0	0	0	0
UO ₂ F ₂	0.2	2.7	14.1	24.6	14.7	0.5	57
HF	0.3	4.7	25.5	41.3	26.2	1.1	99.1

Table 5 UO₂F₂ and HF Mass Source Term for 10 min Release Case for the Portsmouth GDP (in terms of mass) (total UO₂F₂ mass = 30,958 kg, total HF mass = 8,031 kg)

mass (kg)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	unit 7	unit 8	total
UF ₆	0	0	0	0	0	0	0	0	0
UO ₂ F ₂	49.7	825.3	4,377	7,628	4,556	148.1	4.2	0.6	17,589
HF	21.4	374.8	2,055	3,325	2,100	82.3	2.4	0.3	7,962

Table 6 UO₂F₂ and HF Mass Source Term for 10 min Release Case for the Portsmouth GDP (in terms of mass fraction to total available mass)

fraction (%)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	unit 7	unit 8	total
UF ₆	0	0	0	0	0	0	0	0	0
UO ₂ F ₂	0.2	2.7	14.1	24.6	14.7	0.5	0.01	0.002	57
HF	0.3	4.7	25.6	41.4	26.1	1.0	0.03	0.004	99.1

Table 7 UO₂F₂ and HF Mass Source Term for 30 min Release Case for the Paducah GDP (in terms of mass) (total UO₂F₂ mass = 92,873 kg, total HF mass = 24,160 kg)

mass (kg)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	total
UF ₆	0	0	0	0	0	0	0
UO ₂ F ₂	472	3,198	12,260	22,850	13,040	998	52,810
HF	236	1,600	5,902	9,758	6,141	516	24,150

Table 8 UO₂F₂ and HF Mass Source Term for 30 min Release Case for the Paducah GDP (In terms of mass fraction to total available mass)

fraction (%)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	total
UF ₆	0	0	0	0	0	0	0
UO ₂ F ₂	0.5	3.4	13.2	24.6	14.1	1.1	57
HF	1.0	6.6	24.4	40.4	25.4	2.1	99.9

Table 9 UO₂F₂ and HF Mass Source Term for 30 min Release Case for the Portsmouth GDP (in terms of mass)) (total UO₂F₂ mass = 92,873 kg, total HF mass = 24,160 kg)

mass (kg)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	unit 7	unit 8	total
UF ₆	0	0	0	0	0	0	0	0	0
UO ₂ F ₂	494	3,250	12,310	22,860	12,970	947	38	31	52,850
HF	246	1,601	5,926	9,761	6,097	489	21	15	24,155

Table 10 UO₂F₂ and HF Mass Source Term for 30 min Release Case for the Portsmouth GDP (In terms of mass fraction to total available mass)

fraction (%)	unit 1	unit 2	unit 3	unit 4	unit 5	unit 6	unit 7	unit 8	total
UF ₆	0	0	0	0	0	0	0	0	0
UO ₂ F ₂	0.5	3.5	13.3	24.6	14.0	1.0	0.04	0.03	57
HF	1.0	6.6	24.5	40.4	25.2	2.0	0.09	0.06	99.9

Figure 1 Summer ventilation pattern of one unit of the process building

C-337 Building : 6 units & 10 cells/unit, 60 cells

Cell Floor Volume = $55.4 \times 10^6 \text{ ft}^3 / 60 \text{ cells} = 9.23 \times 10^5 \text{ ft}^3 / \text{cell}$

Cell Floor Ceiling Height = 53 ft

Cell Floor Volume to Cell-Housing Elevation :
 $(9.23 \times 10^5 \text{ ft}^3 / \text{cell}) \{ (10.7 + 8.2) / 53 \} = 3.3 \times 10^5 \text{ ft}^3 / \text{cell}$ for cell-housing elevation

Cell Floor Area = $1,045,440 \text{ ft}^2 / 60 \text{ cells} = 17,424 \text{ ft}^2 / \text{cell}$

Air Supply Fan Capacity = $6.06 \times 10^6 \text{ cfm} / 60 \text{ fans} = 1.01 \times 10^5 \text{ cfm} / \text{cell (or fan)}$

Motor Exhaust Fans Capacity :
 if transformer exhaust opens, = 56,250 cfm/cell
 if transformer exhaust closed, = 75,000 cfm/cell

Roof Exhaust = Air Supply - Motor Exhaust

Volume

$V (\text{penthouse}) = (125.6)(31.3)(8.2) = 32,237 \text{ ft}^3$

$V (\text{cell-housing main building}) = (125.6 + 16.6 + 5.8)(31.3 + 2 \times 7)(10.7) = 71,745 \text{ ft}^3$

$V (\text{duct, east}) = (13.7)(20)(6.2) = 1,695 \text{ ft}^3$

$V (\text{duct, west}) = 1,695 \text{ ft}^3$

$V (\text{total cell-housing}) = 107,372 \text{ ft}^3$

$V (\text{vol between cell-housing main building}) = (40)(10.7)(125.6 + 16.6 + 5.8) = 63,348 \text{ ft}^3$

$V (\text{vol between penthouses}) = (40 + 2 \times 7)(8.2)(125.6 + 16.6 + 5.8) = 65,539 \text{ ft}^3$

$V (\text{vol at east+west ends of penthouse}) = (16.6 + 5.8)(8.2)(31.3) = 5,752 \text{ ft}^3$

$V (\text{vol occupied by east duct}) = (13.7)(40)(6.2) = 3,390 \text{ ft}^3$ (to be subtracted)

$V (\text{total volume between cell-housings}) = 131,249 \text{ ft}^3$

$V (\text{total vol at east+west ends}) = 3.3 \times 10^5 - (107,128 + 131,249 + 3,390) = 87,989 \text{ ft}^3$

Figure 2 Schematic drawing of typical cell housing

Figure 3 MELCOR control volumes of the C-337 building of the Paducah GDP

Figure 4 MELCOR control volumes of one unit of the process building

Figure 5 MELCOR nodalization of the C-337 building of the Paducah GDP

Figure 8 Air mass flow rate through cell housing leakage flow paths for 10 min UF_6 release case in the Paducah GDP

Figure 9 UF₆ mass reaction rate in various locations of the building for 10 min UF₆ release case in the Paducah GDP

Figure 10 Pressure variations in control volumes for 10 min UF_6 release case in the Paducah GDP

Figure 11 Source term mass of UF₆, UO₂F₂ and HF for 10 min UF₆ release case in the Paducah GDP

Figure 12 UO_2F_2 source term mass from each unit for 10 min UF_6 release case in the Paducah GDP

Figure 13 HF source term mass from each unit for 10 min UF_6 release case in the Paducah GDP

Figure 14 Atmospheric material source term (air & moisture) from each unit for 10 min
 UF_6 release case in the Paducah GDP

Figure 15 Total material mass source term (air, moisture, UF_6 , UO_2F_2 & HF) from each unit for 10 min UF_6 release case in the Paducah GDP

Figure 16 Fractional UO₂F₂ and HF mass source term from units 1 and 2 for 10 min UF₆ release case in the Paducah GDP

Figure 17 Fractional UO₂F₂ and HF mass source term from units 3 and 4 for 10 min UF₆ release case in the Paducah GDP

Figure 18 Fractional UO₂F₂ and HF mass source term from units 5 and 6 for 10 min UF₆ release case in the Paducah GDP

Integrated enthalpy source term (TJ)

Figure 19 Enthalpy of total material for 10 min UF_6 release case in the Paducah GDP

Figure 20 Enthalpy of UO_2F_2 source term for 10 min UF_6 release case in the Paducah GDP

Figure 21 Enthalpy of HF source term for 10 min UF_6 release case in the Paducah GDP

Figure 22 Source term temperature for 10 min UF_6 release case in the Paducah GDP

Figure 23 Air mass flow rate through cell housing leakage flow paths for 10 min UF₆ release case in the Portsmouth GDP

Figure 24 UF_6 mass reaction rate in various locations of the building for 10 min UF_6 release case in the Portsmouth GDP

Figure 25 Pressure variations in control volumes for 10 min UF_6 release case in the Portsmouth GDP

Figure 26 Source term mass of UF₆, UO₂F₂ and HF for 10 min UF₆ release case in the Portsmouth GDP

UO₂F₂ mass source term (10^3 kg)

Figure 27 UO₂F₂ source term mass from each unit for 10 min UF₆ release case in the Portsmouth GDP

Figure 28 HF source term mass from each unit for 10 min UF_6 release case in the Portsmouth GDP

Integrated atmospheric mass source term (10^6 kg)

Figure 29 Atmospheric material source term (air & moisture) from each unit for 10 min UF_6 release case in the Portsmouth GDP

Figure 30 Total material mass source term (air, moisture, UF_6 , UO_2F_2 & HF) from each unit for 10 min UF_6 release case in the Portsmouth GDP

Figure 31 Fractional UO₂F₂ and HF mass source term from units 1 and 2 for 10 min UF₆ release case in the Portsmouth GDP

Figure 32 Fractional UO_2F_2 and HF mass source term from units 3 and 4 for 10 min UF_6 release case in the Portsmouth GDP

Figure 33 Fractional UO₂F₂ and HF mass source term from units 5 and 6 for 10 min UF₆ release case in the Portsmouth GDP

Figure 34 Fractional UO₂F₂ and HF mass source term from units 7 and 8 for 10 min UF₆ release case in the Portsmouth GDP

Figure 35 Enthalpy of total material for 10 min UF_6 release case in the Portsmouth GDP

Figure 36 Enthalpy of UO_2F_2 source term for 10 min UF_6 release case in the Portsmouth GDP

Figure 37 Enthalpy of HF source term for 10 min UF_6 release case in the Portsmouth GDP

Figure 38 Source term temperature for 10 min UF_6 release case in the Portsmouth GDP

Figure 39 Air mass flow rate through cell housing leakage flow paths for 30 min UF₆ release case in the Paducah GDP

Figure 40 UF₆ mass reaction rate in various locations of the building for 30 min UF₆ release case in the Paducah GDP

Figure 41 Pressure variations in control volumes for 30 min UF_6 release case in the Paducah GDP

Figure 42 Source term mass of UF₆, UO₂F₂ and HF for 30 min UF₆ release case in the Paducah GDP

Figure 43 UO₂F₂ source term mass from each unit for 30 min UFG release case in the Paducah GDP

Figure 44 HF source term mass from each unit for 30 min UF_6 release case in the Paducah GDP

Figure 45 Atmospheric material source term (air & moisture) from each unit for 30 min
 UF_6 release case in the Paducah GDP

Figure 46 Total material mass source term (air, moisture, UF_6 , UO_2F_2 & HF) from each unit for 30 min UF_6 release case in the Paducah GDP

Figure 47 Fractional UO₂F₂ and HF mass source term from units 1 and 2 for 30 min UF₆ release case in the Paducah GDP

Fractional mass source term from Units 3&4 $\times 10^{-3}$

Figure 48 Fractional UO₂F₂ and HF mass source term from units 3 and 4 for 30 min UF₆ release case in the Paducah GDP

Figure 49 Fractional UO₂F₂ and HF mass source term from units 5 and 6 for 30 min UF₆ release case in the Paducah GDP

Figure 50 Enthalpy of total material for 30 min UF_6 release case in the Paducah GDP

Figure 51 Enthalpy of UO_2F_2 source term for 30 min UF_6 release case in the Paducah
GDP

Integrated HF enthalpy source term (GJ)

Figure 52 Enthalpy of HF source term for 30 min UF_6 release case in the Paducah GDP

Figure 53 Source term temperature for 30 min UF_6 release case in the Paducah GDP

Figure 54 Air mass flow rate through cell housing leakage flow paths for 30 min UF_6 release case in the Portsmouth GDP

Figure 55 UF_6 mass reaction rate in various locations of the building for 30 min UF_6 release case in the Portsmouth GDP

Figure 56 Pressure variations in control volumes for 30 min UF_6 release case in the Portsmouth GDP

Figure 57 Source term mass of UF₆, UO₂F₂ and HF for 30 min UF₆ release case in the Portsmouth GDP

Figure 58 UO_2F_2 source term mass from each unit for 30 min UF_6 release case in the Portsmouth GDP

Figure 59 HF source term mass from each unit for 30 min UF_6 release case in the Portsmouth GDP

Figure 60 Atmospheric material source term (air & moisture) from each unit for 30 min
 UF_6 release case in the Portsmouth GDP

Figure 61 Total material mass source term (air, moisture, UF_6 , UO_2F_2 & HF) from each unit for 30 min UF_6 release case in the Portsmouth GDP

Figure 62 Fractional UO₂F₂ and HF mass source term from units 1 and 2 for 30 min UF₆ release case in the Portsmouth GDP

Figure 63 Fractional UO₂F₂ and HF mass source term from units 3 and 4 for 30 min UF₆ release case in the Portsmouth GDP

Figure 64 Fractional UO₂F₂ and HF mass source term from units 5 and 6 for 30 min UF₆ release case in the Portsmouth GDP

Figure 65 Fractional UO₂F₂ and HF mass source term from units 7 and 8 for 30 min UF₆ release case in the Portsmouth GDP

Figure 66 Enthalpy of total material for 30 min UF_6 release case in the Portsmouth GDP

Figure 67 Enthalpy of UO_2F_2 source term for 30 min UF_6 release case in the Portsmouth GDP

Figure 68 Enthalpy of HF source term for 30 min UF_6 release case in the Portsmouth GDP

Figure 69 Source term temperature for 30 min UF_6 release case in the Portsmouth GDP

Appendix A

**MEASUREMENTS OF AIR LEAKAGE
THROUGH CELL HOUSING WALL STRUCTURES**

by

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June 11, 1996

Measurements of Air Leakage Through Cell Housing Wall Structures

The cell housing wall is constructed of steel with 3/8-inch transite siding bolted in place. The tops of the housings are 20-gauge ribbed steel with removable hatches for ease of equipment removal. The bell ends of the compressors are connected to the housings with heavy, reinforced plastic shroud bolted to the ends of the compressor with a metal ring. Although the housing seams are tightly closed, the cell housing was not designed to provide 100 percent secondary confinement in the event of a rupture inside the housing. Atmosphere in the housing will heat up due to heat convection/radiation from equipment surfaces such as compressors. A significant temperature difference between inside and outside the housing develops buoyancy force that convects air naturally through cracks, untightened seams, and other leak paths. The quantity of this leakage was calculated on the basis of an energy balance for the cell using temperature and pressure data collected in various locations in the cell housing. During normal operation, the maximum air flow magnitude was estimated to be $9 \text{ m}^3/\text{s}$ (19,000 cfm) [R.C. Riepe, Paducah Plant Process Building Ventilation Studies, KY-D-3249, 1974]. This magnitude of air flow was evaluated based on total amount of heat transferred by air leaked through the housing. This air leakage heat loss was computed as the difference between the total heat gain in the cell housing and heat losses accounted for by all other heat transfer modes such as convection and radiation at the cell housing surfaces, heat loss at R-114 piping, cell housing floor heat loss, heat loss at condensers, and lube-oil heat loss. Total heat gain in the cell was calculated as compressor shaft energy minus condenser water heat gain, and various heat losses were calculated based on measured temperatures.

Since aerosol transport and settlement largely depend on air circulation in the building, it was necessary to verify $9 \text{ m}^3/\text{s}$ (19,000 cfm) of air leakage through the walls during normal operation. We used a simple and direct method to drive a ball-park figure of the air leakage magnitude. First, size of cracks (or openings at the cell housing walls) was estimated, and air flow velocity at the cracks was measured. Second, temperatures of few surfaces of the cell housing walls were measured for comparison with the old data. Measurements were made for cell 3 of unit 5 in X-333.

Identifying and quantifying all the leak paths are non-trivial tasks. Air leaks into the cell housing at lower locations, and heated air is leaked out at upper locations. Therefore, instead of trying to identify cracks and openings in entire housing surface, we looked into

only most possible leak-out paths. These (at least at the Portsmouth GDP) exist on top portion of the cell housing (i.e., penthouse ceiling). Penthouse ceiling is covered with ribbed steel plates of about 5-1/2 inch width. It was easily seen and measured that about 1/2-inch gap opening exists between each plates; therefore, we can assume that 1/12 of the penthouse ceiling surface has openings to allow out-leakage. In addition, several irregular holes were observed. Since total opening size of such holes is not significant, they were excluded from consideration. By assuming the openings of the penthouse ceiling to represent the vast majority of out-leakage pathways, we were able to estimate air leakage rate through the cell housing. Air velocity measured at such openings varies between 0.2032 to 0.254 m/s (40 to 50 fpm), as seen in Table 1. Since total ceiling surface area is 365.2 m² (3,931 ft²), approximate opening area will be 30.4 m² (1/12 of total area). Therefore, the leakage rate can be estimated to be 6-8 m³/s (13,100 ~ 16,400 cfm). Additionally, 0.9652 m/s (190 fpm) of air flow was detected around joints on the wall behind motor exhaust, and 0.3556 m/s (70 fpm) at the 0.297m x 0.127m (11"x5") hole on penthouse ceiling. Since we omitted these and other minor openings and invisible loosed wall seams from consideration, we conclude that the air leakage rate estimated in previous study (i.e., 9 m³/s) is reasonable.

Table 2 lists measured temperatures of a few surfaces of the cell housing with air temperatures near the surfaces. Also similar temperature measurements from old study are listed in the same Table. Each measurement on same surface was made on different spots. Temperatures are generally in a good agreement between new and old (previous) data. There are some differences observed in both surface and adjacent temperatures. However, these temperatures are expected to vary depending on temperature outside the process building. Also slight difference is expected between various cell housings. Adjacent air temperatures also vary depending on the position at which the data are taken. Farther from the surface, lower air temperature will be measured. For old data, there is no record available on how far the thermocouples were placed from the surface to measure air temperature. In obtaining new data, air temperature was measured at about 10 cm distance from the surface. Considering all these differences involved in measurements, we can conclude that old temperature data are reasonable, as verified via new measurements. Since air leak rate through the cell housing wall depends on temperature data, same conclusion as the first approach (i.e., direct measurement of air velocity and size of openings/cracks) is obtained; that is, 9 m³/s of air leak rate is reasonable value.

Also listed in Table 1 is air velocity data at air blower and motor exhaust suction. There are three air-supply blowers per cell; therefore, using a measured flow area (4.82 m^2 per blower) and air velocity of $3.048\text{--}4.572 \text{ m/s}$ ($600\text{--}900 \text{ fpm}$), air flow rate per cell basis is to be $44\text{--}66 \text{ m}^3/\text{s}$. This measured air flow rate through the air supply binnacles agrees well with $48 \text{ m}^3/\text{s}$ ($1.01 \times 10^5 \text{ cfm}$) of air flow rate determined by equipment technical specification. For air suction rate of motor exhaust, measured flow rate is $2.94\text{--}3.4 \text{ m}^3/\text{s}$ ($6240\text{--}7200 \text{ cfm}$), which agrees well with $3.36 \text{ m}^3/\text{s}$ (7125 cfm) per motor according to technical specification.

The considerable assistance and access provided to the authors by R. Maines, M. Hasty and P. Holmes of PGDP is gratefully acknowledged.

Table 1. Leaked Air Velocity and Temperature ⁽¹⁾

Locations	Air Velocity (fpm)			Air Temperature (F)		
Slits on Penthouse Ceiling (5-1/2" gap @ every 6")	40	50	40	110	150	—
Crack on Penthouse Ceiling (11" x 5" hole)	70	—	—	199	—	—
Crack on Wall Behind Motor Exhaust	190	—	—	120	—	—
Thermal Buoyancy on Penthouse Side Wall (Surface 3 - Fig. 1)	35	40	—	125	—	—
Air Blower (97" H x 77" W)	800	900	600	89	89	90
Motor Exhaust Suction ($\pi \cdot (32''^2 - 12''^2) / 4 = 0.446 \text{ m}^2$)	1300	1500	1400	115	118	—
Access Door @ Low-Elev. (Open)	550	475	—	60	—	—
Access Door @ Mid-Elev. (Open)	600	500	—	60	—	—
Access Door @ High- Elev. (Open)	600	550	—	60	—	—
Leak Between Wall and Access Door @ Low-Elev. (closed)	350	—	—	—	—	—
Leak Between Wall and Access Door @ Mid-Elev. (closed)	400	—	—	—	—	—
Leak Between Wall and Access Door @ High-Elev. (closed)	450	—	—	—	—	—

(1) New data were taken by S.H. Kim & R.P. Taleyarkhan (guided by P. Holmes) at following conditions:

- [illegible]

Table 2. Housing Surface and Adjacent Air Temperatures⁽¹⁾

Node ⁽⁴⁾ (Fig.1)	Description of Surfaces	New Data ⁽²⁾						Old Data ⁽³⁾	
		Surface Temp, T_{surf} (F)			Air Temp, T_{air} (F)			T_{surf} (F)	T_{air} (F)
1	Penthouse top	172	176	156	130	130	128	164	118
2	Penthouse Sidewalls	157	169	165	118	124	123	151	112
3	Penthouse End- East	148	148	151	110	113	115	151	112
4	Penthouse End- West	162	153	151	115	111	112	151	112
5	Horizontal-East	132	135	127	112	110	104	163	112
13	Compressor Housing-	151	152	—	109	110	—	153	93
14	Asbestos behind motors	132	136	—	118	120	—	153	93

(1) For conditions of collecting data, refer to Table 1-note.

(2) New data were collected for 3,300 HP of average stage power.

(3) Old data were collected for 3,308 HP of average stage power.

(4) Node indicates surface identification that is shown in Fig. 1.

Figure 1. Cell Housing Surface Identification

**COMPUTATIONAL FLUID DYNAMICS TRACKING
OF UF₆ REACTION PRODUCTS RELEASE INTO A
GASEOUS DIFFUSION PLANT CELL HOUSING**

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* Managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under contract DE-AC05-96OR22464.

COMPUTATIONAL FLUID DYNAMICS TRACKING OF UF₆ REACTION PRODUCTS RELEASE INTO A GASEOUS DIFFUSION PLANT CELL HOUSING

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ABSTRACT

A three-dimensional (3-D) computational fluid dynamics (CFD) model has been developed using CFDS-FLOW3D³ Version 3.3 to model the transport of aerosol products formed during a release of uranium hexafluoride (UF₆) into a gaseous diffusion plant (GDP) process building. As part of a facility-wide safety evaluation, a one-dimensional (1-D) analysis of aerosol/vapor transport following such an hypothesized accident is being performed. The objective of this study is to supplement the 1-D analysis with more detailed 3-D results. Specifically, the goal is to quantify the distribution of aerosol passing out of the process building during the hypothetical accident. This work demonstrates a useful role for CFD in large 3-D problems, where some experimental data are available for calibrating key parameters and the desired results are global (total time-integrated aerosol flow rates across a few boundary surfaces) as opposed to local velocities, temperatures, or heat transfer coefficients.

NOMENCLATURE

Symbol	Description	Units
A	Cell-wall leakage area	m ²
K	Form loss coefficient	-
$\dot{m}$	Mass flow	kg/s
P_i	Pressure internal to cell wall	Pa
P_e	Pressure external to cell wall	Pa
ρ	Density	kg/m ³

¹Managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under contract DE-AC05-96OR22464.

²Managed by Lockheed Energy Systems, Inc., for the U.S. Department of Energy under contract DE-AC04-84OR21400.

³CFDS-FLOW3D is a commercially available computational fluid dynamics program developed by AEA Technology Engineering Software, Inc.

κ	Turbulent kinetic energy	m ² /s ²
ϵ	Eddy dissipation	m ² /s ³

INTRODUCTION

In the United States, the gaseous diffusion process is used to produce enriched uranium for power generation and defense purposes. The process uses large quantities of the hazardous material uranium hexafluoride (UF₆) that is piped throughout the plant through large process lines. In the event of a break in a UF₆ line, the UF₆ will immediately undergo an exothermic chemical reaction (producing very high temperatures) with the moisture (H₂O) in the air to form hydrogen fluoride (HF) and aerosolized uranyl fluoride (UO₂F₂) that could then be spread inside and outside of the process building. As part of the facility-wide safety evaluation, a one-dimensional (1-D) analysis of aerosol/vapor transport following such an hypothesized severe accident is being performed (Kim et al., 1996). The objective of this study is to supplement the 1-D analysis with more detailed three-dimensional (3-D) results. Specifically, the goal is to quantify the distribution of aerosol passing out of the process building during the hypothetical accident.

A U.S. gaseous diffusion plant (GDP) contains multiple process buildings. The process building currently under consideration contains six "units." A unit is a group of ten "cells." A single cell contains eight axial-flow compressors that pump gaseous UF₆ through large cylindrical steel vessels called "converters." Each cell is contained within a sheet-metal enclosure called a cell housing. These enclosures are not air tight, but allow substantial leakage through openings and panel seams. Figure 1 shows the geometry of the cell with the eight trapezoidal protrusions to accommodate the eight compressors, each attached by a shaft passing through the cell wall to one of eight compressor motors located outside of the enclosure. The upper portion within the sheet-metal enclosure (on the level above the trapezoidal protrusions) is referred to as the penthouse. Within each unit, air is circulated outside the cell housing by the combined action of (1) the air supply blowers (three per cell) that pump air into the building, (2) the compressor motor suction (eight per cell) that pull air out of the building, and (3) the roof vent exhaust that

Fig. 1. Geometry of the gaseous diffusion cell with computational domain including the surrounding process building air.

allows air flow in either direction, but will typically vent the remainder of air out of the building.

A computational 3-D fluid dynamics (CFD) model has been developed using CFDS-FLOW3D² Version 3.3 to model the transport of aerosol products formed during a release of UF_6 into the cell housing. Because the flow domain is large (dimensions of 53 m long $\times$ 26 m wide $\times$ 16 m high), it was recognized from the beginning that a very coarse discretization was required to obtain a solution with existing computational resources (IBM RISC 6000 Model 580 with 128 Mbytes of RAM). Using such a coarse discretization would necessarily compromise the physical accuracy of the simulations. However, it is the relative distribution of aerosol flow at the boundaries of the problem that was desired, not specific local velocities and temperatures within the unit. Existing temperature and flow distribution data were also used to calibrate the steady-state solution, thus improving the accuracy of the predictions.

MODEL DESCRIPTION

An input model was developed for the CFDS-FLOW3D solver by defining the computational domain and discretization, boundary conditions, fluid properties, and solution strategy. The geometry of the problem was defined using the CFDS-FLOW3D mesh generator SOPHIA that allows the user to define 1-D edges, extrude these into two-dimensional (2-D) faces, and subsequently extrude the faces into 3-D blocks that are then discretized. The computational flow domain is shown in Fig. 1, with the rectangular holes in the floor corresponding to the locations of the two air-supply blowers that are interior to the computational domain and the eight compressor motor exhaust ducts (only five of which are visible in the figure). The blowers and motors are represented by rectangular hexahedra located as shown in Figs. 2 and 3. Approximately 50,000 control volumes were used in the discretization.

Although not shown in Fig. 1, the cell housing internals were also discretized for the flow solution. The equipment contained within the cell housing was estimated to fill between 50 and 60% of the cell volume. Refining the details of the air flow in and around this equipment is intractable, due to the large number of computational cells required, and unnecessary, since the details of the flow inside the cell housing are unimportant. However, it was still desired that the model contain the

Fig. 2. Typical motor air suction boundary condition (one of eight).

Fig. 3. Air supply blower as modeled in CFDS-FLOW3D simulations.

correct total mass of air inside the cell and maintain fairly well-mixed conditions, since the equipment is actually distributed throughout the cell. A simple solution to this dilemma is to represent the cell internals as a porous media. By using the CFDS-FLOW3D porous media model, the cell volume was defined to contain 56% solid equipment and 44% air. The porous media model allows the user to provide additional flow resistance to account for small-scale momentum losses; however, no additional flow resistance was added since it was anticipated that these momentum losses would be very small.

The air was treated as incompressible, with a buoyancy force added through the linearized Boussinesq approximation, because compressibility effects are small. Six solid hexahedra were defined to represent the heated surface of the eight converters inside the cell housing. A fixed boundary temperature was assigned to the surfaces of the hexahedra. This surface temperature was then adjusted during the steady-state solution process until the measured penthouse air temperature was matched by the computed flow solution. To match the measured penthouse air temperature, the total amount of heat transfer from the equipment to the air must be accurate. To transfer the

correct amount of heat, the equipment temperature must be increased above the measured average equipment temperature. This increase is necessary because the heat transfer area of the six solid hexahedra is significantly less than the true equipment surface area.

The temperature of the air exiting the roof vent was also known from measurements taken during plant operation. This measurement was matched by specifying a heat flux on the exterior of the cell wall passing into the exterior air. This heat flux represents heat that is transmitted by conduction through the thin sheet metal wall.

To accommodate leakage of mass, enthalpy, and aerosol through openings (seams) in the sheet metal walls, 129 pairs of sources and sinks on either side of the cell wall were specified. Two "patches" are defined on each of the 129 quadrilateral surfaces comprising the discretized sheet metal cell wall that separates the heated air inside the cell housing from the forced-convected air outside. A patch is merely a CFDS-FLOW3D label for a 2-D segment attached to the computational domain which can be used in the user FORTRAN to identify certain computational cells. One patch was specified for the inside wall of each segment, and one for the outside.

A substantial amount of FORTRAN coding was supplied to the CFDS-FLOW3D steady-state simulation to simulate the leakage through the cell wall of mass and energy. Specifically, the user FORTRAN was written to accomplish the following purposes:

- Determine the magnitude of leakage mass flow through the cell wall based on the local pressure difference.
- Generate source/sink terms for the pressure (mass continuity), enthalpy and user scalar (aerosol) equations consistent with the calculated leakage through the cell wall.
- Monitor the mass flow and aerosol flow at the wall, cell door, blower exits, and motor suction locations.

At each of the 129 wall segments, an average internal pressure, P_i , and average external pressure, P_e , are calculated by considering the pressures in each of the computational cells bordering the wall segment. The leakage mass flow rate for one segment, $\dot{m}$, is then calculated using the simple form-loss relationship

$$\dot{m} = \sqrt{\frac{2\rho A^2(P_i - P_e)}{K}} \quad (1)$$

where ρ is the density, A is the leakage area, and K is the form-loss coefficient. The total leakage mass flow rate through the cell wall has been measured, and this information was used to calibrate the loss coefficient K .

The available plant data that were used in developing the computational model are given in Table 1. Some of these values could have been computed directly by the CFD model. Instead of doing so, however, the measured values are used as calibration points to minimize the inaccuracy that accompanies the use of such a coarse discretization.

STEADY-STATE SOLUTION

The flow field within the cell, through the cell wall (via various leakage pathways, including an open door and gaps between sheet metal pieces comprising the wall), and outside the cell (but within the unit) was calculated. The usual equations for transport of mass, momentum (three directions), enthalpy, and aerosol mass, as well as two additional

equations used for κ - ϵ turbulence closure, were then solved. The particle transport model in CFDS-FLOW3D does not allow transient computations, hence the aerosol mass was represented as a user scalar variable, and deposition of aerosol by settling was neglected.

The turbulent Schmidt number is assumed to be 0.9 (default value in CFDS-FLOW3D), and a very low laminar diffusivity is used (i.e., diffusion of the aerosol occurs via turbulent transport only).

The first solution obtained with the model assumed a steady-state at typical operating temperatures and flow rates. During the typical steady state, air is drawn into the cell housing near the base of the housing wall and through the door, then heated and pushed out through the seams in the top of the cell housing. Hence, a steady circulation through the cell housing occurs. The objective of this initial steady-state simulation was to determine the typical flow pattern (to be used as an initial condition for a transient simulation), and to determine the fate of the air that is passed through the cell housing.

Table 1. Assumed data used in calibrating the steady state and defining geometry and boundary conditions.

Parameter	Value
Motor suction area	0.3 m ²
Motor suction velocity	11.18 m/s
Air supply blower area	1.672 m ² (3 ft × 6 ft)
Air supply temperature	310 K
Air supply blower flow rate	15.57 m ³ /s (33,000 cfm)
Air temperature near top of cell housing (penthouse)	360 K
Total leakage flow through cell wall	9.0 m ³ /s (19,000 cfm)
Roof vent exit air temperature	330 K

Fig. 4. Isothermal surface showing developed thermal plume during typical steady-state.

A unit source of 1 kg/s of aerosol (defined by a user scalar variable) was released inside the cell housing, distributed uniformly, and the steady-state solution was obtained. For the steady-state solution, no heat source is included to represent the reaction following the release of UF_6 . This solution was calibrated to the measured through-cell circulation air flow rate (19,000 cfm), cell housing internal air temperature (360 K), and roof exhaust temperature (330 K) by adjusting leakage area, equipment temperature, and cell wall exterior convected heat flow.

The steady-state velocity vectors and one isothermal surface are shown in Fig. 4. The surface, at 330 K, shows the plume of hot air leaving the cell housing and rising to the process building ceiling. The surface also corresponds closely to a constant-user-scalar (aerosol concentration) surface since the aerosol rides along with the hot air that has left the cell housing. Results showed that 50% of the aerosol released is exhausted out the roof vent. The remaining 50% of the aerosol exits the unit building through the motor exhaust, or is passed out of the computational domain to an adjacent cell. A very small amount (less than 1%) of the circulated air is re-entrained into the cell housing.

After calibration, the calculated steady-state volumetric flow rate through the cell wall is $8.94 \text{ m}^3/\text{s}$, the steady-state penthouse temperature is 360.7 K, and the average temperature of air passing through the roof vent is 329.0 K. These quantities were calibrated to the measurements in Table 1 by adjusting the equipment surface temperature and the available cell-wall leakage area. The resulting mass flow and user-scalar transport balance is shown in Table 2.

Table 2. Results of steady-state calculation, mass and aerosol inventory, negative value indicates loss from computational domain.

Location	Mass Flow (kg/s)	Aerosol Flow (kg/s)
Motor Suction	-30.64	-0.3617
Roof Vent	-22.71	-0.4992
Blower 1	17.81	0.00
Blower 2	-8.88	-0.069
Blower 3	17.76	0.00
Blower 4	-8.91	-0.072
Blower 5	17.78	0.00
Blower 6	17.78	0.00
TOTAL	0.00	-1.00
Cell Wall	10.21	1.007
Cell Door	1.98	0.013*

* This number is not exact due to the method of calculation for flow through an interior surface such as the cell door.

TRANSIENT SOLUTION

A transient solution was obtained by starting from the steady-state flow field and a zero initial condition assumed for the aerosol concentration. The hypothetical accident was defined by a release of 26.458 kg/s of aerosol into the cell housing, accompanied by a heat-of-reaction source of $9.635 \times 10^6 \text{ W}$, lasting 5 min (300 s). The transient simulation assumed the actual heat source, and a net amount of 300 kg of user scalar (representing the aerosol) was released into the cell housing over the 300-s period. The aerosol and heat sources were again uniformly distributed through the cell internals.

The time step was fixed to 0.5 s for a requested 1500-s transient, the first 300 s of which would represent the release of aerosol into the cell environment. The simulation was terminated after only 521 s of problem time, due to a pressing deadline. These 521 s of problem time required 10 d of IBM RISC6000 Model 580 processing time. At this time, only about half of the 300 kg of user scalar (aerosol) released during the first 300 s had passed out of the computational domain. Of that aerosol that had passed out of the domain, 69% was exhausted through the roof vent boundary.

The resulting aerosol mass flow through the cell housing wall and out each of the boundaries during the transient is shown in Fig. 5. At about 330 s large oscillations in the mass flow in and out of the cell housing are observed. This is caused by poor convergence at the requested 0.5-s time step. However, the oscillations appear in the mass flow through the cell wall and not in the boundary mass flows. Also, the trend in the aerosol flow rate at the boundaries appears to be a reasonable continuation of the results before the oscillations began. Table 3 shows the fate of the 300 kg of user scalar as of 521.5 s of simulation time. Figure 6 shows the ratio between aerosol mass passing through the motor exhaust and total aerosol mass passing out of the computational domain as a function of time.

Fig. 5. Fraction of aerosol lost from the computational domain that passes through the motor exhaust as a function of time.

Fig. 6. Aerosol mass flow (total generated is 1 kg/s) through cell wall and mass flow boundaries during the transient simulation.

CONCLUSIONS

The results indicated that in the event of a break of a UF_6 line in the gaseous diffusion cell, at least 69% of the aerosol produced from the UF_6/H_2O reaction that passes out of the building would wind up being exhausted out of the roof vent in the process building.

This work demonstrates a useful role for CFD in large 3-D problems, where some experimental data are available for calibrating key parameters and the desired results are global (total time-integrated aerosol flow rates across a few boundary surfaces) as opposed to local velocities, temperatures, or heat transfer coefficients. A coarse discretization and large time step were required to meet the work schedule demands. All of the essential physics were included in the simulation except particle settling. This aspect was neglected due to the limitation of the CFDS-FLOW3D particle dynamics model. Some difficulties were encountered with convergence at the 0.5-s time step; however, the simulation was judged to be adequate for its purpose in providing the supplemental results to the 1-D accident simulations.

Table 3. Fate of aerosol contaminants up until 521.5 s of transient simulation.

Location	Total Mass (kg)	Percent of Release	Percent of Flow out of Domain
Out through Motor Exhaust	28.5	9.5	20.1
Out through Roof Vent	98.1	32.7	69.3
Out through Blower Boundaries	14.9	5.0	10.6
Remaining in Cell	9.4	3.1	
Remaining in Unit	149.1	49.7	
Total	300.0	100.0	100.0

REFERENCES

- Kim, S. H., Taleyarkhan, R. P., Carter, J. C., Keith, K. D., Schmidt, R. W., and Dyer, R. H., March 1996, "Modeling and Analysis of Postulated UF_6 Release Accidents in Gaseous Diffusion Plant," *Proceedings, 4th International Conference on Nuclear Engineering*, published by the American Society of Mechanical Engineers, New Orleans, Louisiana.