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Coupled Fire and Aerosol Analyses Using the FATE 2.0™ Computer Program

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Abstract

FATE 2.0™ is a graded-approach computer program for nuclear and chemical facility analyses coupling fire, explosion, and aerosol phenomena with fluid flow and heat transfer models. The current code version incorporates fire models and improvements to source term and combustion models. Coupling of fire and facility transport models and ability to consider a large facility (hundreds of control volumes and interconnections) directly addresses some concerns expressed by DNFSB Recommendation 2004-2. FATE is created and maintained under the FAI Quality Assurance Program and use of FATE and its predecessors has been audited many times for DOE facilities.

Introduction

Motivation

This paper is motivated in general by the release of FATE 2.0™ computer program[1] to succeed, combine, and improve upon a number of models used at Hanford and elsewhere within the DOE complex, and specifically because FATE capabilities directly address some concerns expressed by DNFSB Recommendation 2004-2 regarding static confinement analyses. FATE has been used for process design, accident, and source term analyses as will be summarized next. Its new fire model capability is similar to that of CFAST, and is embedded within a longitudinally used and validated multiple compartment model allowing arbitrary topology and capable of handling hundreds of control volumes and flow paths. This capability therefore integrates the energy and mass source drivers of a fire accident with source term, fluid, and aerosol transport models, including any pertinent feedbacks, and avoiding the difficulty of iterating between two computer code calculations.

Background and Scope of Use

FATE 2.0™, Facility Flow, Aerosol, Thermal, and Explosion Model, for PCs and workstations is used for design, off-normal, and accident analyses including source term and leak path factor prediction for nuclear and chemical facilities. FATE is the successor to computer codes used extensively for design and safety analyses for U.S. Department of Energy projects at the Hanford site and elsewhere, and recent references are given here.

HADCRT originally stood for Hanford Double Contained Receiver Tank model, and contained models for combustion of gases and solvent vapors along with models for aerosol entrainment during combustion and depressurization (blowdown). These models were exercised for Tank Farms, the Waste Treatment Plant (WTP) [2,3,4], Waste Encapsulation and Storage Facility (WESF), and Plutonium Finishing Plant (PFP).

HANSF originally stood for Hanford Spent Fuel, and contained models for chemical reactions of metallic fuel and sludge. The HANSF MCO (multi-compartment overpack) model was used for process development and the technical safety basis for spent nuclear fuel cold vacuum drying and interim storage[5], and the HANSF Sludge model is still being used for various process and accident analyses involving metallic uranium bearing sludges[6,7].

Quality Assurance

FATE is created and maintained under the FAI Quality Assurance Program, which is a subtier QA Program under the Westinghouse Quality Management System (QMS). Both programs meet the requirements of 10CFR50 Appendix B, ISO-9001:2000 and NQA-1-1994. This includes NQA-1A Addenda Subpart 2.7 for computer software controls.

The FAI QA Program and the Westinghouse QMS are ISO-9001 certified by Lloyds Register Quality Assurance, certificate number UQA 0102162, expiration date of 11/30/2005. The FAI organization is audited for compliance with the above requirements on an annual basis as part of our internal audit program.

General Model Summary

FATE models facilities using well-mixed or stratified-layer (zone) control volumes connected by flow paths that allow pressure-driven, density-driven counter-current, and diffusion flows. Within these control volumes extra details are simulated as required by models, for example, aerosol entrainment requires definition of velocity profiles.

FATE may be thought of as combining the features of MELCOR and CFAST in a single computer program, with additional features pertinent to DOE facilities. General capabilities of FATE 2.0 include:

- Fire model: Fire definition includes burn rate and yield tables. A plume model provides mixing of combustion products with surrounding air defining composition and energy entering the smoky layer. The smoky layer model involves accounting for separate gas layers in all control volumes, and propagation of separate layers throughout a facility including forced flow and counter-current (density-driven) flow. Aerosol transport occurs with lower and smoky layers. Aerosol settling occurs from the smoky layer to lower layer and embedded surfaces.

- Multiple-compartment thermodynamics and general species: Facility rooms have separate pressure, temperature, and composition, and when the fire model is invoked these are separate for the lower and smoky layers. Compound property libraries are input so that elements and chemicals pertinent to a given situation may be included by specifying data such as the name, molecular weighty, heat for formation, vapor pressure versus temperature, second virial coefficient versus temperature, specific heat versus temperature, etc. Bookkeeping considers condensed, gaseous, and aerosol species.
- Facility nodalization and flow: Compartments are connected in arbitrary topology by flow paths specified by the user, so that a complex facility may be accurately represented. Compartments may represent rooms, parts of rooms (hallways are commonly divided), and vent lines, and flow paths may represent doors, gratings, check valves, or simply an open connection. Flows are pressure-driven, density-driven counter-current, and diffusional.
- Aerosol behavior: Aerosol phenomena considered are coagulation, sedimentation, transport with flow, deposition on bends and filters, deposition by condensation, aerosol formation by boiling and fog formation, and aerosol formation by entrainment. Powder, liquid, and sludge waste may be entrained by combustion or flow to form aerosols.
- Flammability and combustion of gases, vapors, and aerosols: Any input compound may participate in flammability and combustion; examples include solvent vapors, hydrogen, and U metal or hydride aerosols. The user defines flammability limit criteria for individual fuels and oxidants, and LeChatelier's law is followed. The user also prescribes allowed chemical reactions for combustion.
- Heat transfer: Standard heat transfer models are used for convection of liquids and gases to structures including condensation. Structures have internal temperature distributions and may be linked for 2D and 3D heat transfer.
- Thermal radiation networks: Radiation network definitions are simplified via a set of view factor models and automatic network balancing. When required, as during a fire, view factors are calculated at every time step.
- Event-oriented simulation: The user prescribes intervention criteria and actions for scenario evolution so that event tree branches may be followed by the code based upon calculated results.
- Sources and time-dependent conditions. The user may prescribe liquid, gas, and aerosol source histories and environmental conditions with time.
- Nuclear fuel and sludge models include pertinent chemical reactions, and it is easy to add new reaction correlations.

For leak path factor analysis, the most important model included in FATE but not present in MELCOR is for density-driven counter-current flow of gases. For many aerosol release situations, either there is little energy driving pressure differences in a facility, or else the energy driver is not sustained. Therefore, a 24 hour leak path factor is almost certainly influenced by density-driven counter-current flow which allows gases to be exchanged between compartments in the absence of pressure differences.

Fire Model Summary

There are four basic features of FATE that together comprise the fire model:

- Pilot fires specification (burn rates, yields, heat release)
- Plume Model
- Stratified layer composition; i.e., conservation equations for a smoky layer in each control volume and equations for inter-compartmental flow of lower and smoky layers, and
- Radiation heat transfer with automatic view factor calculation and a palette of models for common geometries.

This formulation recognizes that many aspects of fire modeling problems are part of the generic features of the code. Adding fire models to the FATE framework provides advantages to zone models (CFAST, etc) by incorporating multi-compartment heat transfer and inter-compartmental flow phenomena without the computational expense of CFD-based fire analysis tools. Examples of bottom line goals are to predict if conditions are inhabitable and estimate time available for evacuation. Passive heat sink temperatures are of great concern because another oft-used bottom line goal is to predict survivability and operability of critical equipment under fire conditions.

Figure 1 shows a pilot fire and plume in a process facility with a number of compartments that communicate via doors and ventilation ducts, and contain heat sinks such as ceilings, walls and internal equipment. This is the familiar construct of regions, heat sinks and junctions, with the addition of pilot fire and plume in one compartment (region). This figure typifies compartment fire modeling by showing an idealized hot smoky layer above a relatively cold, clean, lower layer. This assumption neglects the true nature of the interface, which at various stages of the fire can be ill-defined or non-existent, and presumes that the smoky layer quickly propagates horizontally along the ceiling. In reality, the smoky plume initially strikes the ceiling and spreads outward until it reaches the confines of compartment walls, at which point the smoky layer proceeds downward. Nevertheless, the two-layer idealization is useful and accurate enough that a number of code and analytical techniques employ it for compartment analysis. Fire test data is often reduced to this ideal.

Smoky layer growth then depends on the balance between the pilot fire and plume source and the inter-compartmental flows in both the smoky and lower layers. The fuel burning rate, plume entrainment rate, and fuel properties, namely heat of combustion and product yields, determine the rate at which mass and energy enter the smoky layer. Between the base of the fire and the bottom of the smoky layer, plume entrainment mixes the lower layer gases with the combustion products, thereby increasing total mass flow to the smoky layer, but decreasing the incoming temperature. Inter-compartmental flows, noticeably complicated by the presence of two layers, depend greatly on junction orientation and elevation. As an example, Figure 1 shows that the smoky layer must advance below the top of a door before it can proceed to the neighboring compartment. In one junction, inter-compartmental flow can now consist of pure lower layer flow, pure smoky layer flow or a combination of the two. The smoky layer can be thin if the compartment ceiling contains a hatch that allows smoke to escape immediately to a region above, or if an operating ventilation duct is located near the ceiling to draw smoky layer gases from the region.

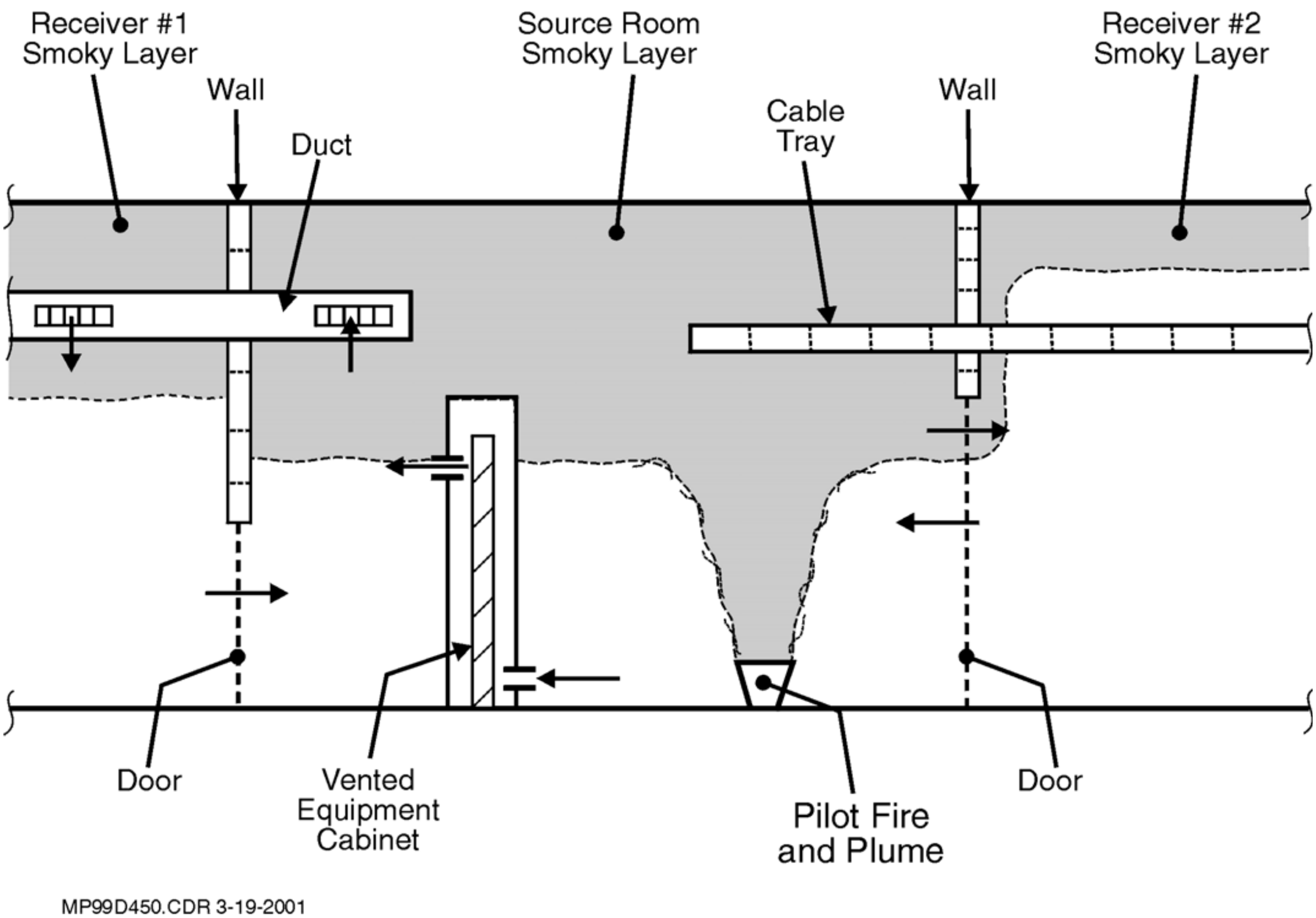

Figure 1. FATE Fire Model Features.

Validation Examples

FATE model validation includes regression testing to reproduce past results, separate phenomena testing for individual models, and integral testing for overall performance of many models for typical applications. Individual phenomena models are validated against experimental data and hand calculations. These include chemical reaction, fluid flow, heat transfer, combustion, and aerosol models that have been in long use at the Hanford site for situations ranging from analysis of the potential for thermal runaway of containers with uranium metal to filter temperature response to loading by hot soot particles. Details are given in the FATE manual[1] and other cited references.

While separate effects testing exists for components of the FATE fire model, integral results are the most interesting and compelling to demonstrate proper model function. FAI has participated in the International Collaborative Fire Model Project (ICFMP) and results for two benchmark exercises are presented here; FAI is presenting results of several new benchmark exercises to the ICFMP in May, 2005.

ICFMP Benchmark Exercise 2, Part I[8] consists of three cases based on a series of full-scale experiments inside a test hall with dimensions 19 m high by 27 m long by 14 m wide (i.e. floor area 378 m^2). Each case involves a single fire (2 - 4 MW), and for which there are experimental measurements of gas temperature and doorway velocity. The height of a turbine hall within a nuclear power plant (approximately 25 m) is similar to that of the test hall although it is acknowledged that the area of a turbine hall (approximately 3500 m^2) is much greater. However, the test hall is one of the largest enclosures for which fire test data is available for comparison with model predictions.

Figure 2 shows the geometry of the hall, comprising a rectangular space with a pitched roof structure above. A Cartesian axis system is defined, with the origin as indicated. All dimensions are in meters. The four walls are labeled as west (x=0), east (x=27 m), south (y=0) and north (y=13.8 m). Here the west and east walls known collectively as the end walls and the south and north walls as the side walls.

In cases 1 through 3 there are two doorways, 0.8 m wide by 4 m high, one located in each end wall. Both doorways open to the external ambient environment, and are located such that the centre is 9.3 m from the south wall (y=9.3 m). The doorway openings are labeled as the west doorway (door 1) and the east doorway (door 2).

Figure 3 shows the internal geometry of the test hall for Part I, including the location of the fire source and the location of instrumentation. Four thermocouple trees and two sets of velocity probes are shown as a series of open circles. The thermocouple trees are numbered sequentially 1 through 3 from left to right with tree #4 located directly over the fire source. Thermocouples for the first three trees are numbered sequentially 1 through 10 from floor to ceiling. The velocity probes appear in the east and west doorways.

FATE calculations are presented here for BE-2 Case 1, a small fire (1.5 MW peak burning rate) with closed doors and no ventilation Figures 4 and 5, and Case 3, a large fire (3.2 MW peak) with doors open and ventilation on, Figures 6 and 7. In both cases, agreement between FATE and the experiment are seen to be very good. This integral agreement demonstrates correct overall function of the models comprising the FATE fire model.

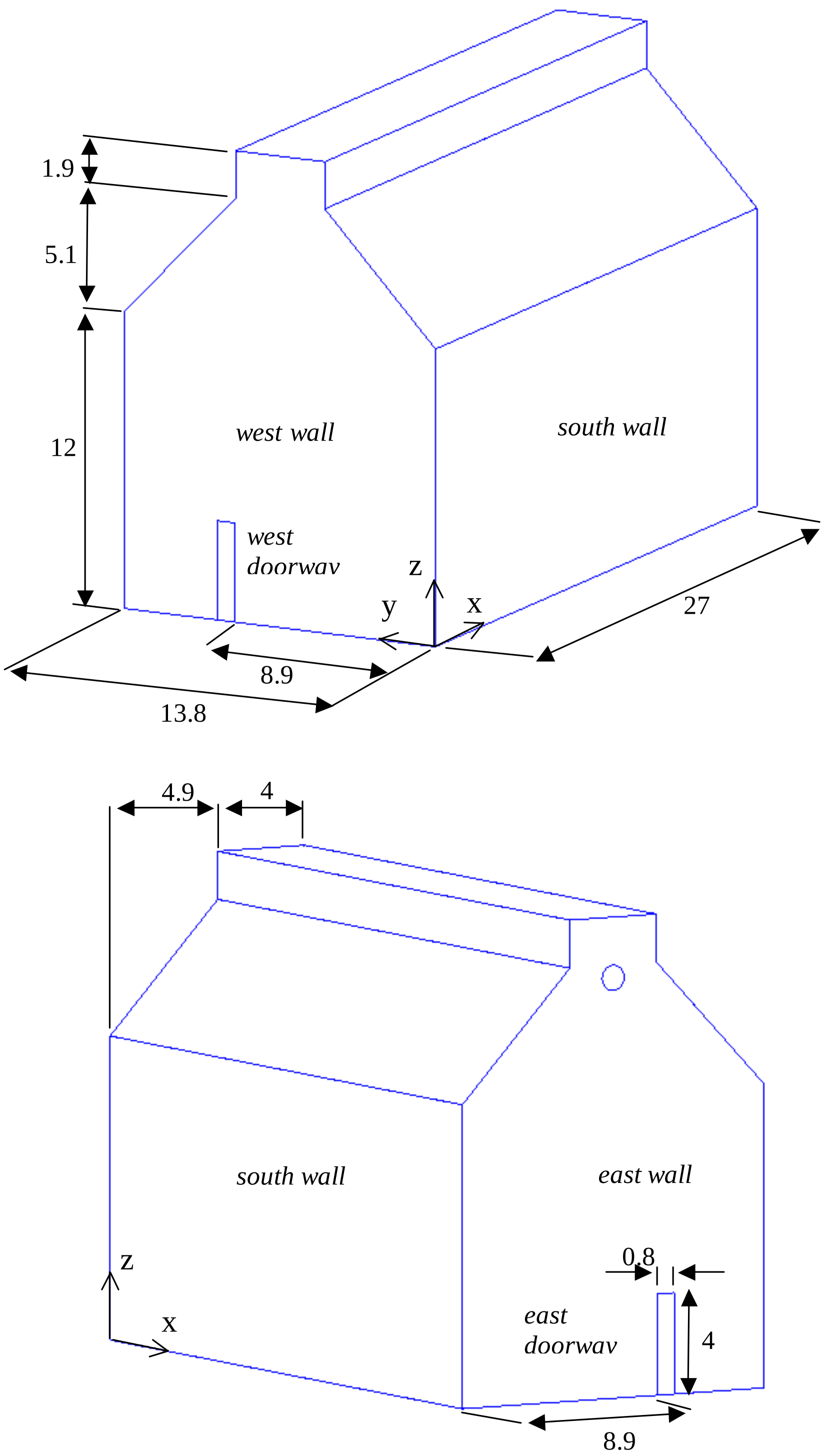

Figure 2. Hall and Dimensions for ICFMP BE-2 Part I.

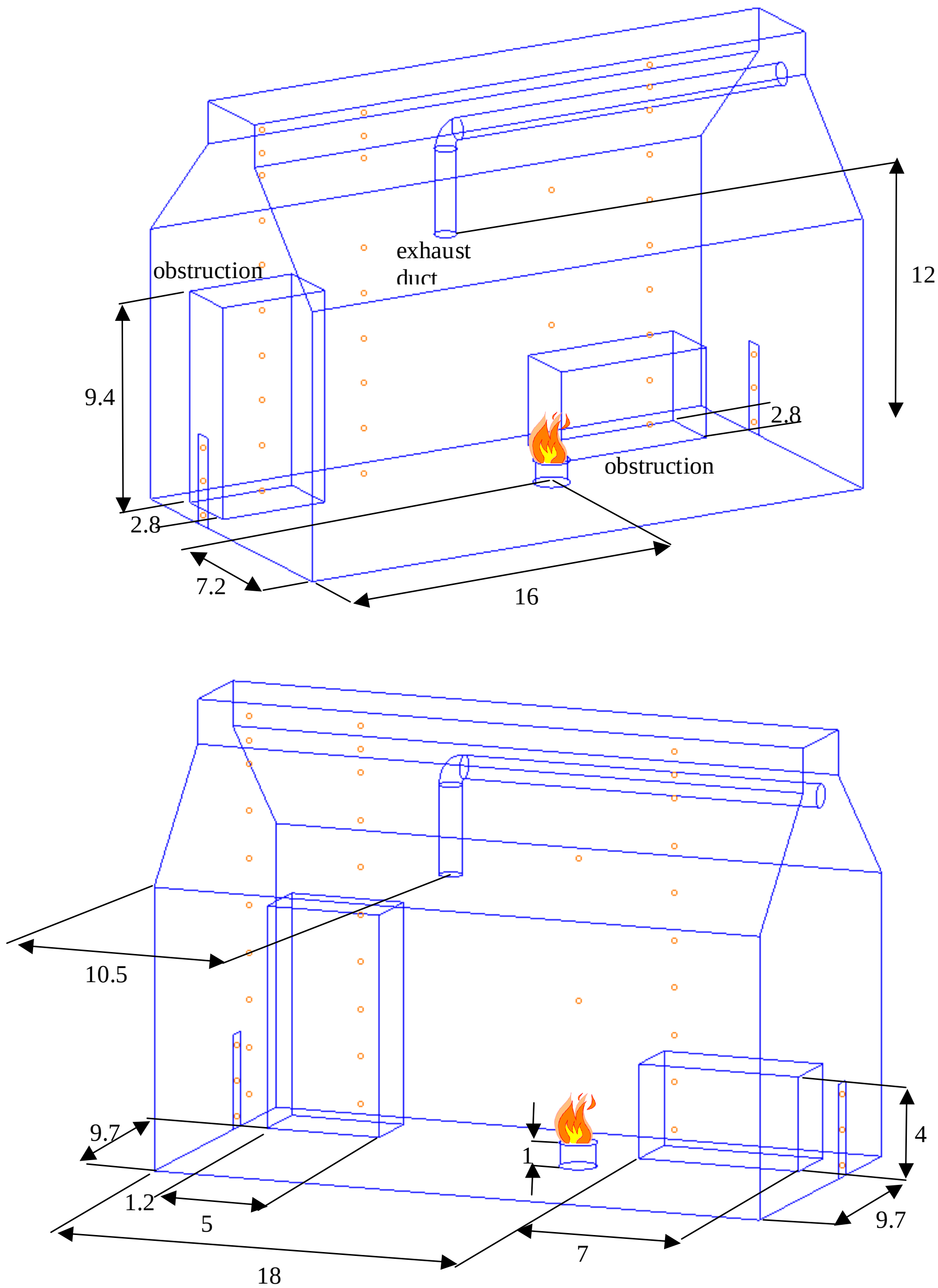

Figure 3. Internal Geometry for ICFMP BE-2 Part I.

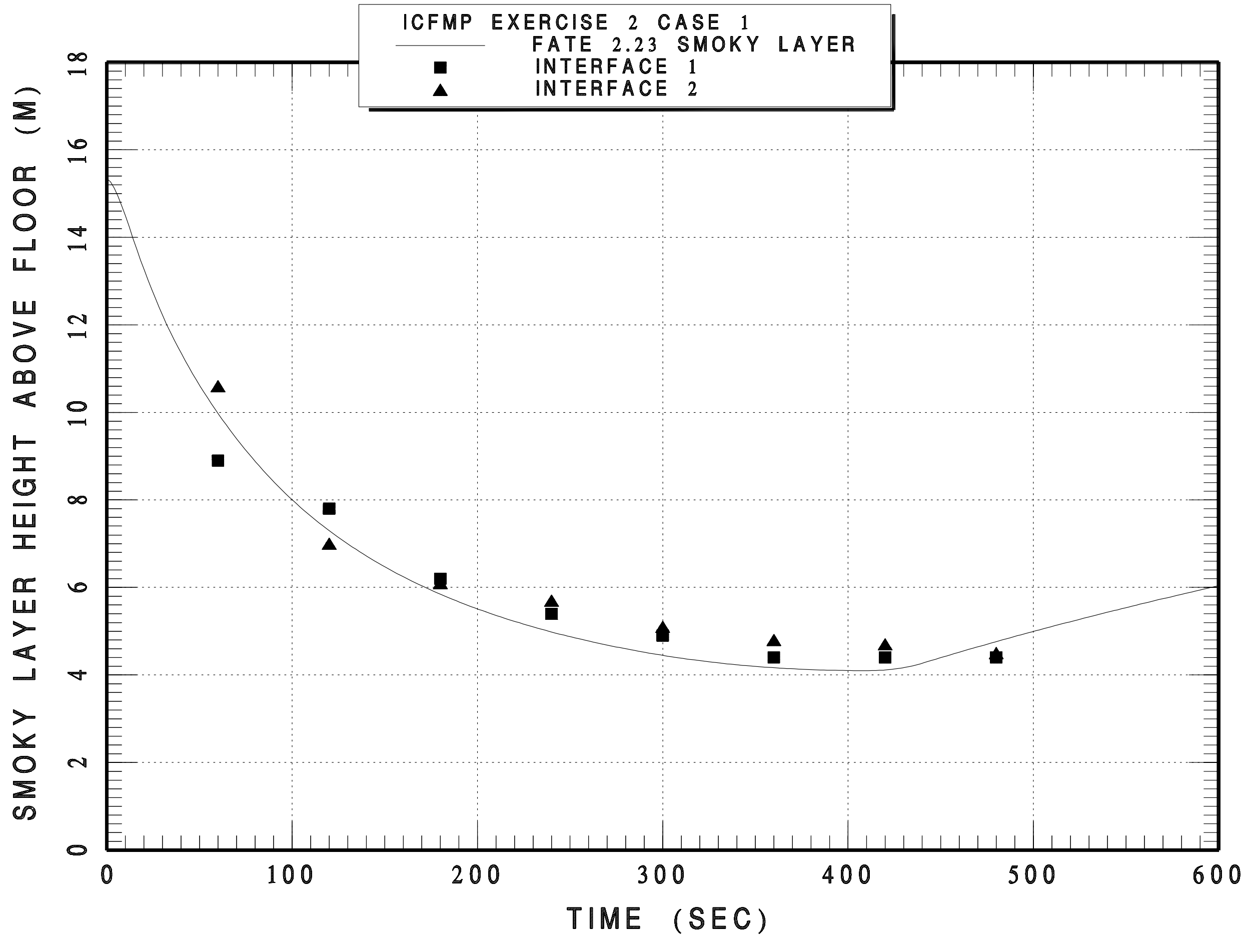

Figure 4. ICFMP BE-2 Case 1 Smoky Layer Height.

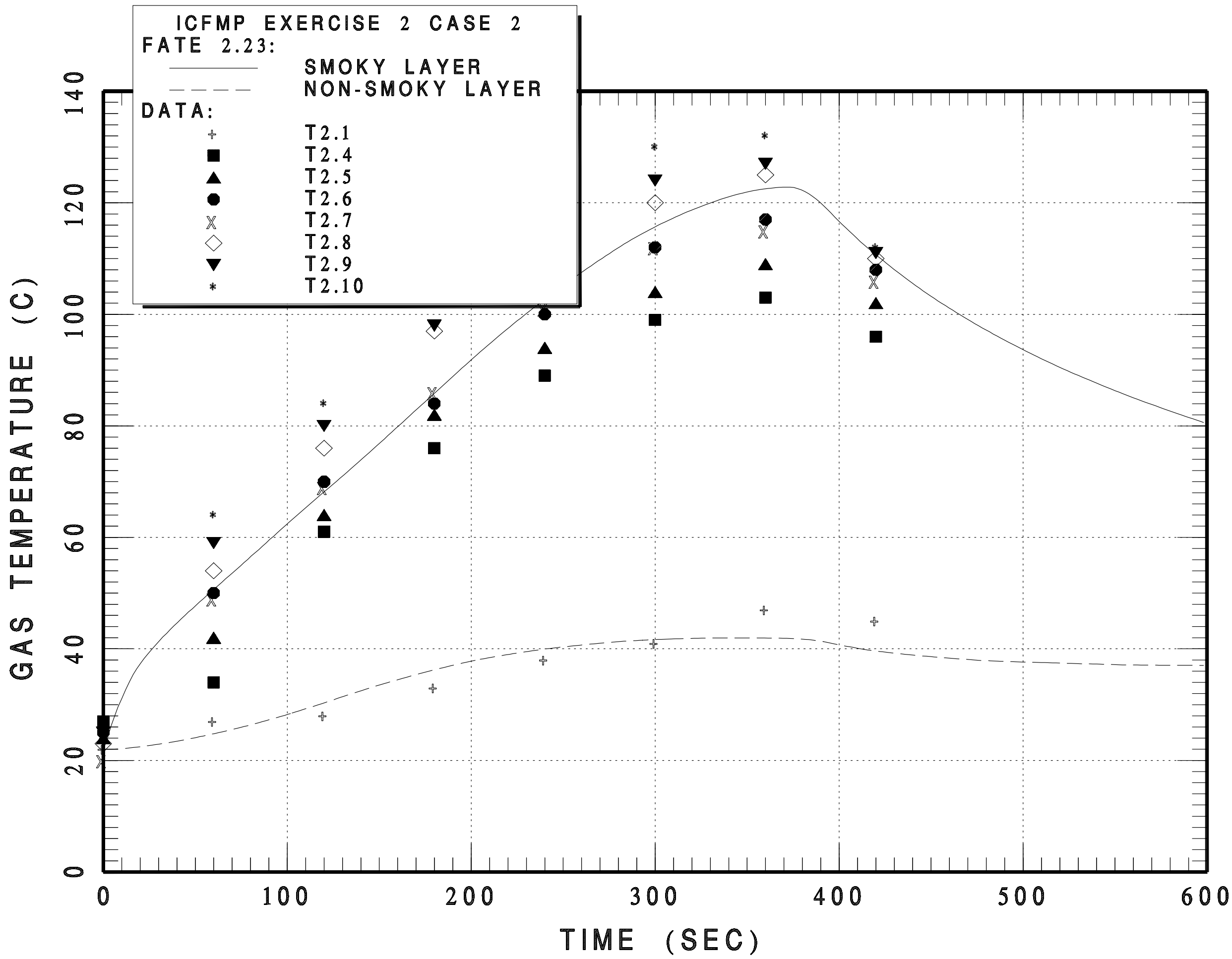

Figure 5. ICFMP BE-2 Case 1 Gas Temperatures Compared to Measurements.

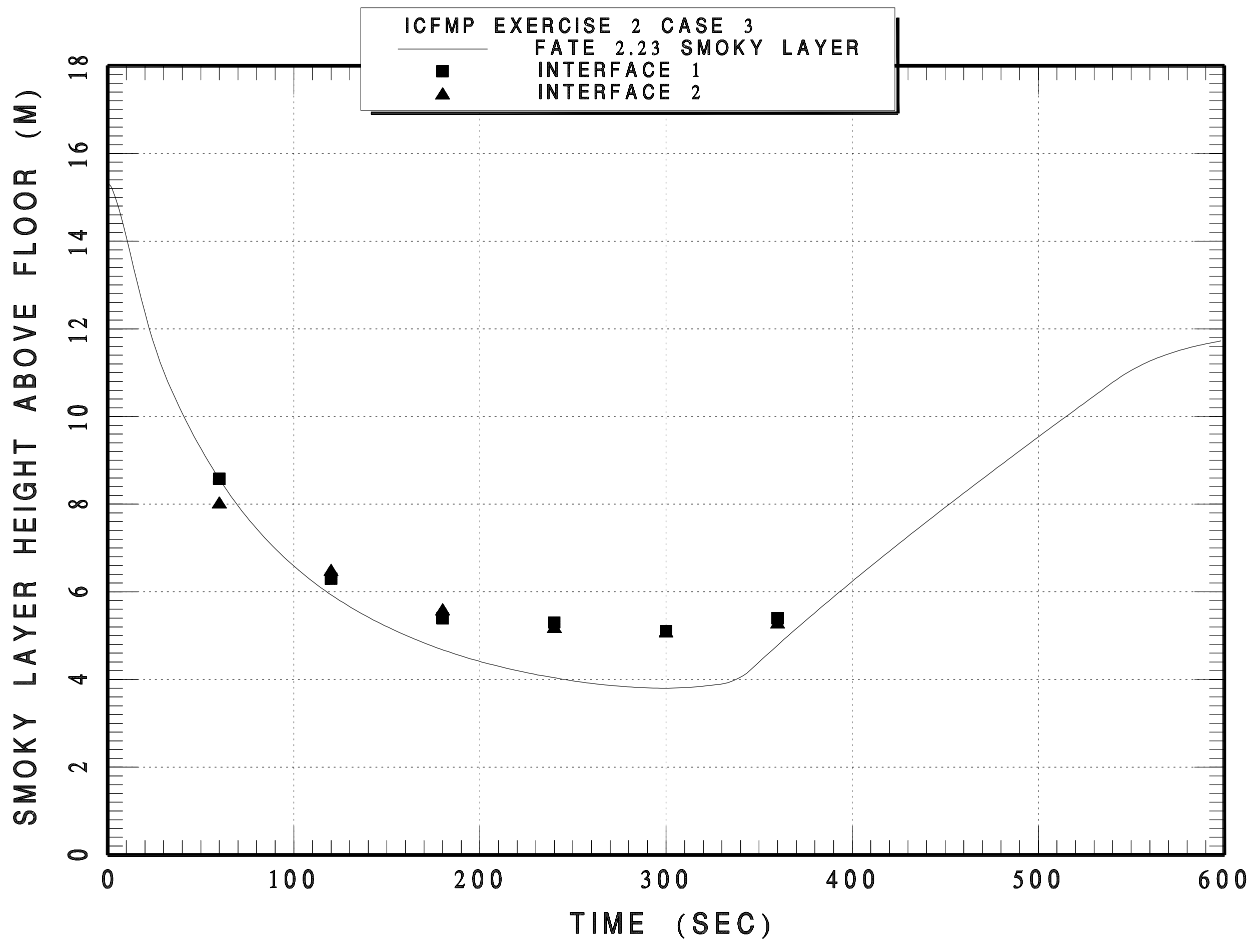

Figure 6. ICFMP BE-2 Case 3 Smoky Layer Height.

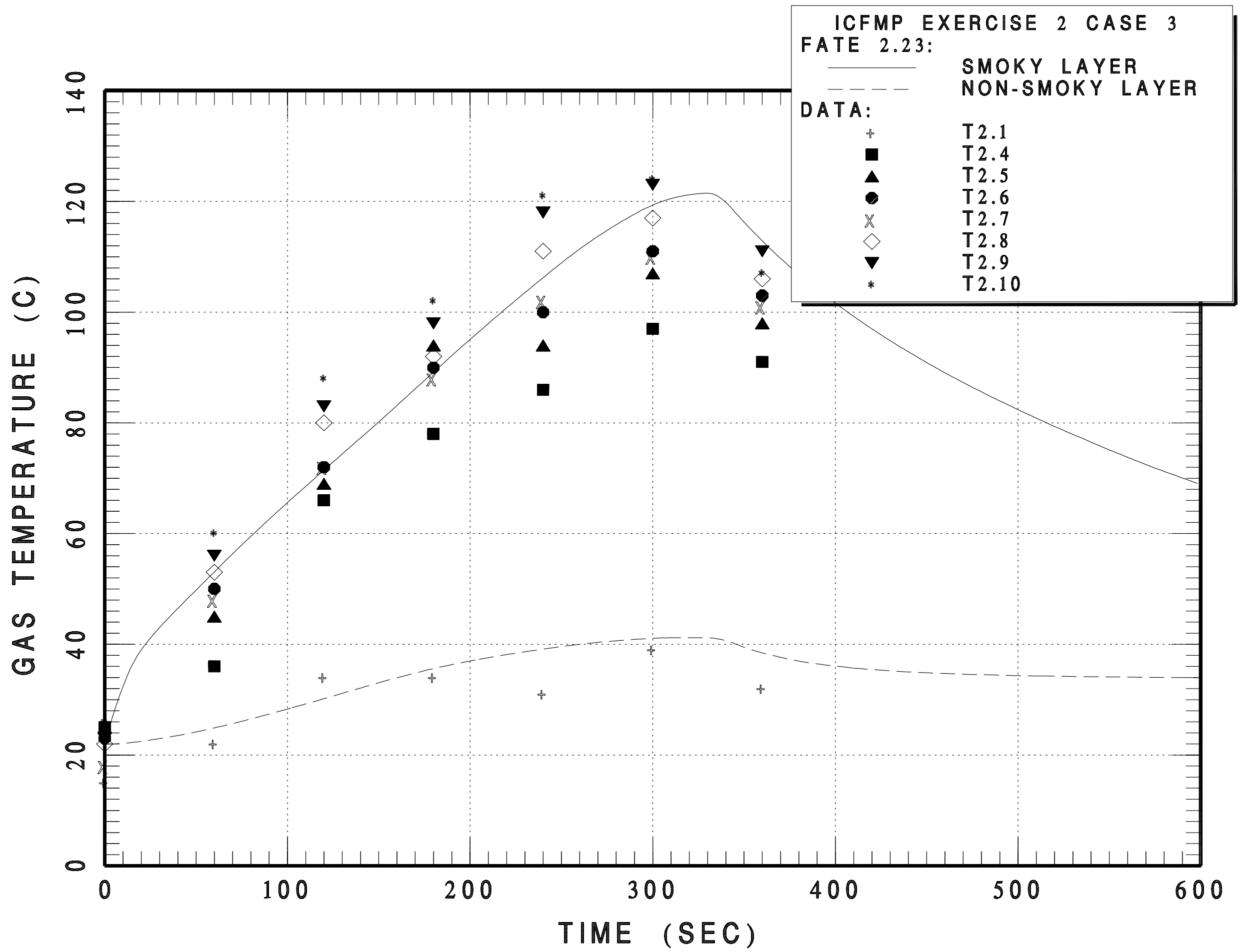

Figure 7. ICFMP BE-2 Case 3 Gas Temperatures Compared to Measurements.

Large Facility Fire Example

This paper concludes with an example large facility fire calculation. This example is based upon analysis of a real facility, but details of the facility and actual calculated accident cases are withheld here. The purpose of the example is simply to demonstrate application of FATE to a facility of substantial size and indicate the practical nature of this application.

Figure 8 is a schematic plan view of one level of the facility. Over 100 control volumes and nearly double that number of flow paths are used for the rooms alone, not counting the HVAC system which is omitted purposely for this example. All doors are open to provide the maximum leak path factor. A 1 MW fire is placed in a central location with HVAC shut down; the fire itself burns out in 20 minutes. A 60 Pa wind-induced pressure gradient is imposed upon the building in the direction from the top to bottom of Figure 8 (referred to as North to South for convenience). A source term of 1 g UO_2 aerosol is released to the smoky layer during the first 15 minutes of the fire; since the source is 1 g, the number of grams released is numerically identical to the leak path factor.

Because all doors are open, little pressurization occurs due to the fire itself, and a quasi-steady pressure gradient is established from North to South in the facility. Ordinarily in a room with closed doors, the fire would cause first pressurization and then depressurization (negative gauge pressure) would occur after fire extinction. Smoky layer temperature is shown in Figure 9, and smoky layer propagation is shown in Figure 10. These figures merely show that the fire room becomes rather hot, and combustion products and aerosols are indeed transported throughout the facility. The list of rooms shown includes major corridors along the nearest route from the fire room to the environment. High temperature differences cause density-driven counter-current flow which distributes aerosol (soot and UO_2) among corridors and rooms near the fire room. The fire room has detailed wall and ceiling heat structures, but these were neglected for corridors and rooms not near the fire, so that the smoky layer in the fire room is observed to cool down but the smoky layer in some other rooms does not, and this in itself tends to artificially promote counter-current exchange flow. This is not a model limitation, just a choice made for simplicity of the example.

Figure 11 indicates aerosol release, where the time scale is now hours (versus minutes for the previous figures). Fire energy and mass sources are responsible for short-term mixing between compartments, while long-term aerosol release is driven by the wind-induced pressure gradient. Note that inclusion of HVAC paths would not likely increase the given leak path factor because all the doors are open. The value of the leak path factor is about 42% at 8 hours and releases have nearly terminated.

In summary, this large facility fire example shows the importance of both counter-current flows and wind-induced pressure gradients for calculation of a 24 hour leak path factor in the absence of HVAC. Also, the advantage of having a fire model including smoky layer growth and transport directly embedded in FATE is clear, because no special input tricks are required as might be the case if output of one code were used to drive another.

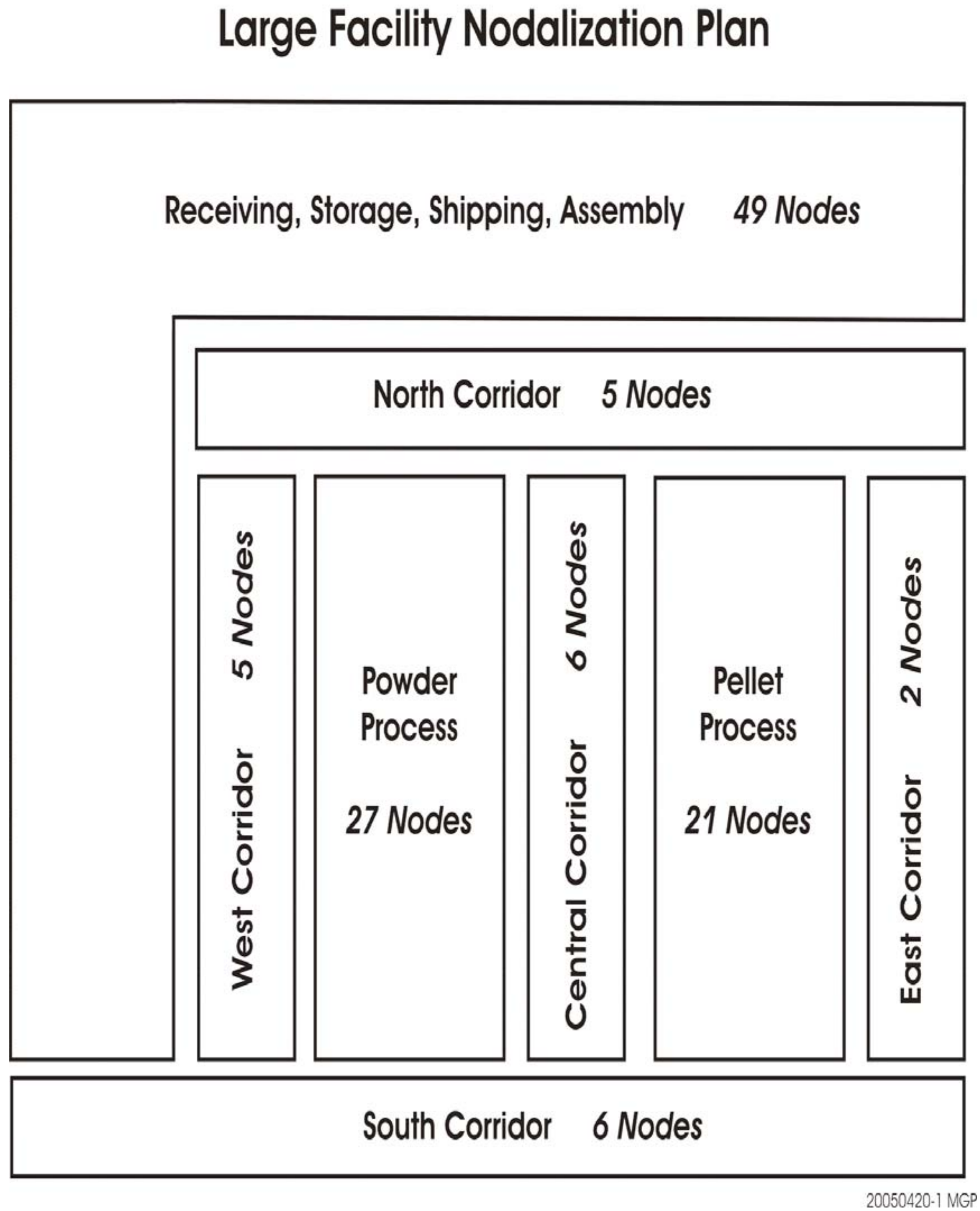

Figure 8. Large Facility Fire Example Nodalization Summary.

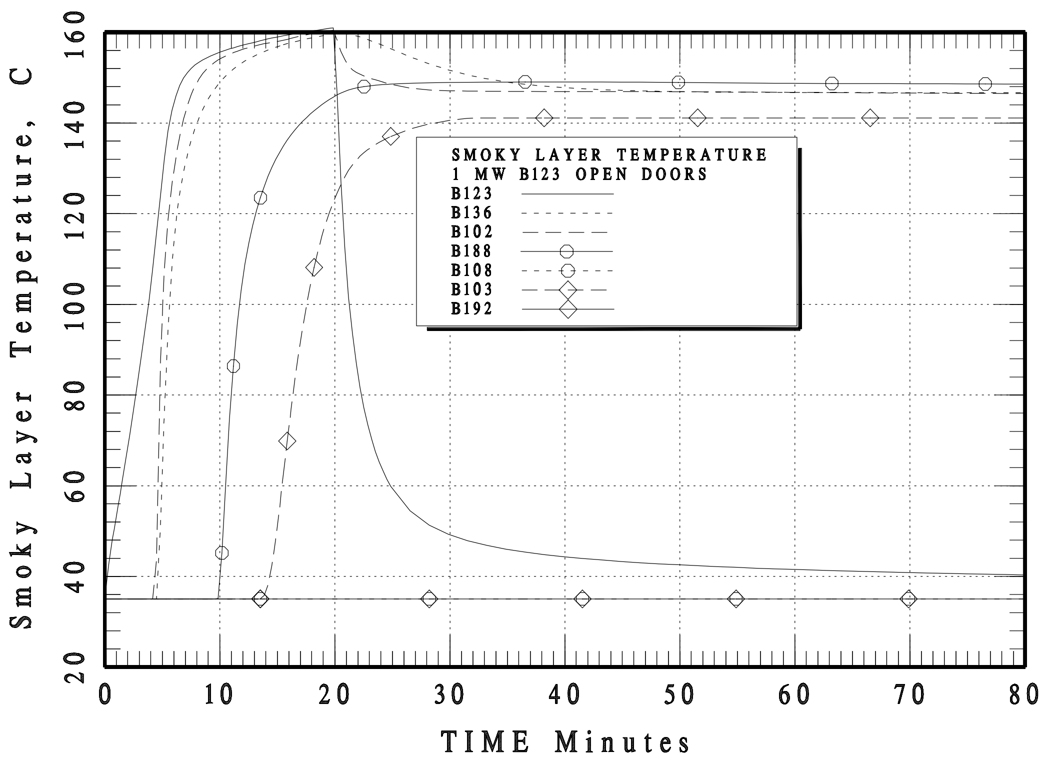

Figure 9. Facility Fire Example, Smoky Layer Temperature History.

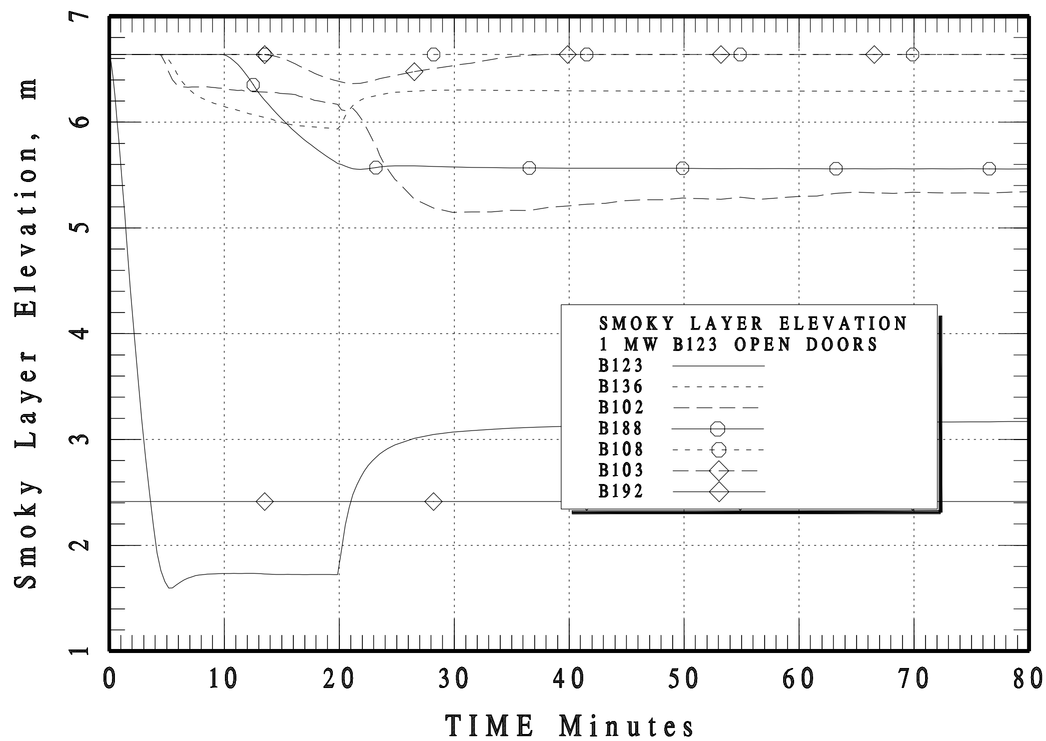

Figure 10. Large Facility Fire Example, Smoky Layer Propagation History.

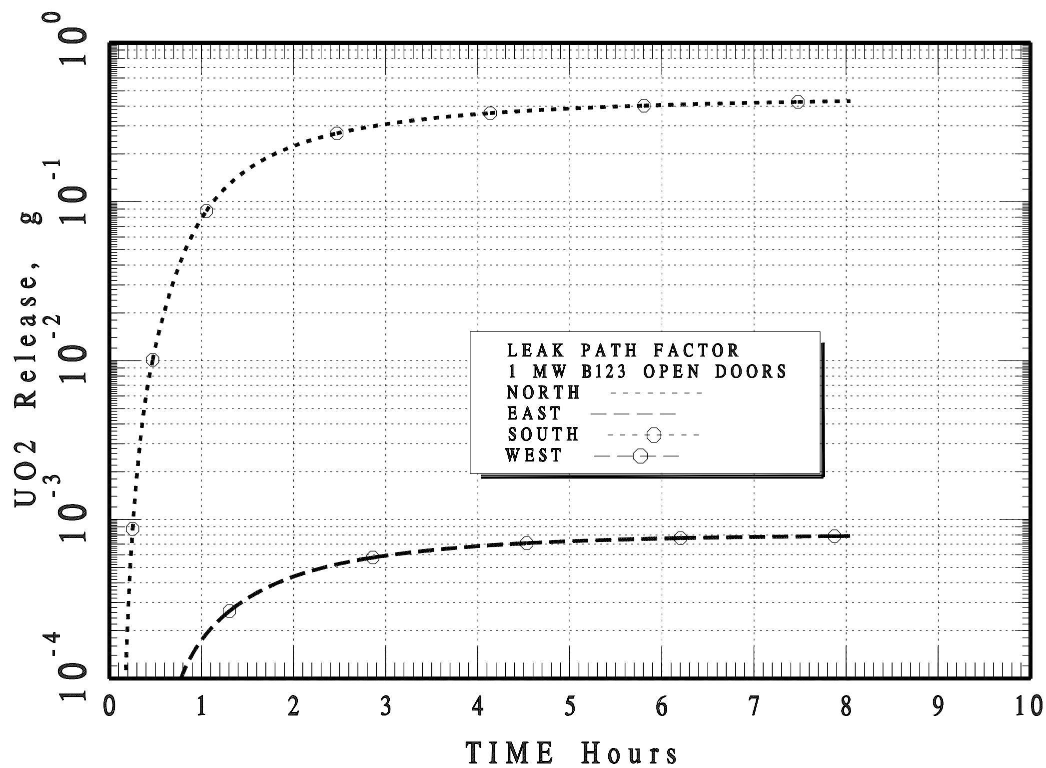

Figure 11. Facility Fire Example, UO_2 Release History.

References

1. Plys, M.G., *FATE 2.0: Facility Flow, Aerosol, Thermal, and Explosion Model, (Improved and Combined HANSF and HADCRT Models),* FAI/04-71, SNF-23281, 2 volumes, Fluor Hanford, Inc., Richland, WA, November 2004.

2. Crowe, R. D. and R. D. Lanning, *Analysis of a HLW Process Vessel Hydrogen Deflagration Using HADCRT Computer Code,* 24590-HLW-U0C-30-00004, Rev. A, Bechtel National Inc., Richland, Washington, 2002.

3. Crowe, R. D. and R. D. Lanning, *Analysis of HLW Melter Unplanned Pour Using HADCRT Computer Code*, 24590-HLW-U0C-30-00003, Rev. D, Bechtel National Inc., Richland, Washington, 2002.

4. Crowe, R. D. and R. D. Lanning, *Beyond Design Basis Event - LAW Melter Offgas Release Event Using HADCRT Computer Code*, 24590-LAW-U0C-20-00002, Rev. A, Bechtel National Inc., Richland, Washington, 2003.

5. Piepho, M. G., *Thermal Analysis of Cold Vacuum Drying of Spent Nuclear Fuel*, HNF-SD-SNF-CN-023, Rev. 2, Fluor Federal Services Inc., Richland, WA, March 2000.

6. Plys, M. G., *Independent Calculation for Hanford Sludge Transportation and Storage (FAI/02-11)*, HNF-10439, Rev. 0, Fluor Hanford Company, Richland, Washington, 2002.

7. Plys, M. G. and S.J. Lee, *Thermal Analysis of KE-KW Transfer Line and Pump Pits for Revised Sludge Solids (FAI/05-27, Rev. 1)*, KBC-25186, Fluor Hanford Company, Richland, Washington, 2005.

8. USNRC, International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications – Specifications for Benchmark Exercise # 2 Fire in a Large Hall (February, 2002).