

FATE Unified Modeling Method for Spent Nuclear Fuel and Sludge Processing, Shipping and Storage – 13405

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ABSTRACT

A unified modeling method applicable to the processing, shipping, and storage of spent nuclear fuel and sludge has been incrementally developed, validated, and applied over a period of about 15 years at the US DOE Hanford site. The software, FATE™, provides a consistent framework for a wide dynamic range of common DOE and commercial fuel and waste applications. It has been used during the design phase, for safety and licensing calculations, and offers a graded approach to complex modeling problems encountered at DOE facilities and abroad (e.g., Sellafield). FATE has also been used for commercial power plant evaluations including reactor building fire modeling for fire PRA, evaluation of hydrogen release, transport, and flammability for post-Fukushima vulnerability assessment, and drying of commercial oxide fuel. FATE comprises an integrated set of models for fluid flow, aerosol and contamination release, transport, and deposition, thermal response including chemical reactions, and evaluation of fire and explosion hazards. It is one of few software tools that combine both source term and thermal-hydraulic capability. Practical examples are described below, with consideration of appropriate model complexity and validation.

INTRODUCTION

FATE was originally developed to quantify process safety and source terms for fuel cycle facilities including high level waste tanks, vitrification, and spent nuclear fuel. FATE thus couples thermal-hydraulic and aerosol models including:

- Thermodynamics and heat transfer within compartments
- Pressure-driven flows and density-driven recirculation flows between compartments in a topology truly representing the facility
- Performance of engineered systems such as ventilation, cooling, filters, etc.
- Specialty models for energy release and species conservation during a fire, gas phase or dust explosion
- Aerosol source and aerosol transport and deposition, along with species conservation for radionuclides and toxic materials, including aerosol/vapor phase transitions

- Correlations for uranium metal reactions with air, moist air, and water/water vapor under various conditions

The unique capabilities of FATE are illustrated here through specific applications where the software has been used to simulate processing, shipping, and interim storage of spent nuclear fuel and sludge. Examples include:

- Vacuum drying of metallic spent nuclear fuel and the determination of the potential for thermal instability
- Shipping of spent nuclear fuel sludge which contains reactive metal
- Integral response of transport and storage containers and an interim storage facility including evaluation of the potential for accumulation of flammable gas
- Source term evaluation during a facility fire and the importance of stratification,
- Evaluation of a dry cask storage container

These examples identify parameters that can be varied for either a best-estimate calculation or a conservative evaluation and emphasize the importance of

- Threshold phenomena for systems with the potential for thermal runaway
- Density-driven counter-current flows and stratification phenomena for transport of aerosols and contamination
- The ability to independently check complex integral code calculations

APPLICATIONS

Drying of Damaged Fuel and Scrap Material

A key process step in remediation of metallic spent nuclear fuel is vacuum drying, in order to move such fuel from pool storage to dry storage. This drying process is complicated by the fact that it must accommodate failed fuel elements, scrap pieces of fuel elements, and scrap particulate. Physical and chemical processes that must be considered in order to effectively and safely vacuum dry these materials include:

- Exothermic oxidation of exposed metallic surfaces including particle depletion
- Potential thermal instability
- Degradation of particulate thermal conductivity at low pressures
- Multiple component diffusion

FATE models for the individual phenomena are based upon experimental data, and integral process simulations have been validated against closed-form solutions. The integrated model has been used in support of the conceptual, preliminary, and final design phases for vacuum drying of damaged metallic fuel and scrap particulate from the Hanford K Basins [1]. Iteration between design alternatives and calculations led to a design that is demonstrably robust with minimal need for safety-related technical specifications and material characterization.

The main Hanford SNFP process steps are fuel cleaning, scrap sorting, loading of fuel and scrap into baskets, loading of baskets into Multi-Container Overpack (MCO) vessels, transportation of MCOs to the Cold Vacuum Drying Facility (CVDF), MCO drainage and Cold Vacuum Drying (CVD), transportation of dried and sealed MCOs to the Canister Storage Building (CSB), and placement of the MCOs into vault tubes at CSB for interim storage (IS). Each MCO can hold 5 or 6 baskets, where the basket size depends upon the specific fuel design.

Figure 1 illustrates an MCO with 5 fuel baskets, which was the configuration used for the majority of the previous SNFP campaign. The fuel baskets were redesigned as compartmentalized scrap baskets to hold larger fuel pieces, and subsequently modified further by including copper block inserts so as to accommodate fuel particulate. Figure 2 illustrates a scrap basket with copper inserts in place, leaving slots into which fuel particulate (so called Knock-Out Pot or KOP material) is placed. FATE was used in development of this design.



Fig. 1. Cutaway of an MCO with 5 fuel baskets.

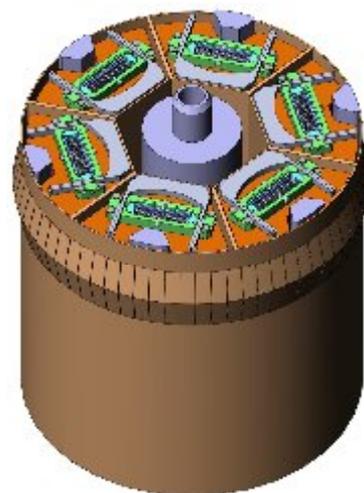


Fig. 2. Copper inserts in a scrap basket.

For the baseline CVD process development, the greatest challenge involved creating the technical safety basis for design and licensing of the scrap baskets. Each scrap basket has six outer compartments made from copper so that heat generated within fuel scrap can be efficiently conducted outward to the periphery, where it is transferred across a gap to the MCO wall. The FATE model for CVD of metallic fuel particulate is shown in Figure 3, and includes control volumes for each basket elevation with flows driven by pressure, density differences, and diffusion.

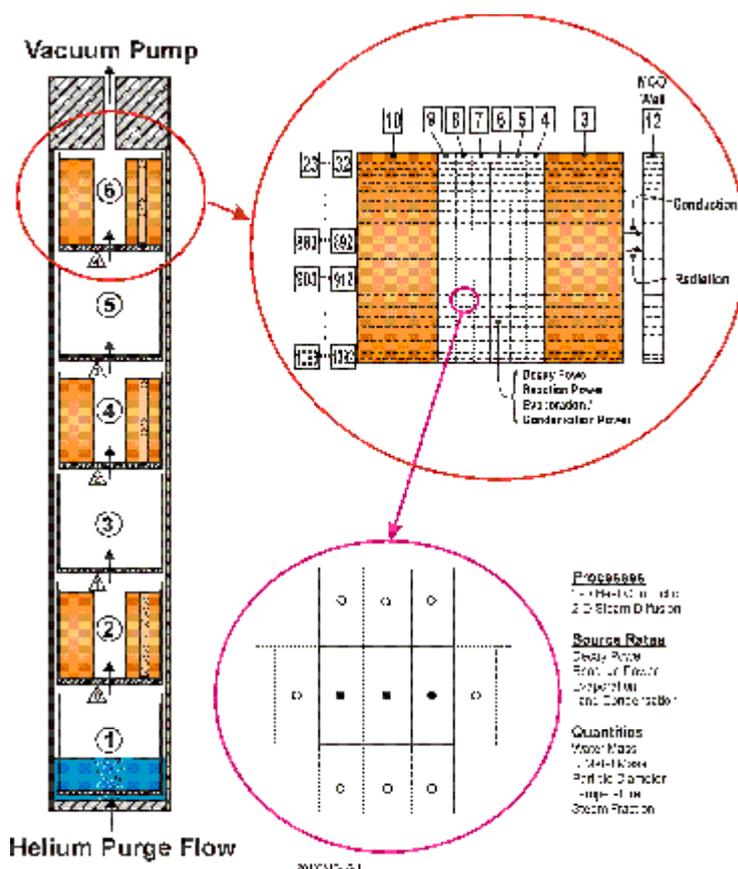


Fig. 3. FATE model for vacuum drying of metallic fuel particulate.

The permeability of a metallic fuel scrap bed determines whether or not convective flow is possible or if diffusion limitations might exist. In the case of Hanford fuel scrap, permeability was sufficiently high to ensure that a supply of water vapor for reactions would always be available. However in the case of fuel particulate in the insert geometry described above, permeability is low enough that diffusion limitations are an important factor in limiting the fuel oxidation rate. Furthermore, diffusion can be important for vacuum drying applications where inert gas is diffusing into the debris against the outflow of water vapor. FATE models have been

used to develop vacuum drying processes for metallic fuel and scrap, including demonstration of an appropriate pressure rebound criterion corresponding to the required minimum residual water. Key lessons learned from this work are the importance of:

- Identification of governing phenomena, acquiring data for their quantification, and using those data to create simple models
- Quantifying design tradeoffs using simple models
- Using simple models to check the implementation of individual phenomenological models in an integral calculation, and to check the integral calculation itself

The results of the investigation explain crucial differences between behavior of metallic fuel scrap and particulate; in particular, the manifestation of thermally unstable behavior is quite different for the two cases, and is far more benign for the case of fuel particulate. The phenomena investigated and quantified are also pertinent to remediation of spent metallic nuclear fuel presently stored in fuel pools. Interaction between design alternatives and model development has resulted in a robust design that requires no significant change in aspects of the process used for previous campaigns for fuel and scrap, and no significant characterization is required to verify the technical safety basis.

Sludge Transport and Storage Containers

Sludge that evolves from degraded metallic fuel and scrap will remain in storage pools after the fuel, scrap, and larger particulate have been removed. Removal and transport of such sludge presents unique challenges. FATE is presently being used to support design of Sludge Transport and Storage Containers (STSCs) for transport (and subsequent interim storage) of accumulated Hanford K Basins sludge which has been consolidated into engineered storage containers.

In general the loading of this sludge into an STSC will occur in one or more batches, and each batch will undergo a settling period in which solids preferentially accumulate in layers depending on particle sizes and material density. Sludge segregation into metal-rich and metal-free layers during loading is influenced by variations in sludge type, batch loading volume, total uranium and uranium metal content, and STSC internal design. Once loading is complete, an appropriate layer of cover water is added, providing a heat sink and radiation shielding, and the STSC is purged before it is enclosed in a Sludge Transport System (STS) Case for shipment to the T Plant facility for storage. During shipment, the STS Cask is potentially exposed to several days of solar heating and ambient temperature extremes. Figure 4 and Figure 5 illustrate FATE modeling of a STSC and STS Cask during transport.

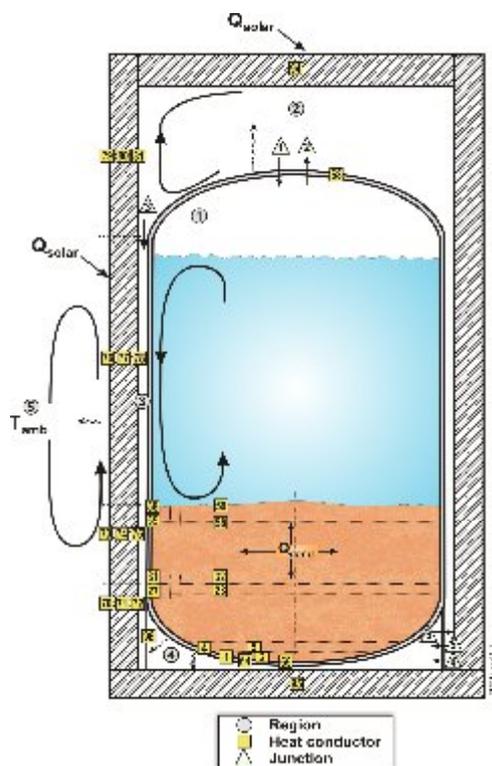


Fig. 4. FATE model for the STSC and STS Cask.

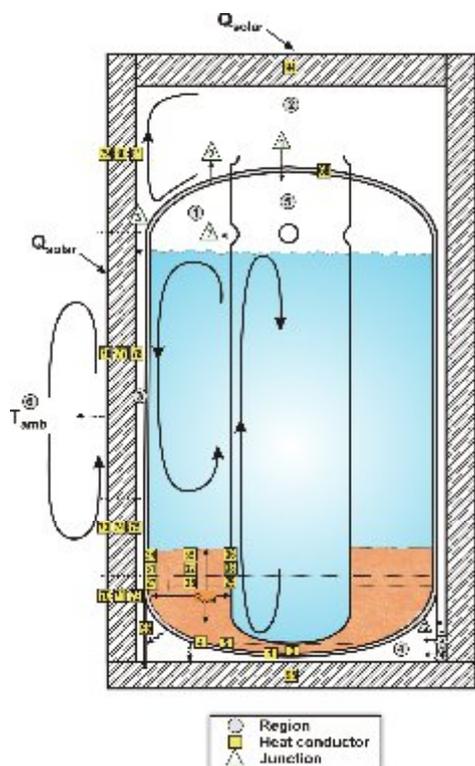


Fig. 5. FATE model for the STSC and STS Cask with a water core insert.

The FATE model accounts for sludge layers of different composition, according to settling calculations that are performed separately. Thus the model considers that metal oxidation and decay heat are concentrated in one or more sludge layers which depend on knowing the sludge composition, material properties, and particle sizes. Multi-dimensional heat transfer within the STSC is modeled between sludge layers, the adjacent STSC wall segments, and the overlying water. Sludge composition can be chosen to reflect either best estimate (design basis) conditions or more conservative safety basis conditions (such as higher uranium metal content).

The evolution of hydrogen and oxygen (from oxidation and radiolysis) is tracked within both the STSC and the shipping Cask, which communicate through filtered vents on the STSC. Heat transfer within and through the Cask, and external to the Cask, is modeled and accounts for solar insolation and heat transfer to or from the environment. The result is a detailed transient model for the temperature, pressure, and gas composition within the STSC and Cask. This facilitates decisions regarding the types and volumes of sludge that can be safely transported in an STSC, the available time window for transport, as well as the benefit gained from STSC design details regarding ventilation of the lower support skirt and the possible inclusion of a water-filled insert

or inner core (Figure 5). The core insert would provide an additional heat sink and a more coolable geometry for sludge types with higher uranium content, but at the expense of less volumetric sludge capacity in a given STSC. FATE has been used to optimize the sludge loading process to ensure safe stable conditions while minimizing the number of STSCs.

T Plant Interim Storage

STSCs containing K Basins sludge are designated for storage at the T Plant facility. T Plant is a repurposed fuel processing building, comprising a large open hall (canyon), a loading bay, a number of process (storage) cells, and an HVAC system which ventilates each cell and exhausts through the building HEPA filters and stack. Upon arrival at T Plant each STSC/Cask is vented to remove built up pressure, and then purged. FATE has been used to estimate the required time for each process step to ensure that flammable conditions are avoided, and to evaluate process design options such as purging by continuous flow or pressure cycling.

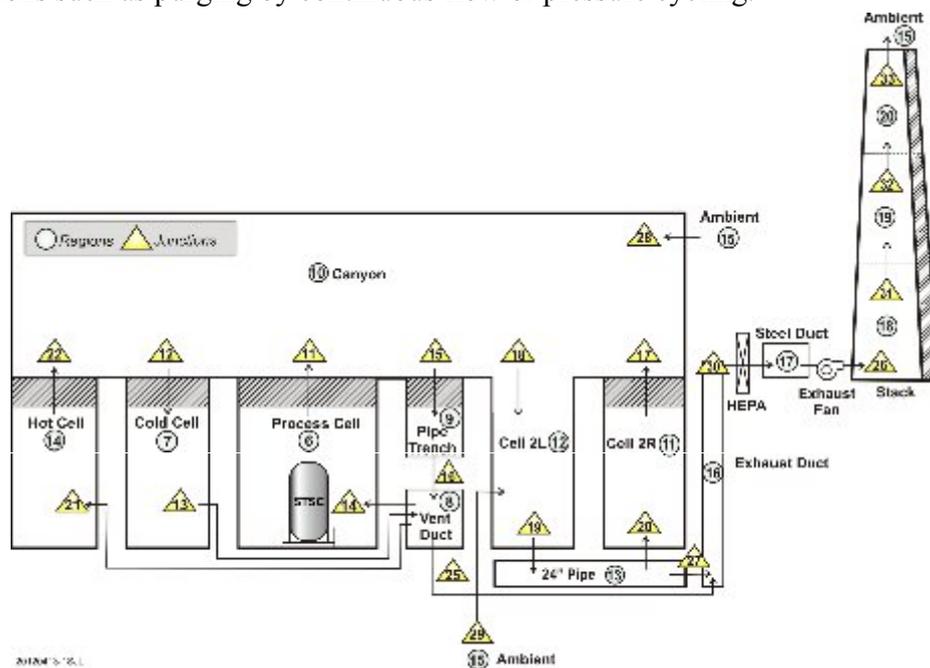


Fig. 6. FATE model for T Plant storage facility.

Subsequent STSC storage configurations within T Plant have been evaluated using FATE to model the entire building, as shown in Figure 6. This model considers the number of STSCs within a given cell and the number of cells with or without STSCs (i.e., “hot” or “cold” cells) and evaluates the impact of details such as air gaps between the cell cover blocks (or if the covers are even in place) as well as building breathing and hydrogen accumulation in the event that HVAC is disabled. In addition to the usual heat and mass transfer models, the simulation

considers the ventilation fans, HEPA filter resistance, and exhaust stack heat sinks. The key results include peak sludge temperature and hydrogen levels in a safety basis STSC and the T Plant cells during storage. Of particular interest are the long term thermal stability of the sludge and the potential development of flammable gas mixtures, along with the rate of water loss in an STSC and the potential for freezing.

Dry Cask Storage of SNF Assemblies

A HI-STORM™ 100 Cask System multi-purpose container (MPC) and HI-TRAC™ transfer cask loaded with spent PWR fuel were analyzed using FATE for steady-state thermal behavior in an isolated loss-of-flow condition. The FATE model is illustrated in Figure 7. Peak cladding temperatures were demonstrated to be within the allowable limit of 570°C for short term operations. In the loss-of-flow case, heat transfer from the fuel to the environment was split almost equally between combined conduction/radiation radially to the basket periphery and convection of naturally circulating helium fill gas within the MPC, with thermal radiation from the fuel to the MPC lid accounting for the remainder. The effect of insolation was considered.

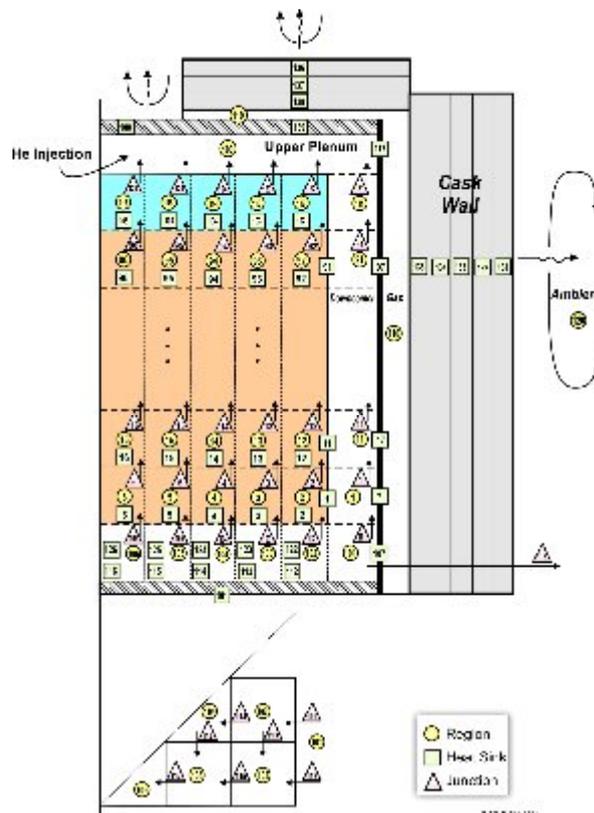


Fig. 7. FATE model of an MPC with MPC-32 Fuel Basket in HI-TRAC™ Transfer Cask.

The forced helium dehumidification (FHD) step was also evaluated, as FATE can accommodate the closed-loop forced helium dehumidification process. Boundary condition information was used to construct a model that can accommodate the geometric and thermal conditions for the individual fuel assemblies, fuel cells, canister cylinder and transfer cask that form the basic configuration. Specific design details which affect fluid flow and heat transfer were considered, such as MPC flow geometry, upper and lower fuel spacers, friction and form losses along a fuel assembly, as well as effective thermal conductivity of the fuel basket, transfer cask water jacket and upper lid. In the case of forced helium dehumidification, the injected helium gas tends to travel into the downcomer to the exhaust, with little effect on the natural circulation of the helium through the center fuel channels.

Contamination Release

Fire and explosion risk is generally increased during decommissioning because of the ignition frequency associated with hot work, handling of oil and solvents, and either cleanup or the potential for creation of fine particulate (dust). As a facility is dismantled, its topology for air flow evolves, and this affects the transport of released contamination: doors will be left open or removed, walls may be breached for equipment removal, and ventilation supply and exhaust balances will change. Accident simulation must consider how these changes impact the potential for contamination release, and thus must take into account both physical effects, such as the formation and deposition of aerosols, as well as structural characteristics which enable density driven and stratified flow. Depending on the geometry, the principal transport mechanism is often density-driven, counter-current flow of hot gas in one direction and cold air returning in the opposite direction [2].

In a fire scenario soot and contamination are transported throughout the facility with the hot gas layer. Transport can be enhanced due to high heat release rates associated with pool fires from spilled and ignited solvents. Contamination release in explosion scenarios is typically by entrainment of deposited material. Liquid pools or films can be atomized, and deposited dust can become airborne given sufficient gas flow during venting [3].

Contamination release is generally quantified in terms of the “Leak Path Factor” LPF, which represents the fraction of originally released contamination that leaks from a facility to the environment [4]. FATE provides an integral plant thermal-hydraulic and aerosol analyzer with capabilities similar to those of advanced LWR severe accident codes, but with generalizations to consider chemical phenomena applicable to general fuel cycle and waste treatment plants. FATE models address fire, solvent vapor flammability, and dust explosion hazards, including quantification of potential radiological and toxic releases.

To quantify the transport and ultimate fate of radioactive contamination released during a fire, thermal-hydraulic, fire, and aerosol models are fully integrated in FATE and include:

- Thermodynamics and heat transfer within compartments
- Pressure-driven flows and density-driven recirculation flows between compartments in a topology truly representing the facility
- Performance of engineered systems such as ventilation, cooling, filters, etc.
- Specialty models for energy release and species conservation during a fire, gas phase, or dust explosion, which drive the transient
- Aerosol source and aerosol transport and deposition along with species conservation for radionuclides and toxic materials, including aerosol/vapor phase transitions

FATE simulation can be applied to normal decommissioning operations wherein contamination release from unit operations is the source to drive the facility models. An example situation [5] is shown in Figure 8, which shows a simplified plan view of a reactor building floor outside containment. Three process rooms (numbered 17, 18, and 19) are accessed by a hallway (zones numbered 1 through 16). Flow paths are indicated with open rectangles and consist of normally closed double doors and, for the process rooms, additional overhead vents for ventilation overflow (not shown). Dotted lines indicate open corridor flow areas. The path into Room 1 (upper left) is a normally closed fire door (no vent) and the path from Room 16 (upper right) opens into a large, open volume for operations.

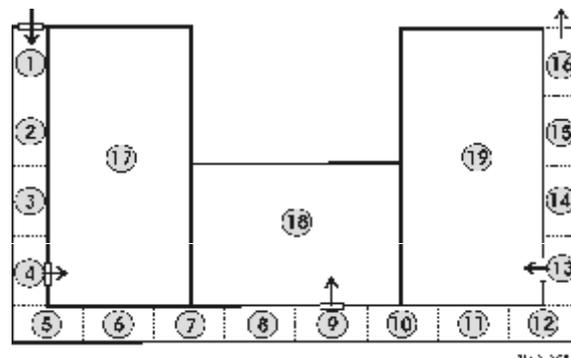


Fig. 8. FATE model for a simplified reactor building.

A fire or explosion in Room 18, whose doors would be open for operations, would cause smoke and contamination to enter the hallway and potentially move down the hallway in both directions. If the door to Room 1 (upper left) is closed as it should be, the hallway in that direction is a “dead end” for smoke accumulation and retention of contamination. If, on the other hand, the door to Room 1 is left ajar for operations, or opened during accident response, an

external pressure imbalance (from wind or the building ventilation system) could cause the smoke to flow preferentially toward the exit from Room 16 (or toward the door left ajar). The position of just one door can be readily shown to have a large impact on contamination release.

In FATE, all control volumes can potentially be “stratified” regions whose upper layer, sometimes called the “smoky layer,” has a different composition, energy, and temperature than that of the lower layer (Figure 9). The top and bottom elevations and orientations of each flow path determine which layer from a donor region may enter the flow path (in principle both layers can) depending on the elevation of the interface between upper and lower layers. In this illustration the transport through the door on the left is by forced flow, whereas the door on the right experiences stratified counter-current flow. In addition, layers are allowed to mix if a density inversion occurs. Aerosols can settle from either layer onto surfaces, and from the smoky layer to the lower layer.

The key tradeoff influencing the LPF is settling time versus transport time. In closed-door scenarios, settling time exceeds transport time, and in open-door scenarios, the opposite is true. In the above example, when the fire door in Node 1 is closed a “dead end” corridor is formed in which substantial amounts of contamination can be deposited. Stratified counter-current flow of hot gases above cold gases carries aerosols from the source room through the corridor and to the ambient, but is much less efficient than forced flow.

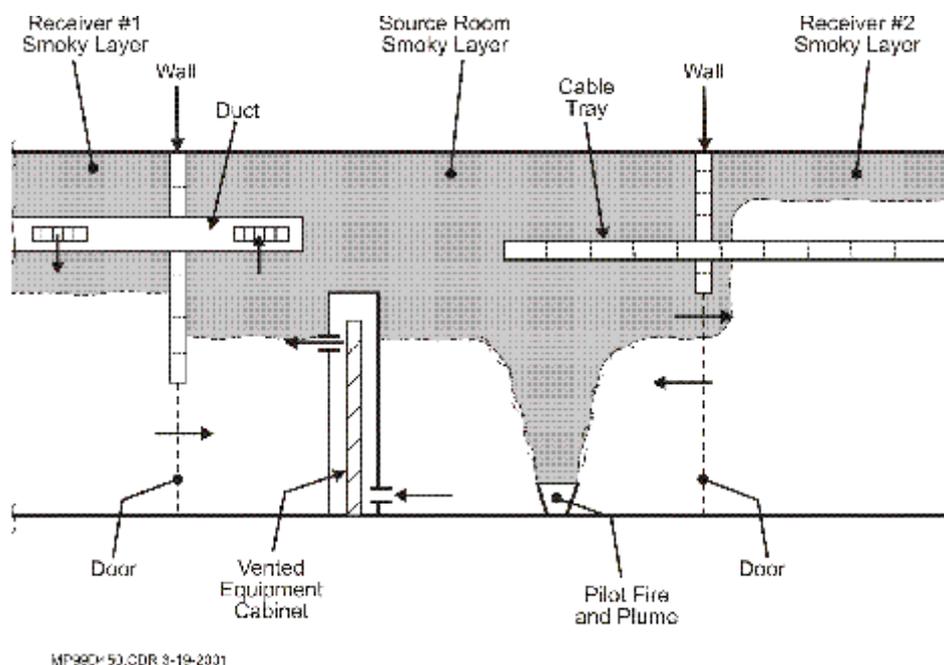


Fig. 9. FATE fire modeling features.

Aerosols are transported by flow, and therefore aerosol transport depends upon which layer is being transported. In static situations, counter-current density-driven flow can dominate over pressure driven flow. This buoyancy-driven exchange flow mechanism is explicitly considered by FATE. Under active ventilation, FATE can be used to simulate a complete loss of supply isolation function in order to illustrate how crucial this function is to proper confinement. If the HVAC system continues to supply air to otherwise isolated process and support rooms, it can push aerosol contamination throughout the facility.

Crucially for fire scenarios, the HEPA filter resistance changes as aerosols accumulate. In FATE, the decontamination factor (DF) for a clean filter is input, and this is assumed to not change. However, the user can specify either a curve fit or a table to represent the change in filter resistance as a function of captured aerosol mass. It is typical for filter resistance to double with the addition of between 50 and 400 grams of aerosol, depending on the area of the filters. Furthermore, the temperature of the filter can be calculated if desired.

Contrasting the fire and vapor explosion scenarios, the key difference with respect to LPF is the duration of the driving source. Fire scenarios clearly have a great potential to drive contamination release compared with other transients that are relatively brief, such as vapor explosions or accidental depressurization.

Model Validation

The above mentioned models are conducive to problems of increasing complexity, from simple benchmark exercises, to individual waste transport containers, to large storage or processing facilities. Individual models have been validated against analytical solutions and experimental data, and have been developed under a NQA program. Two examples are shown below.

FATE aerosol calculations have been compared against data from Test AB-5 taken at the Containment Systems Test Facility (CSTF). CSTF was an 850 m³ carbon steel vessel, and during Test AB-5 a sodium fire aerosol was pumped in at a rate of about 445 g/s for 900 s and then allowed to settle for over a day [6]. From Figure 10, it is evident that the aerosol essentially achieves steady-state during the source period, and about 5 orders of magnitude in concentration were experienced during the test. The aerosol correlation used by FATE agrees well with data, and is somewhat conservative for the lean concentrations at the end of the experiment.

Solid and liquid fire sources are typical input to an analysis, and FATE allows fuel burn stoichiometry and rates to be user-specified. However, a mechanistic model is employed for entrainment of surrounding gases by combustion products which form a plume source to a stratified layer. The Ricou-Spalding entrainment law [7] is applied in a manner that joins

momentum and buoyancy-driven plumes. FATE benchmark calculations have been validated against experiments [8] in which low density gas was injected into containers of higher density gas to generate plumes and stratified layers. In Figure 11 the position of the stratified layer interface predicted by FATE models is in accord with the reference data.

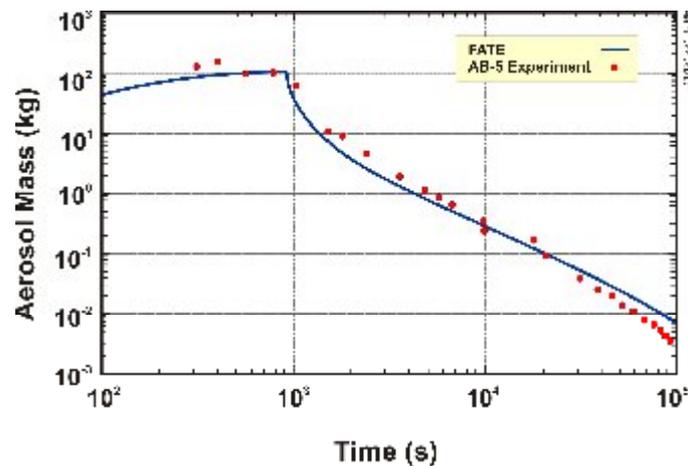


Fig. 10. AB-5 experiment aerosol concentration history.

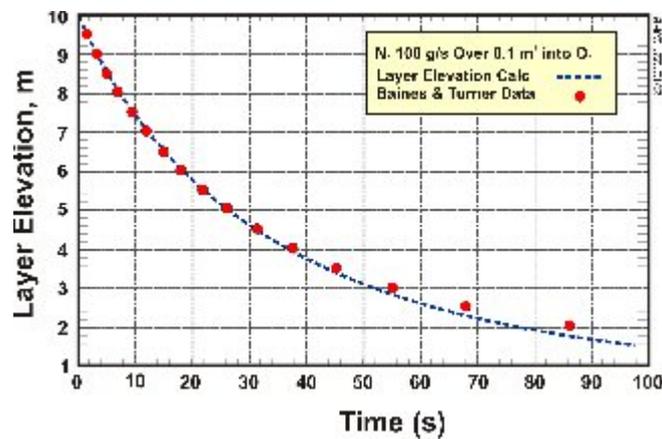


Fig. 11. Stratified Layer and Plume Entrainment Validation.

Threshold Phenomena

For thermal stability of metallic fuel, scrap, or particulate, the stability threshold is the point where the process moves from a stable zone to an unstable zone [1]. This threshold can be investigated, without resorting to detailed simulation, through the use of ignition theory [9]. This method has been employed for the scrap technical safety basis and for the particulate safety basis in order to guide design and eventually check the results of detailed calculations. The essential

step in ignition theory is to write a steady-state heat balance for the system, equating the reaction energy source and losses to some external boundary condition. The energy source is given by the product of the heat of reaction and the water vapor consumption rate used in the diffusion equation. The result is a closed form solution and an independent check.

In the particulate case (Figure 2), the thermal boundary condition is taken to be the (variable) copper block temperature, and it is desired to find that temperature which divides stable from unstable cases. The stability criterion is found by considering particle and gas properties and the width of the particulate slot. The resulting formulation may be used to create a stability map relating key process parameters. An example illustration, Figure 12, relates combinations of reactive particle size d and the metal/water reaction rate multiplier, which are the principal uncertainties, and this map indicates that thermal stability is expected for the safety basis quantities selected for the design. Detailed calculations using FATE have consistently agreed with the simple stability criterion: whenever the copper block temperature exceeds the criterion threshold, unstable behavior and temperature escalations are observed.

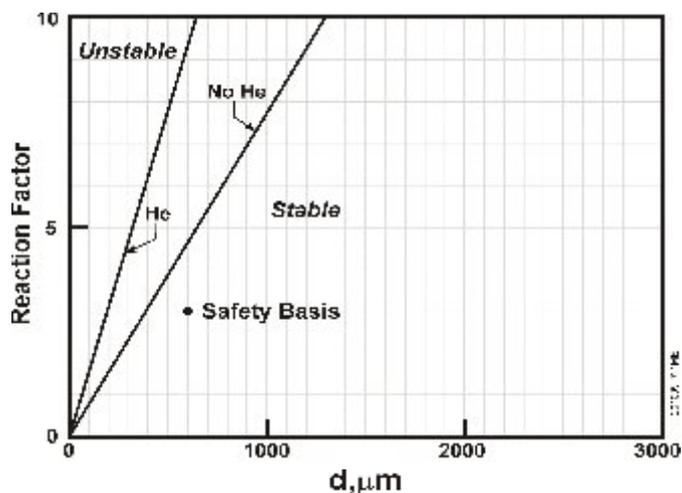


Fig. 12. Thermal stability map for fuel particulate.

Integral Verification

The physical models described above for vacuum drying of fuel particulate [1] were combined to create a simple analytical model for integral verification of FATE results. The simple model begins with an equation for the time history of the copper block temperature. Heat sources to the copper block are decay and chemical reaction power, and heat is lost to the MCO wall. The temperature for the reaction rate is found by Taylor series expansion of the rate law (also done to derive the stability criterion), and it uses a model for thermal conductivity at reduced pressure to relate the copper block temperature to the average particulate reaction temperature. An equation for the reaction zone length is used to quantify the total heat source. The result is a nonlinear

ordinary differential equation for the copper block temperature derivative, which has an exact solution. Figure 13 compares the simple model with the FATE calculation for a safety basis case. The block temperature increases while residual water at the bottom of the MCO is available for evaporation, and it decreases when the water has been depleted at about 10.5 hrs.

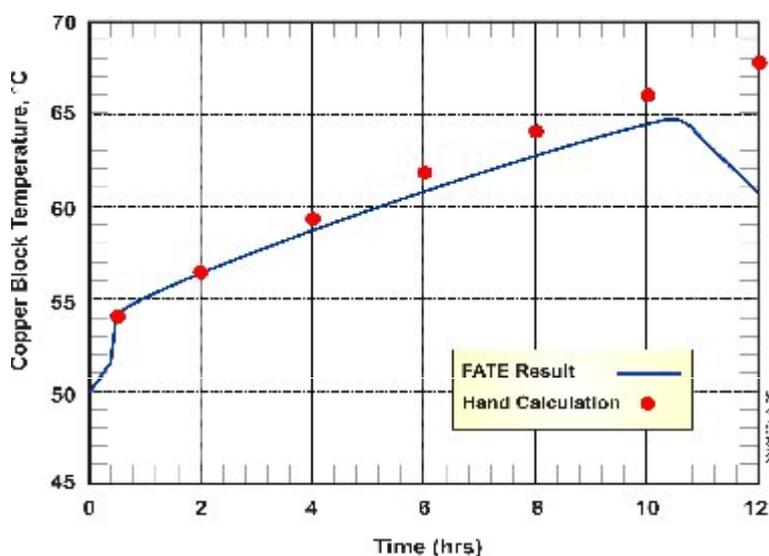


Fig. 13. Comparison of an integral simple model and FATE results for vacuum drying of fuel particulate.

CONCLUSIONS

A variety of customized models is available in FATE. Beyond the usual heat and mass transfer correlations, these couple together such diverse phenomena as aerosol entrainment, transport, and deposition (liquid or dust), plume formation, stratification, flammability, metal-water and other chemical reactions, countercurrent flow, and diffusion in porous media. This diverse mix of validated models has been applied successfully across a broad range of nuclear waste applications, developing technical insights by addressing detailed physics (e.g., transport of water vapor through a fuel crack) and process systems (e.g. transport in building HVAC ducts).

For fuel drying, in cases that are thermally unstable, there is a demonstrable difference between the thermal behavior of fuel scrap and fuel particulate. These classifications are defined by whether or not water vapor flow into the reactive medium is diffusion controlled (particulate, sufficiently low permeability) or convection controlled (scrap, sufficiently high permeability). In the case of fuel scrap, the water vapor reactant is essentially available throughout the reacting medium, which can therefore attain very high temperatures through a majority of its volume. Thus the temperature is determined by the rate of evaporation of residual water – i.e., by the

supply rate of one reactant. In the case of particulate, reactant depletion occurs in the vicinity of a high reaction rate and a moving reaction-front wave forms. The peak temperature of the moving wave decreases as the wave moves from the outer surface of the bed inward, so only a very limited mass of material is at a high temperature at any given time. Generally, the technical safety basis rests upon avoidance of thermally unstable cases, but it is also possible to demonstrate that peak temperatures in unstable cases might be acceptable

Fire and contamination release calculations can only be performed meaningfully with fully coupled models for the fire or explosion, stratification within rooms, inter-compartmental flows that account for stratification and density-driven exchange flows, aerosol behavior, and engineered systems. Through this approach, FATE has been used to evaluate design and scenario features that can form part of decommissioning and teardown strategies for reduction of contamination in the case of accidental releases. For example, for planning purposes, it is best to preserve “dead ends” and to have active ventilation at “open ends.” The correct response to a fire or explosion is to maintain isolation of hallways and if possible to activate a filtered exhaust system, while the worst case response is to allow fire doors to be periodically opened, which allows through-flow for contamination release. It is interesting to observe that intermittent opening and closing of a fire door is in some cases just as bad as just leaving the door open.

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