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Mechanistic Facility Safety and Source Term Analysis

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MECHANISTIC FACILITY SAFETY AND SOURCE TERM ANALYSIS

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Abstract

A PC-based computer program was created for facility safety and source term analysis at Hanford. The program has been successfully applied to mechanistic prediction of source terms from chemical reactions in underground storage tanks, hydrogen combustion in double contained receiver tanks, and process evaluation including the potential for runaway reactions in spent nuclear fuel processing. Model features include user-defined facility rooms, flow path geometry, and heat conductors, user-defined non-ideal vapor and aerosol species, pressure- and density-driven gas flows, aerosol transport and deposition, and structure to accommodate facility-specific source terms. Example applications are presented here.

Motivation and Background

Motivation for this work was to provide an easy-to-use, fast-running, PC-based implementation of mature technology developed for commercial nuclear safety analysis to bring Hanford source term evaluations to a similar level of sophistication. Four key points of the effort are:

- (1) Application of commercial methods at Hanford and the potential benefit to its use elsewhere in the DOE system,
- (2) Delivery of the program to Hanford engineers for in-house use rather than use of a proprietary code by a subcontractor,
- (3) Combining thermal-hydraulic, chemistry, and aerosol models into a single integrated analysis, and
- (4) Flexibility to create modules for facility-specific situations.

The resulting computer program is based upon extensive experience in modeling combined fluid flow, heat transfer, fission product release, and aerosol transport and deposition for accident analysis of commercial nuclear reactors. Example computer programs which contain similar facility models are MAAP 4.0 [Henry, Paik, and Plys, 1994; Schlenger-Faber et al, 1996] and MELCOR [Gauntt et al, 1997]. Recent example applications of these programs to predict hydrogen distribution in large facilities may be found in [Wolf, Holzbauer, and Cron, 1999] and [S.J. Lee et al, 1999].

The computer programs cited above are quite complex and contain detailed models for nuclear reactor primary system and secondary components, but also represent the state-of-the-art for control volume based complex facility models (as opposed to multidimensional flow and heat transfer representations, which are computationally far more complex). This is an appropriate level of sophistication for fuel cycle facility modeling given uncertainties inherent in prediction of chemical reaction and physical entrainment mechanisms for initial release of toxic and radioactive species. However, drawbacks to use of these codes include run time, licensing, user learning curves, relative difficulty in addition of general chemical species not considered in commercial nuclear facilities, and relative difficulty in addition of fuel cycle facility specific source term phenomena.

To address the key points listed above and transfer of this technology to Hanford personnel for analysis of DOE facilities, a generic program named AMAZON was created whose features are described below. AMAZON is essentially a mechanistic/parametric model to predict source term to the environment given the material at risk (tank waste or metallic fuel) by evaluating the release fraction (through a chemical equilibrium model, entrainment rate correlations, or fission product release rate correlations) and leak path factor (aerosol models predict deposition in the source regions and facility regions connected via flow paths).

First use of AMAZON was for analysis of hypothetical runaway organic-nitrate reactions in Hanford waste tanks. AMAZON was extended to create an organic-nitrate consequence model named ORNATE (ORGanic NitrATE) by adding an experimentally-based reaction rate law and fission product release rate equations based on chemical equilibrium. Both general and tank-specific analyses were performed with ORNATE, but because follow-on efforts in characterization and statistical analysis have shown propagating organic-nitrate reactions to not be credible [Meacham et al, 1998], no such examples will be given here.

Further work with AMAZON has been performed under a Quality Assurance program fully compliant with 10CFR50 Appendix B. Behavior of metallic uranium fuel in multi-canister overpack (MCO) containers is modeled via the appropriately-named subroutine MCO and the resulting computer program is named HANSF (HANford Spent Fuel) [Plys et al, 1999]. Its main purpose is evaluation of processing, shipping, and storage of spent nuclear fuel including exothermic chemical reactions of uranium metal and water release by decomposition of hydrates.

Currently, the HADCRT program was created by including a mechanistic model for aerosol release during combustion and post-combustion venting of a double-contained receiver tank. HADCRT may be used for entrainment due to combustion events in multi-compartment facilities. Analysis of these hypothetical events is in progress at the time of this writing.

General Model Description

AMAZON allows compartments in a facility to be individually modeled and connected via an arbitrary network of flow paths, containing (or joined by) a list of heat conductors, much the same as MAAP4 and MELCOR cited above. A region may be either well-mixed or stratified and contain a mixture of gases and aerosols. At present, well-mixed models are used for multiple compartment applications, and the stratified model is a "smoky layer model" used for single compartment fires.

Gases may condense on walls or form aerosols, and aerosols may evaporate. Generally the model assumes thermal equilibrium is maintained between gases and aerosols, but this requirement is relaxed for entrainment during combustion processes. Names and physical properties of the species are user-specified and include curve fits for specific heat, second virial coefficient, heat of vaporization, viscosity, thermal conductivity, etc. Using the non-ideal gas model, water and solvents for example may be represented with sufficient accuracy for tank analyses.

Heat transfer within walls, floors, and internal structures is represented by a one dimensional conduction model. The user specifies thermal transport properties of materials that may be sandwiched together for a conductor of variable properties. Conductor surfaces in a region may be joined in a thermal radiation network. Conductors may also be networked to simulate two or three dimensional heat transfer.

Intercompartmental flow models account for pressure and density differences between regions. One-dimensional compressible flow model with a choking limitation is used for pressure-driven flow. In

large facilities, pressure differences are low and density differences cause counter-current exchange of gases between regions which are represented by correlation of experimental data [Epstein, 1988]. Flow path models include provision for check valves, lifting of covers, one-time failure threshold, and aerosol decontamination by bends and filters. Gases and aerosols are transported via flow paths.

Aerosol deposition is considered in each region through correlations to numerical solutions of the exact equation for the aerosol size distribution and deposition rate [Epstein and Ellison, 1988]. This technique has been extensively validated and greatly simplifies aerosol source term analysis. The particle size distribution follows one of two distribution families for a source-driven or decaying aerosol, or it may be interpolated between them. In this model the aerosol size distribution is the same for all species, which is typically correct for physical entrainment problems, and is a good approximation for aerosols formed by condensation of vapors released by reactive vaporization when the temperature of the reactive material does not vary quickly.

Time-dependent sources of gases and aerosols may be specified on input, or a specific model for sources may be written and easily added to the program architecture as is the case HANSF and HADCRT. Time-dependent boundary conditions such as conductor temperatures, region temperatures, and region pressures may be user-specified. Thus the general AMAZON model can handle source term problems a priori when the feedback between region conditions and the initial source rate is negligible.

Example Calculations

An example application for safety evaluation of the Hanford spent nuclear fuel (SNF) cold vacuum drying (CVD) process is shown here from [Plys et al, 1999]. About 6 MT of SNF are contained in an MCO which is a stainless steel cylinder about two feet in diameter and 12 feet tall inside. During CVD, water outside the MCO keeps the wall at about 50 C and supplies energy for evaporation. Helium injection and vacuum pumping occur according to a process schedule.

Figure 1 is a schematic of regions and heat conductors used to represent an MCO containing Hanford metallic SNF. Basket regions are connected via flow paths, and ports as shown are flow paths to the balance of the system. Each basket contains a network of heat conductors representing either fuel elements or fuel scrap. Fuel elements in a basket form a thermal radiation network, while scrap is modeled by a series of conductors. The MCO-specific model calculates reaction rates between fuel and gases, and calculates thermal conductivity of the porous scrap material (including a radiation component) but most other aspects of this model are generic. Other MCO-specific models include a kinetic model of uranium oxide hydrate thermal decomposition, simulation of the process vacuum pump, and entrainment of oxide particulate.

Figure 2 illustrates histories of temperatures at various elevations and the pressure history during a prolonged vacuum pumping phase of CVD. In these plots time is given in thousands of seconds and the calculation duration is two days; temperature is in degrees Kelvin and pressure is in thousands of Pascals, up to 20,000 Pa or about 3 psi. Fuel is initially covered with a thin film of water after the MCO is drained, and vacuum pumping leads to evaporative cooling. Little water is assumed present on the scrap, which has large reactive surface area relative to fuel in fuel baskets, so scrap dries out early and increases in temperature. Scrap temperature passes through a maximum as the pressure decreases because the kinetic rate of reaction between water vapor and uranium depends upon water vapor pressure. Dryout occurs at about 50,000 seconds and thereafter fuel temperatures increase to steady values while the pressure depends upon the rate of helium injection.

This model is capable of predicting thermal excursions due to runaway reactions between fuel and

oxidant, although the model does not, by scope of design, represent eutectic melting and relocation which is a beyond design basis event. Current calculations demonstrate thermal stability and safety of the process.

Another example calculation is presented here for work in progress to predict the source term from hypothetical combustion accidents in double contained receiver tanks (DCRTs). The example shown here is purely to illustrate model features and does not represent a specific DCRT or accident. Figure 3 presents a schematic of the nodalization, which features four compartments (tank headspace, tank vault, pump pit, and filter pit). A detonation is hypothesized to occur in the tank headspace, which causes entrainment of aerosols from the waste liquid surface and from solids adhering to the wall. Note that detonations are not considered likely by the authors, but deflagrations yield very little aerosol release and it is easier to see results when a detonation is postulated.

Transient histories are illustrated in Figure 4. Pressure and temperature are illustrated over a time period of 100 milliseconds, and reactants are burned within the first 1.6 ms; the pressure scale is given in increments of 0.1 MPa which is effectively in atmospheres, and the temperature scale is in K. The adiabatic, complete combustion temperature and pressure are attained during the burn, and values decrease due to venting and heat transfer to the copious amount of entrained aerosol. Here 11 kg is given as the limiting amount of material at risk, and it is all entrained. Gas concentration and aerosol mass histories are illustrated over a time scale of 2 seconds; the aerosol mass scale is in kg. Over a period of about 0.1s liquid water aerosol is evaporated until a relative humidity of 100% is reached, and this accounts for the plateau achieved by the gas concentrations and total aerosol mass. Masses of liquid waste and solid aerosol are shown as they enter thermal equilibrium (with a time constant of 0.1 s), while the solid line which declines from 11 kg to about 3 kg represents total aerosol at all times. Of the 11 kg entrained, only about 0.3 kg are released to the environment, i.e. about 3% of the initial release actually yields a source to the environment in this case.

Summary

In summary, the AMAZON/ORNATE/HANSF/DCRT tool provides a mechanistic treatment of facility phenomena leading to a source term. It is easy to use and it exemplifies a successful transfer of commercial nuclear technology to engineers on site at Hanford. It provides a consistent framework so that different facilities may be analyzed to a similar level of detail but with pertinent phenomena considered at an appropriate level.

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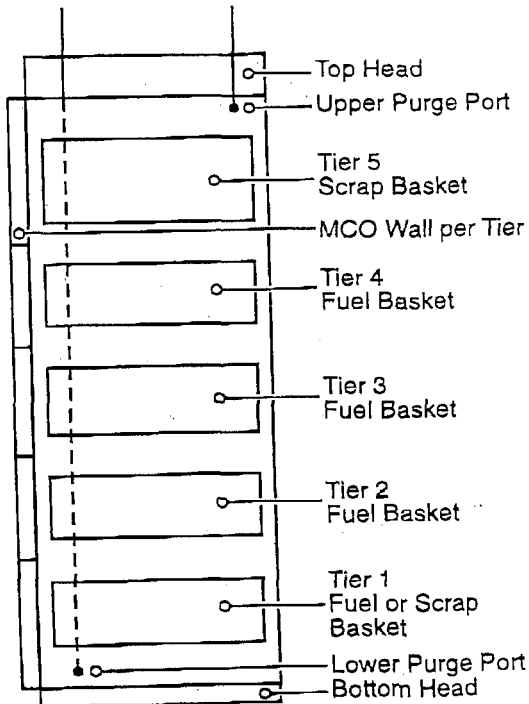
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L. Wolf, H. Holzbauer, and T. Cron, Detailed Assessment of the Heiss Dampf Reaktor Hydrogen-Mixing Experiments E11, Nuclear Technology, Vol. 125, pp. 119-135, February, 1999.

Figure 1. Schematic Multi-Canister Overpack (MCO) Control Volumes and Flow Paths.



MP986085.CDR 6-19-98

Figure 2. Temperature and Pressure Histories for Cold Vacuum Drying Example Problem.

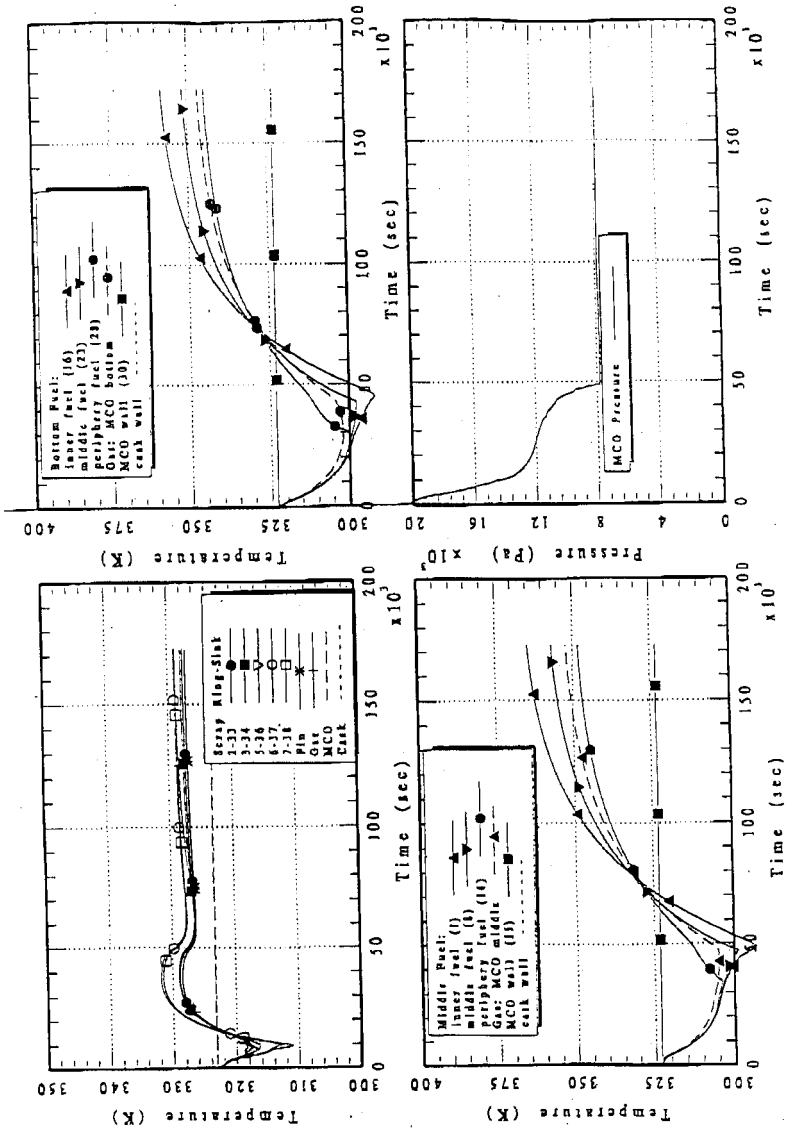


Figure 3. Schematic Nodalization for Double Contained Receiver Tank (DCRT) Example Problem.

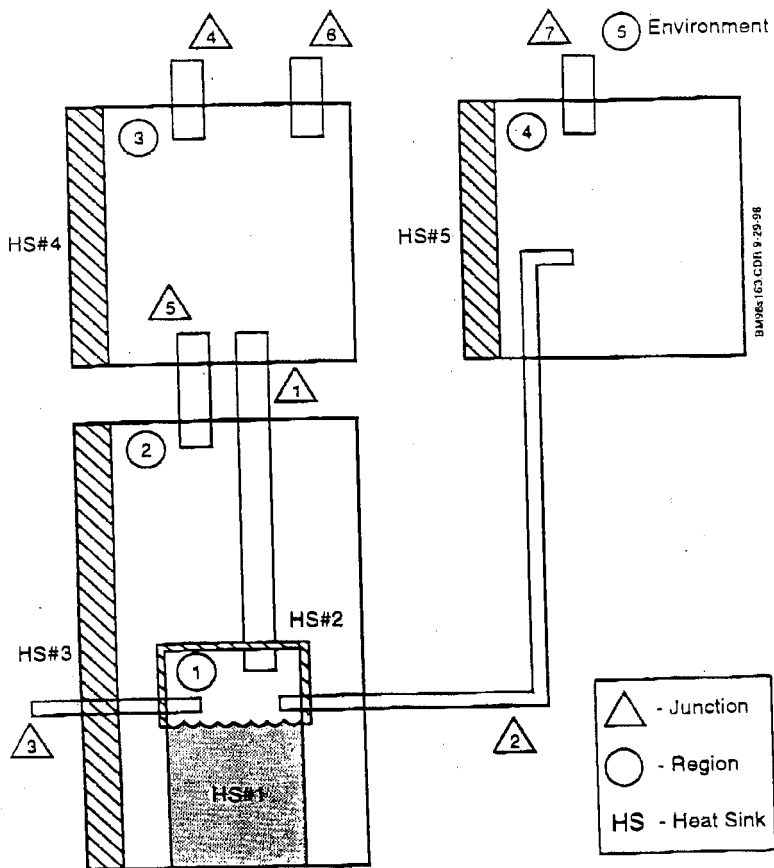


Figure 4. Temperature, Pressure, Concentration, and Aerosol Histories for DCRT Example Problem.

