FAI/04-71, (Volume 1 of 2)

FATE™ 2.0:
FACILITY FLOW, AEROSOL, THERMAL, AND EXPLOSION MODEL
(Improved and Combined HANSF and HADCRT Models)

Submitted To:

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November 2004

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1.0 INTRODUCTION

1.1 Scope and Purpose

This document describes new models that constitute the FATE™ 2.0 computer code (FATE is a Trademark of Fauske & Associates, LLC.), which combines and updates models used for design, off-normal, and accident analysis at fuel cycle facilities. FATE is an acronym for facility Flow, Aerosol, Thermal, and Explosion model. The word facility emphasizes the multiple-compartment nature of the analysis, and the other words used for the acronym signify major capabilities essential to both design and source term analysis of fuel cycle facilities.

FATE 2.0 is a successor code to the HADCRT, HANSF MCO, and HANSF Sludge computer codes, as described in Section 1.4 below. These computer codes have been extensively used for design and safety basis quantification for numerous U.S. Department of Energy projects and facilities at the Hanford site.

This document is a supplement to individual code manuals as follows:

Table 1-1: Summary of Code Versions and References.

User's Manual Hanford Reference	Content	Code Version	Reference
HNF-16784	HADCRT 1.4C Updates	HADCRT 1.4C	[Plys, et al., 2003B]
SNF-3650, Rev. 3	HANSF MCO Models	HADCRT 1.4B	[Plys, et al., 2003A]
SNF-13042, Rev. 0	HANSF Sludge Models	HADCRT 1.4A	[Plys, et al., 2002B]
SNF-10607, Rev. 0	HADCRT 1.4 Models	HADCRT 1.4	[Plys, et al., 2002A]

All model updates to HADCRT 1.4C are reiterated here so that only the HADCRT 1.4 manual is required to fully describe generic facility models.

This document also comprises a major portion of the Quality Assurance (QA) information for FATE 2.0.

1.2 Purpose of Computer Code Update

The purpose of this computer code update is to: (a) Introduce major new general facility phenomena models for combustion, entrainment, thermal radiation, and simulation control, (b) Describe other important generic facility model phenomena and solution technique upgrades, and (c) Correct errors and address user inquiries regarding HADCRT 1.4C.

FATE 2.0 combines general facility models and the HANSF MCO and sludge models to ensure consistency of the platform and minimize long-term maintenance.

1.3 Major FATE Models

New major models introduced by this code version are:

1. Combustion of gases, vapors, and aerosols. Any compound whose properties are given through input may be a fuel, oxidant, or product of gas and aerosol phase reactions. Examples pertinent to DOE facilities include hydrogen, solvent vapors, and metallic aerosols (U metal or U hydride).

2. Entrainment of deposits to form aerosols. General waste types are defined that may be entrained from surfaces by combustion or flow between compartments.

3. Thermal radiation networks. A suite of view factor models is provided to automatically calculate heat transfer in thermal radiation networks.

4. Event-oriented simulation. A set of intervention criteria are defined, allowing scenario definition to proceed in a conditional manner, rather than through a priori specification.

General major models of FATE are:

1. General species. Any element or compound whose properties are input is tracked in mass and energy conservation, in a condensed, gaseous, or aerosol state, and aerosols are in equilibrium with their vapors.

2. Region thermodynamics. Temperature, pressure, and properties of liquid and gas species in a compartment are found by constitutive relations including non-ideal gas modeling.

3. Intercompartmental gas flows. Regions (facility compartments) may be connected in an arbitrary manner via flow paths, and 3 key flow types are considered: Pressure-driven flow, density-driven counter-current flow, and diffusion.

4. Aerosol behavior. Aerosol coagulation, sedimentation, transport, and deposition on pipe bends and filters are considered. Aerosols are also created by boiling.

5. Heat conduction and convection. Heat conductors provide detailed temperature distributions in one dimension and may be linked for 2D or 3D heat flow, and conductors interact with liquids and gases.

6. Sources and time-dependent conditions. Sources of mass and energy may be added, and boundary conditions may be varied as a function of time.

Important new features for user convenience or numerics in this version are:

1. Aerosol bookkeeping for material deposited on HEPAs and bends.
2. Automatic pressure initialization in interconnected regions.
3. Automatic initialization of heat conductor temperatures.
4. Growth of heat conductors by adding material.
5. Implicit heat and mass transfer between heat conductors, pools, and gases.
6. Relative specification of heat conductor elevations.
7. Thermal radiation from heat conductor "fin" surfaces.

1.4 Quality Assurance Status

FATE and its progenitor HADCRT, HANSF MCO, and HANSF Sludge models are created and maintained under the Fauske & Associates, LLC (FAI) QA Program. The present code upgrade and its documentation are performed under FAI procedure FAI-IG-3.7, Maintenance of Configured Computer Programs, and procedures which it references. Section 2.0 describes how QA documentation is organized.

1.5 FATE, HADCRT, and HANSF Computer Code Background and Names

The FATE 2.0 computer program is the successor computer program to the HADCRT 1.4C computer code and its HANSF MCO and Sludge models.

The original scope of HADCRT was to predict combustion and aerosol entrainment phenomena in a single region, the headspace of a Hanford Double Contained Receiver Tank (DCRT), hence the acronym for its name. HADCRT relied upon a large generic set of models for thermodynamics, intercompartmental gas flow, heat convection and conduction, and aerosol behavior, which form the core of a multiple-compartment facility model. The HADCRT specialty models were invoked by the facility model. Users of the general facility model have called the code HADCRT, insofar as they were able to pronounce the acronym.

HANSF is the acronym for HANford Spent Fuel, and the HANSF computer code is invoked by the same facility model for the purpose of modeling Multi-Canister Overpack (MCO) containers with spent metallic nuclear fuel, and for modeling sludge with chemically reactive components. Users of these models have called the code HANSF because it was easier to pronounce, and for project continuity.

All functional capability of the HADCRT 1.4C, HANSF MCO, and HANSF Sludge models is retained by FATE 2.0. However, the original DCRT combustion and entrainment models are considered obsolete because they are superseded by far more general models as described herein.

The name FATE replaces the name HADCRT because the original scope of the DCRT models is now generalized, and the new acronym more accurately reflects the previously existing general scope of the model for facility and source term analysis.

Version number 2.0 is used because the 1.x versions of the HADCRT models are now replaced by a new general suite of models for combustion and entrainment. So, the new name FATE 2.0 reflects an increase in version number followed by renaming the computer code.

1.6 FATE Capability and Application Background

FATE and its progenitor program versions share the same top-level generic capabilities to model heat and mass transfer, fluid behavior, and aerosol behavior in a fuel cycle or chemical processing facility. This generic capability is described in a recent ANS paper [Plys, et al., 2000]. Phenomenological capabilities include:

- Multiple-compartment representation,
- Pressure-driven, counter-current, and diffusion gas flows,
- Transport of gases and aerosols between compartments,
- Vapor-aerosol equilibrium,
- Entrainment of aerosol from liquid and deposited particulate,
- Deposition of aerosols via gravitational sedimentation, impaction, etc.,
- Combustion,
- Heat transfer and condensation on structures, and
- Liquid pool in each compartment exchanging heat and mass with gas and with submerged structures.

Generic models may be used to model normal processes, operational transients, and accidents at fuel cycle facilities such as K basins, the Canister Storage Building (CSB), Tank Farm facilities including underground waste tanks, pits, and multi-room vaults, the future Waste Treatment Plant (WTP), and other facilities such as T-Plant, WESF, WRAP, and PFP. A typical use is to predict radiological consequences of an accident involving combustion, including attenuation of radionuclides within the facility (the so-called leak path factor). Example analyses include double-shell tank gas release (tank bump) analysis [Epstein, et al., 2000], combustion in double-contained receiver tanks [Siciliano and Puigh, 1999], and combustion in the WTP [BNFL and FAI, 1999].

Recent large-scale analyses have been conducted with FATE's HADCRT facility model for the Hanford WTP [Crowe and Lanning, 2002A, 2002B, and 2003]. The first analysis considered a sudden leak of low activity waste (LAW) melter off-gas into the melter facility, tracked hazardous gases and radioactive aerosols throughout the facility including the HVAC system, and was used to predict leakage into occupied areas and the environment. The second predicted temperatures, pressures, and flows resulting from hydrogen combustion in process vessels, including the vessel vent system and HVAC systems for the high level waste (HLW) facility. The third analyzed the impacts of an unplanned pour from the HLW melter, which include local heating of concrete walls and floor by radiation and convection, local gas temperatures and pressurization, and maximum temperatures seen by downstream HEPA filters.

FATE's HANSF/MCO model (HANSF for short) was developed to include specific models for fuel behavior inside a multi-canister overpack (MCO) container for shipping, processing, and storage of Hanford SNF. HANSF has models for fuel oxidation, hydrogen production, hydrate decomposition, ice formation, and numerous other phenomena pertinent to MCO process analyses. Together with the generic capability, HANSF is also capable of estimating the aerosol source term from accidents such as depressurization of an MCO or from hydrogen combustion. Before HANSF/SLUDGE was created, HANSF/MCO was simply referred to as HANSF. Example analyses conducted with HANSF are HNF-2256 [Plys, et al., 1998] and HNF-SD-SNF-CN-023 [Piepho, 2000]. In HNF-2256, a "cradle to grave" analysis of MCO behavior from vacuum drying through dry storage was conducted. Analyses from CN-023 form the basis for the SNF SAR.

FATE's HANSF sludge models were created to model thermal and chemical properties of Hanford SNF sludge within the integral model framework. This allows a complete analysis of behavior internal to sludge, such as oxidation, heat generation, hydrogen generation, and prediction of the sludge temperature profile, coupled with behavior external to sludge, such as calculation of pressures and gas concentrations in a sludge container, exchange flows between a sludge container and a facility, and gas concentrations throughout a facility. Using the same nodalization, the calculations can include accident analysis such as combustion and depressurization, with creation, transport, and deposition of aerosols, providing estimates of the aerosol source term, facility leak path factor, and source to the environment. Analyses of sludge container behavior in transport and at T-Plant are described in [Plys, 2002].

FATE can be used for design and scoping evaluations as well as accident analyses, and indeed it is common to first create a design via scoping and then, via straightforward new inputs, specify an accident scenario. An example of this range of capability is found in [Fuller, 2003], where the sludge model was used to simulate various open port arrangements for a sludge container placed in a cell at T-Plant. A design was found which would prevent the accumulation of a flammable composition in the container, considering simultaneously the buildup of flammable gases in the cell; it was also able to predict the annual water loss rate. This input file was then extended to consider consequences of hydrogen combustion and entrainment from the container, and exposure of the container in a transfer cask to an external fire.

1.7 Ownership

FATE is a trademark of Fauske & Associates, LLC (FAI). The FATE computer code is owned by FAI and is licensed to users. License terms describe license fees and restrictions on the use and dissemination of the code. Licenses were originally written using the computer code names HADCRT and HANSF, but all terms apply to FATE because the computer code is simply renamed.