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Process Options Description for Vitrification Flowsheet Model of INEEL Sodium Bearing Waste

T. T. Nichols

D. D. Taylor

L. Lauerhass

C. M. Barnes

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Process Options Description for Vitrification Flowsheet Model of INEEL Sodium Bearing Waste

**Todd T. Nichols
Dean D. Taylor
Lance Lauerhass
Charles M. Barnes**

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**Idaho National Engineering and Environmental Laboratory
High Level Waste Program
Idaho Falls, Idaho 83415**

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PURPOSE

The purpose of this document is to provide the technical information to Savannah River Site (SRS) personnel that is required for the development of a basic steady-state process simulation of the vitrification treatment train of sodium bearing waste (SBW) at Idaho National Engineering and Environmental Laboratory (INEEL). INEEL considers simulation to have an important role in the integration/optimization of treatment process trains for the High Level Waste (HLW) Program. This project involves a joint Technical Task Plan (TTP ID77WT31, Subtask C) between SRS and INEEL. The work scope of simulation is different at the two sites. This document addresses only the treatment of SBW at INEEL. The simulation model(s) is to be built by SRS for INEEL in FY-2001.

SCOPE

This document provides all the information required a priori for SRS engineers to construct and link unit operation modules in a commercial software simulation application to represent the treatment train for the vitrification of SBW. The information required is of a mid- to high-level nature and consists of the following: 1) a list of specific unit operations, their operating conditions and constraints, and the modeling approaches that will be used in FY-2001 (see Tables I and II); 2) several potential configurations of the unit operations, and their interdependencies via stream connections (see Figure I); and 3) stream compositional makeups (see Table III - VI).

Low-level information, such as assumed partition fractions or separation efficiencies, is not detailed in this document because it is not required for the construction and verification of the simulation. The users' manual supplied by SRS will list values for and explain all such low-level assumptions involved with the simulation's data packs created by SRS. INEEL personnel will coordinate with SRS when selecting values to use for the low-level data during the verification phase of the simulation. The document Savannah River Technology Center (2001) discusses the quality assurance plan for the simulation model.

This document is focused only on the steady-state simulation of the direct vitrification of SBW to be performed in FY-2001. The treatment of newly generated liquid waste (NGLW), tank heels, and solid calcine will not be modeled with the process simulation package in FY-2001, and thus, they are outside the scope of this document.

OBJECTIVES

The purpose of building the simulation model in a commercial software package in FY-2001 is to add thermodynamic equilibrium to the simulation capabilities of the INEEL HLW Program. The modeling of INEEL SBW vitrification is currently performed with linked EXCEL spreadsheets and lacks a physical properties database. The objective for FY-2001 is to perform basic mass and heat balances on individual unit operations and around the entire treatment train. Having an integrated model with a thermodynamic database will increase the ability of INEEL engineers to assess the system-wide impacts of local changes at individual unit operations.

Such capability will help to reduce the life-cycle schedules and costs of HLW projects, which is imperative given the Settlement Agreement commitments and shrinking DOE budgets. There is currently no funding for an integrated pilot plant demonstration of the treatment train, which increases the role of process simulation. Refinements to the physical properties database and unit operation models are planned for the out-years to support future optimization efforts and detailed design of SBW treatment.

Simulation results will be used by engineers and scientists to develop higher-level recommendations for DOE-ID and INEEL program managers regarding the treatment of HLW. As such, it is expected that technical personnel will be the primary end-users of the simulation results, and program management will be an indirect end-user. Simulation will not be used as a formal part of waste form qualification (Nichols, 2000). The reader can refer to Barnes, Lauerhass, Nichols, and Taylor (2000) to learn how the simulation efforts of this project being performed in FY-2001 relate to the project's entire scope and objectives.

SUMMARY

Three potential process configurations will be modeled in the simulator in FY-2001. These are shown in Figure I. All differences between the three configurations reside in the offgas treatment section of the process train. The three configurations were selected to form a reasonable set of unit operations to help assure that INEEL will have models for the process configuration eventually chosen for direct vitrification of SBW. SRS engineers will build three models in the commercial simulation package, one for each configuration.

Table I describes the details of the individual unit operations. A brief overview of each operation is provided, along with the natural phenomena involved, how the phenomena are currently modeled in INEEL's spreadsheet model, the modeling approach SRS plans to use in FY-2001, and constraints/targets. Table II describes the modeling approaches possible for each of the phenomena mentioned in Table I.

Representative compositional makeups of several streams are given in Tables III – VI. The amount of stream information is provided not to over-constrain the simulation results but rather to facilitate a step-wise construction of the unit operations and debugging.

TABLES

Table I: Unit Operation Descriptions

Table II: Phenomena Modeling Approaches

Table III: Representative Compositions of Dilute SBW Feed

Table IV: Representative Compositions in SBW Tank

Table V: Representative Gas Streams

Table VI: Miscellaneous Mass Balance Assumptions

TABLE I: UNIT OPERATION DESCRIPTIONS

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
1. SBW Tank Purpose: Mix SBW (1-3 tank wastes, including UDS) & scrub recycle Phases: Aqueous, solid Primary Species: Ionic species, free acid Key Outputs: Determine precipitation, concentrations of corrosive species (HF, H ⁺ , Cl ⁻—Ref. 0) and solids that may precipitate (recent analyses of solid samples from WM-182, 183, 188 suggest these may include Al, As, Fe, F, Mo, Na, NO ₃ , P, PO ₄ , SO ₄ , SiO ₂ , Zr—Ref. 0, 0) and stream properties for assessment of blending scenarios and equipment/piping sizing & specification (mixing apparatus required?) Op Range: 10-33°C, ambient pressure			
Solid/liquid chemical equilibrium Major species: Al, H, K, Na, NO ₃ Minor species: Ag, As, B, Ba, Ca, Cd, Cr, Fe, Hg, Mo, Ni, Pb, Zr, Zn, Pd, Pu, U, F, Cl, I, PO ₄ , Ru, Se, Si, Sr, SO ₄ , O Salts associated with combinations of ions from the major & minor species lists above Soluble complexes of F ⁻ , Cl ⁻	C. (Black Box)	White or Gray Box	Corrosivity concerns Criticality concerns Presence of tank heel solids would dictate some type of mixing capability in tanks or design measure to prevent precipitation
2. Mixing Tank Purpose: Mix SBW/scrub purge with frit & sugar/carbon/other reductant Phases: Aqueous (inorganic and organic), solid, gas Primary Species: Ionic, gaseous, nitric acid Key Outputs: 2-phase (liquid & solid) properties of stream to melter for mixing requirements (solids assumed to be a pass-through—unaltered by this unit op), equipment and piping sizing & specification; offgas composition; operating temperature of tank; and effect of heating/cooling on reaction/gas phase composition; prediction of liquid-phase reaction rates and their heat generation Op Range: 25-100°C, ambient pressure			
Vapor/liquid chemical equilibrium V/L equilibrium of N ₂ , NO, NO ₂ , HNO ₃ , O ₂ , H ₂ O Chemical equilibrium concentrations of H ₂ , CO, reductant (sugar or formic acid). Temperature dependence of equilibrium limits. Potential heat release from reaction. Decomposition of sulfate to volatile forms (H ₂ SO ₄ /SO ₂ /SO ₃ /H ₂ S). (Provide insight into ways this could be done.)	O. (not modeled)	White or Gray Box	Flammability/explosivity; downstream NO _x treatment
Finite-rate homogeneous chemical reaction Oxidation of sugar/carbon/other reductant to form flammable gases; e.g., H ₂ , CO (Ref. 0). Nitrated organic compounds; e.g., sugar. (Ref. 0)	O. (not modeled)	Gray or Black Box	
Steady state single-phase mixing with volumetric sources Solids concentration in liquid tank effluent. Solids densities for design of mixing capability (Ref. 0).	O. (not modeled)	Gray or Black Box	Slurry mixture going to melter must be spatially and temporally homogenous in solid and liquid

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
3. Melter (joule heated)– evaporation, acid decomposition, glass formation Purpose: Glass formation, acid decomposition, volatiles vaporization Phases: Aqueous (inorganic and organic), solid, gas Primary Species: Aqueous ionic (NO ₃ ⁻ , H ⁺ , OH ⁻ , Cl ⁻ , F ⁻ , SO ₄ ⁻), aqueous molecular (HgCl ₂ , CO ₂ , H ₂ SO ₄ , HCl), Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , H ₂ O, Cl ₂ , SO ₂ , SO ₃ , HF, HCl, HCs[methane, ethane, ethylene, propane, butane, formaldehyde, acetone, benzene, toluene, butadiene, naphthalene Ref 7]), solid (glass formers[SiO ₂ , B ₂ O ₃ , Na ₂ O, Li ₂ O, Fe ₂ O ₃], rad and non-rad metal oxides[Al ₂ O ₃ , CaO, CdO, Fe ₂ O ₃ , FeO, K ₂ O, MnO, Na ₂ O, ZrO ₂ , UO ₂ , P ₂ O ₅], reductant[C ₁₂ H ₂₂ O ₁₁]) Key Outputs: Melter throughput rate and heat requirements/loading; melter offgas, melter offgas solids and glass compositions; glass properties Op Range: 650 – 1300°C, 5 – 12 psia			
Vapor/liquid chemical equilibrium Offgas concentrations of nitrogen oxides, HNO ₃ , speciation of Cs (Cs ₂ O, CsTcO ₄ , CsCl, Cs ₂ CO ₃ , Cs ₂ BO ₂ , CsBO ₂ , CsOH, CsMoO ₄ , CsAlSiO ₄)speciation of Tc (CsTcO ₄ , Tc ₂ O ₇ , HTcO ₄ , TcO ₂ , TcO(OH) ₂ , TcCl ₄ , TcF ₄ , TcF ₆), Sr-90, speciation of Hg (Hg ⁰ , HgO, HgCl ₂ , Hg ₂ I ₂), SO ₂ , SO ₃ , H ₂ SO ₄ , H ₂ S, speciation of Cl (HCl, CaCl ₂ , Cl ₂ , NaCl, KCl, CsCl, SrCl ₂), speciation of I (I ₂), speciation of Ru (Ru ₂ , RuO ₄), HF, F, PICs, CO, CO ₂ , CO ₃ , As, Cd, Pb, Sb, total solids (Ref. 0)	D. (Black Box)	White or Gray Box	Determine concentrations of Cl, Hg, Cs, I, F, NO, NO ₂ , HNO ₃ and other volatiles going to downstream offgas equipment
Finite-rate homogeneous chemical reaction Reduction of noble metals, essential glass forming reactions Effective migration rates of volatiles from glass to melter head space incorporating effects of key melter operating parameters Composition of glass (oxide compounds) leaving melter	C. (Black Box)	Gray or Black Box	Need sufficient residence time/conditions for formation of targeted glass (local equil. mass transfer limited by natural convection) Retain volatile species in glass (e.g., Cs, Tc) Specify glass composition leaving melter to use glass property correlations with composition
Heat transfer between two nondisperse phases Melt rate of cold cap vs temperature and surface area, steady state melter offgas temperature	O. (not modeled)	Black Box	Must maintain cold cap for offgas control ??
Viscous single-phase flow with volumetric sources Flow pattern, rate, residence time, temperature of glass within melter and pour system	O. (not modeled)	Black Box	Melter output glass stream must be flowable to pour into canister
Generation of melter offgas particulates Total solids loading in offgas (to design film cooler), Hg, Cs, Tc, Sr, SO ₄ -2, Cu (for assessment of PCDD/PCDF formation potential)	C. (Black Box)	Black Box	Determine quantity and composition of solids going to downstream offgas equipment to ensure compliance with emissions limits
Liquid droplet entrainment in a gas stream Mass flow rate of fume from glass and/or molten salts to the offgas due to entrainment	C. (Black Box)	Gray or Black Box	Determine liquid carryover with offgas (e.g. sulphate layer)
Waste form properties as functions of processing parameters Glass durability (PCT), viscosity, liquidus temperature, electrical conductivity	O. (not modeled)	Black Box	Target waste site WAC--phase stability, leachability, corrosion Electrical conductivity must be in target range for uniform heating of melter contents. No pooling of metals to avoid short circuit (noble metal content too high, undesirable redox e.g. Fe ⁺² /Fe total > 0.3 is undesirable) Liquidus temperature must be less than operating temperature throughout melter to avoid crystalline phase formation in the

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
			melter and electrical conductivity and flow problems Melter output stream (to-be-glass) must be flowable to pour into canister
Transient thermal conduction Time @ Temperature profiles throughout glass logs (for assessment of phase separation/crystallization potential)	O. (not modeled)	Black Box	The glass transition temperature is dependent upon the cooling history and affects glass durability
4. Cyclone /Knockout (KO) Drum			
Purpose: Gross solids/droplets separation Phases: Solid, gas/Liquid, gas Primary Species: Solid (frit, glass, volatile metals-Cs, Hg), Gas (N2, NO, NO2, O2, CO2, CO, H2, H2O), Aqueous (NO3-, Cl-, F-, H+, H2O, SO4-2, cations from dissolved solids) Key Outputs: Outlet solids loading in gas, outlet gas temperature, PSD of solids Op Range: 350 – 650°C, 5 – 12 psia			
Particle collection by sedimentation Frit, glass, Cs, Hg, salts (in cyclone) Scrub liquor (in KO drum)	C. (Black Box)	Gray or Black Box	Solids loading in gas going to downstream components
Steady state heat exchange between a fluid and its boundary Temperature change of offgas (with solids) during transit through the cyclone	C. (Black Box)	Gray or Black Box	Downstream temperature dependencies (kinetics, heat loads) and MOC constraints
5. Film Cooler			
Purpose: Control solids accumulation on offgas duct wall Phases: Solid, gas Primary Species: Solid (frit, glass, volatile metals-Cs, Hg), Gas (N2, NO, NO2, O2, CO2, CO, H2) Key Outputs: Solids deposition rate, outlet gas temperature, composition and solids loading, diluent (air) injection rate, post-agglomeration PSD of solids Op Range: 350 – 650°C, 5 – 12 psia			
Steady state single-phase mixing with volumetric sources Cooling of offgas solids by injected stream (to determine solids deposition potential) Particle impingement pattern, impaction rate on walls (offgas flowfield and resulting particle trajectories)	O. (not modeled)	Gray or Black Box	Prevent wall fouling from molten particles; ensure aerosol collectibility
Particle impingement due to inertia Frit, glass, Cs, Hg, salts	O. (not modeled)	Gray or Black Box	
Aerosol growth by condensation and agglomeration Size and temperature (“stickiness”) of particles in likely deposition region of offgas ducts	O. (not modeled)	Black Box	
Finite-rate homogeneous chemical reaction Gas phase reactions involving H2O, N2, NO, NO2, O2, CO2, CO, H2	C. (Black Box)	Gray or Black Box	Determine concentrations of NO, NO2, HNO3 going to other offgas system components

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
6. Noxidizer Reduction Chamber			
Purpose: Reduce NO _x to N ₂ Phases: Gas, liquid (fuel) Primary Species: Gas - N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HgCl, HgCl ₂ , HgO, various HCs [set of plausible species includes: acetone, formaldehyde, methane, propane, ethane, ethylene, benzaldehyde, monochloroethane, dichloroethane, benzo(a)pyrene, chlorobenzene, tetrachlorobiphenyl, biphenyl, and 2-3-7-8 TCDD], H ₂ S, SO ₂ , and SO ₃ Liquid - HCs, S Key Outputs: Percent NO _x elimination, outlet gas composition and temperature, NOxidizer fuel rate Op Range: 1100 – 1200°C, 5 – 12 psia			
Gas phase chemical equilibrium NO _x , CO, PIC/HCs, H ₂ S, SO ₂ , SO ₃ , Hg, HgCl, HgCl ₂ , HgO concentrations as a result of NO _x reduction, fuel pyrolysis, and incomplete combustion OR Viscous single-phase flow with volumetric sources (see above) OR Finite-rate homogeneous chemical reaction (see above)	O. (not modeled)	White or Black Box	Reduce concentration of NO _x to acceptable level HC, CO concentrations input to downstream unit operations which control them
OR	O. (not modeled)	Black Box	
OR	C. (Black Box)	Gray or Black Box	
Steady state heat exchange between a fluid and its boundary Required fuel rate to achieve required reduction temperature, and consequent exit gas composition	O. (not modeled)	Gray or Black Box	Downstream temperature dependencies (kinetics, heat loads) and downstream MOC constraints
7. Noxidizer Oxidation Chamber			
Purpose: Oxidize residual CO, HCs to CO ₂ & H ₂ O Phases: Gas Primary Species: Gas - N ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HgCl, HgCl ₂ , HgO, various HCs [set of plausible species includes: acetone, formaldehyde, methane, propane, ethane, ethylene, benzaldehyde, monochloroethane, dichloroethane, benzo(a)pyrene, chlorobenzene, tetrachlorobiphenyl, biphenyl, and 2-3-7-8 TCDD], H ₂ S, SO ₂ , and SO ₃ Key Outputs: Output gas composition (esp. CO, CO ₂ , HCs, Hg speciation, H ₂ S, SO ₂ , SO ₃) and temperature Op Range: 800 – 1000°C, 5 – 12 psia			
Gas phase chemical equilibrium Oxidation of CO, HCs, S, and elemental Mercury OR Viscous single-phase flow with volumetric sources (see above) OR Finite-rate homogeneous chemical reaction (see above—also, N ₂ , NO, NO ₂ oxidation/reduction) OR Finite-rate heterogeneous (or catalytic) chemical reaction (see above)	O. (not modeled)	White or Black Box	Destroy organics in offgas to levels mandated by MACT
OR	O. (not modeled)	Black Box	
OR	C. (Black Box)	Gray or Black Box	
OR	O. (not modeled)	Gray or Black Box	
Steady state heat exchange between a fluid and its boundary	C. (Black Box)	Gray or Black Box	Downstream temperature dependencies (kinetics, heat loads) and downstream MOC constraints

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
Mixture temperature (for kinetic rates), effluent gas temperature			and downstream MOC constraints
8. Venturi Scrubber/Ejector Fume Scrubber Purpose: Remove particulate, acid gases from gas Phases: Aqueous, gas, solid Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HCl, HNO ₃ , H ₂ SO ₄ , HF, melter offgas solids) Aqueous (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, SO ₄ ⁻² , cations from dissolved solids) Key Outputs: Solids loading in gas; output gas & liquid compositions (H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄), temperatures Op Range: 100 – 500°C, 5 – 12 psia			
Venturi scrubber particle collection Solids loading in effluent gas	D. (Black Box)	Gray or Black Box	Minimize solids loading rate/radionuclide carryover to HEPA filters.
Vapor/liquid equilibrium Acid dissociation (HNO ₃ , H ₂ SO ₄ , HF, and HCl) Aqueous Hg speciation (Hg ⁰ , HgCl ₂ , HgCl) Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water OR Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water AND Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases	C. (Black Box)	White or Gray Box	Maintain carryover of Hg to below design levels for downstream GAC beds. Acid gas removal required to meet MACT for downstream processes Minimize liquid carryover to HEPA filters Downstream MOC/process temperature limits
	O. (not modeled)	Gray or Black Box	
	O. (not modeled)	Gray or Black Box	
Liquid droplet entrainment in a gas stream Droplet concentration in offgas going to downstream equipment (HEME/KO Drum)	C. (Black Box)	Gray or Black Box	Minimize liquid carryover to HEPA filters.
9. Packed Bed Quench/Submerged Bed Scrubber/Caustic Scrubber Purpose: Cooling and/or scrub gas with liquid, gross solids separation Phases: Aqueous, gas, solid Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , H ₂ O, HCs, Cl ₂ , SO ₂ , SO ₃ , HF, HCl, HNO ₃), acidic aqueous (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, HSO ₃ ⁻ , HSO ₄ ⁻ , SO ₄ ⁻² , HgCl ₂ , HgCl, Hg ⁺² , cations from dissolved solids), basic aqueous (Na ⁺ , NO ₃ ⁻ , Cl ⁻ , F ⁻ , OH ⁻ , H ₂ O, SO ₃ ⁻² , SO ₄ ⁻² , HgCl ₂ , HgCl, Hg ⁺² , cations from dissolved solids) Key Outputs: Output gas & liquid temperatures, compositions (H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄); solid & liquid loading in gas; UDS in liquid Op Range: 100 – 1200°C, 5 – 12 psia			
Particle collection by sedimentation Solids loading in effluent gas	C. (Black Box)	Gray or Black Box	Minimize solidsloading rate/radionuclide carryover to HEPA filters Characterize UDS in recycle streams

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
Vapor/liquid equilibrium Acid dissociation (HNO ₃ , H ₂ SO ₄ , HF, and HCl) Aqueous Hg speciation (Hg ⁰ , HgCl ₂ , HgCl) Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water OR Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water AND Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases	C. (Black Box)	White or Gray Box	Maintain carryover of Hg to below design levels for downstream GAC beds. Acid gas removal required to meet MACT for downstream processes Minimize liquid carryover to HEPA filters Downstream MOC/process temperature limits
Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water	O. (not modeled)	Gray or Black Box	
Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases	O. (not modeled)	Gray or Black Box	
Liquid droplet entrainment in a gas stream Droplet concentration in offgas going to downstream equipment	C. (Black Box)	Gray or Black Box	Minimize liquid carryover to HEPA filters.
10. Spray Quench Purpose: Rapid cooling of gas with possibility of a single, dry exit stream Phases: Aqueous, gas, solid Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg), aqueous (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, SO ₄ ²⁻ , cations from dissolved solids) Key Outputs: Output gas & liquid temperatures, compositions (H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄), presence/non-presence of liquid; solid & liquid loading in gas; UDS in liquid Op Range: 100 – 500°C, 5 – 12 psia			
Particle collection by sedimentation Solids loading in effluent gas	C. (Black Box)	Gray or Black Box	Minimize solidsloading rate/radionuclide carryover to HEPA filters Characterize UDS in recycle streams
Vapor/liquid equilibrium Acid dissociation (HNO ₃ , H ₂ SO ₄ , HF, and HCl) Aqueous Hg speciation (Hg ⁰ , HgCl ₂ , HgCl) Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water OR Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous	C. (Black Box)	White or Gray Box	Maintain carryover of Hg to below design levels for downstream GAC beds. Acid gas removal required to meet MACT for downstream processes Minimize liquid carryover to HEPA filters Downstream MOC/process temperature limits Accommodate possible liquid phase accumulation in quench vessel
Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous	O. (not modeled)	Gray or Black Box	

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
phases Vaporization/condensation of water AND Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases	O. (not modeled)	Gray or Black Box	
Liquid droplet entrainment in a gas stream Droplet concentration in offgas going to downstream equipment	C. (Black Box)	Gray or Black Box	Impact of liquid in gas phase to downstream processes Minimize liquid carryover to HEPA filters
11. HydroSonic Scrubber Purpose: Remove particulate Phases: Aqueous, gas, solid Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, melter offgas solids), aqueous droplet (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, SO ₄ ⁻² , cations from dissolved solids) Key Outputs: Output gas & liquid temperatures, compositions (H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄); solids loading in gas, net scrub liquor evaporation Op Range: 100 – 200°C, 5 – 12 psia			
Vapor/liquid equilibrium Acid dissociation (HNO ₃ , H ₂ SO ₄ , HF, and HCl) Aqueous Hg speciation (Hg ⁰ , HgCl ₂ , HgCl) Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water OR	C. (Black Box)	White or Gray Box	Maintain carryover of Hg to below design levels for downstream GAC beds. Acid gas removal required to meet MACT for downstream processes Minimize liquid carryover to HEPA filters Downstream MOC/process temperature limits Accommodate possible liquid phase accumulation in quench vessel
Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water AND		Gray or Black Box	
Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases		Gray or Black Box	
Steady state single-phase mixing with volumetric sources Vaporization/condensation of water Temperature/saturation level of offgas after mixing with throttled steam	O. (not modeled)	Gray or Black Box	Conditions required to model particle collection
Submicron particle collection by steam condensation Solids loading in effluent gas	O. (not modeled)	Gray or Black Box	Minimize solids loading rate/radionuclide carryover to HEPA filters

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
Droplet concentration in offgas going to downstream equipment			
12. Mercury Removal by GAC Adsorption			
Purpose: Remove Hg & organics Phases: Gas Primary Species: Hg species, trace organics, other gas species Key Outputs: Concentrations of Hg and I-129 species in offgas Op Range: 100-200°C, ≈ 5 psia (subatmospheric)			
Adsorption Hg ⁰ , HgCl ₂ , and organics	D. (Black Box)	Black Box	Emissions data for permit applications
Finite-rate heterogeneous (or catalytic) chemical reaction NO _x oxidation of C in GAC bed	O. (not modeled)	Gray or Black Box	Avoid ignition of bed due to heats of reaction from catalytic reactions of NO _x with the sorbent
13. Settling Tank/Scrub Collection Tank			
Purpose: Collect scrub liquor, dissolve solids from scrubber to equilibrium concentration, settle out remainder to reduce solids in streams which originate from the tank (e.g., ion exchange feed); Precipitate Hg out of solution Phases: Gas, aqueous, solids Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, melter offgas solids) Aqueous (NO ₃ ⁻ , CO ₃ ²⁻ , Ca ²⁺ , Cl ⁻ , F ⁻ , H ⁺ , Hg, Hg ²⁺ , H ₂ O, SO ₄ ²⁻ , S ²⁻ , cations from dissolved solids), solids species from melter offgas, CaS Key Outputs: Equilibrium TDS, UDS loading in scrub liquor, UDS composition (to provide design basis for required liquid/solid separations), gas composition, Hg concentration in liquid effluent, precipitation rate of HgS Op Range: 50-80°C (same as scrub temperature), 5 – 12 psia			
Gas/liquid/solid equilibrium HNO ₃ , H ₂ CO ₃ , HCl, HF, H ₂ O, H ₂ SO ₄ , CaS, HgS, CaCl ₂ , CaF ₂ , CaCO ₃ , CaSO ₄ , UDS and condensed volatiles/semivolatiles from melter offgas in scrub liquor, speciation of Cs (Cs ₂ O, CsTeO ₄ , CsCl, Cs ₂ CO ₃ , Cs ₂ BO ₂ , CsBO ₂ , CsOH, CsMoO ₄ , CsAlSiO ₄), speciation of Tc (CsTcO ₄ , Tc ₂ O ₇ , HTcO ₄ , TcO ₂ , TcO(OH) ₂ , TcCl ₄ , TcF ₄ , TcF ₆), speciation of Hg (Hg ⁰ , HgO, HgCl ₂ , Hg ₂ I ₂), , , speciation of I (I ₂), speciation of Ru (Ru ₂ , RuO ₄), CaS, HgS, CaCl ₂ , CaF ₂ , CaCO ₃ , CaSO ₄ (Cs, Tc, Ru, I from Ref. 0)	O. (not modeled)	White or Gray Box	Prevent buildup of regulated species (e.g., Hg) and consequent carryover into downstream offgas system components Define composition of feed streams to secondary waste treatment Define composition of recycle streams Immobilize Hg in a solid form which won't leach from grout
OR Solid/liquid chemical equilibrium UDS and condensed volatiles/semivolatiles from melter offgas in scrub liquor, H ₂ O, speciation of Cs (Cs ₂ O, CsTeO ₄ , CsCl, Cs ₂ CO ₃ , Cs ₂ BO ₂ , CsBO ₂ , CsOH, CsMoO ₄ , CsAlSiO ₄), speciation of Tc (CsTcO ₄ , Tc ₂ O ₇ , HTcO ₄ , TcO ₂ , TcO(OH) ₂ , TcCl ₄ , TcF ₄ , TcF ₆), speciation of Hg (Hg ⁰ , HgO, HgCl ₂ , Hg ₂ I ₂), speciation of I (I ₂), speciation of Ru (Ru ₂ , RuO ₄), CaS, HgS, CaCl ₂ , CaF ₂ , CaCO ₃ , CaSO ₄ (Cs, Tc, Ru, I from Ref. 0)	C. (Black Box)	White or Gray Box	
AND Vapor/liquid equilibrium	C. (Black Box)	White or Gray Box	

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
HNO ₃ , H ₂ CO ₃ , HCl, HF, H ₂ O, H ₂ SO ₄			
Particle collection by sedimentation Hg and solids concentration in scrub liquor to recycle and to purge (grouting)	O. (not modeled)	Gray or Black Box	Characterize UDS in recycle streams Solids concentration in IX column feed must not exceed limit
14. Ion Exchange			
Purpose: Remove contaminants Cs, Sr (and possible Tc and I) from scrub purge Phases: Aqueous Primary Species: Cs, Sr, (Tc and I), and non-rad exchangeable cations (Ca, Na, Mg, K, ...) in scrub liquor Key Outputs: Column design parameters; and rad & hazardous species concentrations in secondary waste (Cs-137, Sr-90, Tc-99, I-129) Op Range: 70-80°C (same as scrub temperature), ambient pressure			
Adsorption Cs, Sr, Tc, I, and competing cations (Ca, Na, Mg, K)	D. (Black Box)	Black Box	Secondary waste meets its disposal WAC specification for rad
15. Scrub Purge Grout Mix Tank			
Purpose: Mix grout additives and ion exchanged scrub purge; neutralization Phases: Aqueous, solid, gas Primary Species: NO ₃ ⁻ , SO ₄ ⁻² , Na ⁺ , Cl ⁻ , CaO, Ca(OH) ₂ , NaOH, Radionuclides, Hg, Cd, As, Ba, Pb, Cr, Key Outputs: Provide design basis for grout system and waste form composition; determine cooling needs of tank Op Range: 70-100°C, ambient pressure			
Vapor/liquid chemical equilibrium Acid/base neutralization (H ⁺ , OH ⁻) and attendant heat release Heats of mixing and formation for major salt species: CaCl ₂ , CaF ₂ , CaO, Ca(NO ₃) ₂ , Ca(OH) ₂ , CaSO ₄ , HCl, HF, HNO ₃ , H ₂ O, H ₂ SO ₄ , NaCl, H ₂ F, NaOH, NaNO ₃ , Na ₂ SO ₄ Vaporization/condensation of water	O. (not modeled)	White or Gray Box	pH of mixture must satisfy constraint for proper grout recipe used Secondary waste meets its disposal WAC; maintain flowability of mixture for pouring into canisters
Steady state heat exchange between a fluid and its boundary Mixture temperature rise due to heats of neutralization and solution	O. (not modeled)	Gray or Black Box	Grout mixture temperature must be maintained below boiling
Waste form properties as functions of processing parameters Acceptability/non-acceptability of grout mixture	O. (not modeled)	Gray or Black Box	Grout must set within reasonable time Grout compressive strength must satisfy disposal site criteria Leachability of RCRA toxic metals must be within LDR limits
16. HEME (mist eliminator, demister)			
Purpose: Collect liquid droplets remaining in offgas (and solids which they contain) prior to final HEPA filtration and Hg removal in GAC columns Phases: Gas, liquid Primary Species: Gas (N ₂ , O ₂ , Ar, CO ₂ , H ₂ O, NO _x), liquid (scrub liquor—HNO ₃ or NaOH, water, HCl, H ₂ SO ₃ , H ₂ SO ₄ , dissolved/undissolved solids in scrub liquor from melter offgas) Key Outputs: Liquid loading and temperature in gas upstream of pre-HEPA gas heater Op Range: 50-175°C, 5 – 12 psia			
Vapor/liquid equilibrium Acid dissociation (HNO ₃ , H ₂ SO ₄ , HF, and HCl) Aqueous Hg speciation (Hg ⁰ , HgCl ₂ , HgCl) Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous	C. (Black Box)	White or Gray Box	Minimize carryover of liquid droplets from venturi or hydrosonic scrubber to prevent fouling of GAC columns and wetting of HEPA filters Minimize solids loading rate/radionuclide carryover to HEPA filters

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
phases Vaporization/condensation of water OR Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water AND Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases			
Interphase mass transfer with one phase disperse Partitioning of NO ₂ , HNO ₃ , CO ₂ , CO, Hg, HgCl ₂ , HgCl, H ₂ O, HCl, HF, H ₂ SO ₄ , SO ₂ , SO ₃ between gas and aqueous phases Vaporization/condensation of water		Gray or Black Box	
AND Interphase heat transfer with one phase disperse Vaporization of water Heat transport in aqueous & gas phases		Gray or Black Box	
Vapor/liquid equilibrium N ₂ , O ₂ , Ar, CO ₂ , H ₂ O, NO _x , HNO ₃ or NaOH, H ₂ O, HCl, H ₂ SO ₃ , H ₂ SO ₄ , and acid salts TDS in liquid	C. (Black Box)	White or Gray Box	Minimize offgas volume to reduce size of downstream equipment Acid gas removal required to meet MACT for downstream processes
17. HEPA Filter Bank/Prefilter Purpose: Collect all particulate remaining in offgas prior to discharge to the atmosphere Phases: Gas, solid Primary Species: Gas (N ₂ , O ₂ , Ar, CO ₂ , H ₂ O, NO _x), solids species from melter offgas Key Outputs: Solids loading rate in HEPA filters, solids loading in plant offgas discharge to atmosphere (solid composition of particulate is obtained as a pass-through) Op Range: 20 – 100°C, 5 – 12 psia			
Particle removal from gas by HEPA filtration Total solids, radionuclide, and hazardous species concentrations in stack gas	C. (Black Box)	Gray or Black Box	Control total particulate loading, annual particulate discharge, and specie-specific discharges to below regulatory limits Control specie-specific radionuclide discharges to below the regulatory limits
18. Gas Heater/Cooler Purpose: Raise or lower offgas temperature to satisfy downstream equipment constraints (e.g., to prevent wetting of HEPA filters) Phases: Gas Primary Species: Gas (N ₂ , O ₂ , Ar, CO ₂ , H ₂ O, NO _x) Key Outputs: Offgas temperature, power input or heater or outlet temperature of heating fluid Op Range: 150-200°C, 5 – 12 psia			
Steady state heat exchange between two fluids in a heat exchanger Exit temperature of heated offgas	C. (Black Box)	Gray or Black Box	Temperature of gas entering HEPA filters and GAC beds must exceed the dew point by a prescribed minimum Temperature of gas entering blowers must not exceed operational temperature limits
19. Condenser/Entrainment Separator Purpose: Lower offgas temperature below the dewpoint to condense out water vapor and thus reduce gas volume Phases: Gas, liquid Primary Species: Gas (N ₂ , O ₂ , Ar, CO ₂ , H ₂ O, NO _x), liquid (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, SO ₄ ²⁻) Key Outputs: Offgas temperature, cooling load or outlet temperature of cooling fluid, water condensation rate Op Range: 25 – 200°C, 5 – 12 psia			

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
Vapor/liquid equilibrium Rate of condensation of water	C. (Black Box)	White or Gray Box	Recover a target fraction of the water vapor present in the offgas (in the event that recovery of water becomes an objective) Reduce volume of offgas to limit required size of downstream components
Steady state heat exchange between a fluid and its boundary Rate of cooling of offgas	O. (not modeled)	Gray or Black Box	
20. Evaporator			
Purpose: Concentrate melter feed, reduce thermal load of melter Phases: Aqueous, gas, solid Primary Species: Gas (N ₂ , NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HgCl ₂ , HCl, HNO ₃ , H ₂ SO ₄ , HF), aqueous (NO ₃ ⁻ , Cl ⁻ , F ⁻ , H ⁺ , H ₂ O, SO ₄ ²⁻ , Hg ⁺² , HgCl ₂ , cations from dissolved solids in feed), solid (UDS in feed, scaling deposits[CaCO ₃ , SiO ₂], precipitates formed by over concentration of the feed) Key Outputs: Overhead (gas) and concentrate (liquid) temperatures and compositions (H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄ , CO ₂ , CO, Hg, HgCl ₂); presence/non-presence, composition, and concentration of solid precipitates in concentrate, presence/non-presence of scale deposits; UDS concentration in concentrate, pressure drop through the evaporator Op Range: 25 – 125°C, 10 – 12 psia			
Two-phase flow with heat transfer Evaporation rate of water from evaporator feed	O. (not modeled)	Gray or Black Box	Predict water loss to determine melter heat duty
Gas/liquid/solid equilibrium Partitioning of NO ₂ , CO ₂ , Hg, HNO ₃ , HCl, HF, H ₂ O, H ₂ SO ₄ , Hg, HgCl ₂ , H ₂ BO ₃ , and acid salts between evaporator bottoms and overheads Precipitation rates of nitrate, sulfate, chloride, fluoride, phosphate salts. Scaling deposits of CaCO ₃ , SiO ₂ (Ref 6) Soluble complexes of F ⁻ and Cl ⁻ with Al ⁺³ , Cr ⁺³ , Fe ⁺³ , Zr ⁺⁴ , H ₂ BO ₃ OR Vapor/liquid chemical equilibrium Partitioning of NO ₂ , CO ₂ , HNO ₃ , HCl, HF, H ₂ O, H ₂ SO ₄ , Hg, HgCl ₂ , and acid salts between evaporator bottoms and overheads Partitioning of Hg between elemental, HgCl ₂ , and HgCl AND Solid/liquid equilibrium Precipitation rates of nitrate, sulfate, chloride, phosphate, fluoride salts	O. (not modeled)	White or Gray Box	Determine composition of evaporator overheads for evaluating MACT compliance of post-offgas system effluent Determine composition of feed to melter to determine melter offgas composition, suitability of feed to melter, and resulting glass properties
	C. (Black Box)	White or Gray Box	
	O. (not modeled)	White or Gray Box	
21. WESP (Wet Electrostatic Precipitator)			
Purpose: Collect liquid droplets remaining in offgas (and solids which they contain) prior to final HEPA filtration and Hg removal in GAC columns Phases: Gas, liquid Primary Species: Gas (N ₂ , CO ₂ , H ₂ O, NO _x), liquid (scrub liquor—HNO ₃ or NaOH, water, HCl, H ₂ SO ₃ , H ₂ SO ₄ , dissolved/undissolved solids in scrub liquor from melter offgas) Key Outputs: Liquid loading and temperature in gas upstream of pre-HEPA gas heater Op Range: 50-175°C, 5 – 12 psia			
Particle collection by wet electrostatic precipitation Solids loading in effluent gas		Gray or Black Box	Minimize solids loading rate/radionuclide carryover to HEPA filters.
Vapor/liquid equilibrium	C. (Black Box)	White or Gray Box	Maintain carryover of Hg to below design levels for downstream

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HgCl ₂ , H ₂ O, HCl, HNO ₃ , HF, H ₂ SO ₄			GAC beds. Acid gas removal required to meet MACT for downstream processes Minimize liquid carryover to HEPA filters Downstream MOC/process temperature limits
22. SCR(Selective Catalytic Reduction)			
Purpose: Reduce NO _x to N ₂ /oxidize unburned hydrocarbons and CO Phases: Gas Primary Species: Gas (N ₂ , NO, NO ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, various HCs) Key Outputs: Percent NO _x elimination/percent HC/CO elimination, outlet gas composition and temperature, ammonia injection rate, ammonia slip to the outlet gas, NO _x oxidizer fuel rate, oxygen/air injection rate Op Range: 400 – 450°C, 5 – 12 psia			
Gas phase chemical equilibrium NO _x , CO, PIC, HC, H ₂ S, SO ₂ , SO ₃ , Hg, HgCl ₂ , HgO, NH ₃ concentrations as a result of NO _x reduction, fuel pyrolysis, and incomplete combustion	O. (not modeled)	White or Black Box	Reduce concentration of NO _x to acceptable level HC, CO concentrations input to downstream unit operations which control them Hg speciation and concentrations to downstream unit operations
OR Viscous single-phase flow with volumetric sources (see above)	O. (not modeled)	Black Box	
OR Finite-rate homogeneous chemical reaction Reduction of gaseous NO _x by injected ammonia: Reduction of gaseous NO _x by injected ammonia: Oxidation of PICs, HCs Oxidation/reduction of Hg, HgCl ₂ , HgCl, HgO	C. (Black Box)	Gray or Black Box	
OR Finite-rate heterogeneous (or catalytic) chemical reaction (see above)	C. (Black Box)	Gray or Black Box	
Steady state heat exchange between a fluid and its boundary Mean gas temperature in reaction chamber	O. (not modeled)	Gray or Black Box	Downstream temperature dependencies (kinetics, heat loads) and downstream MOC constraints
23. Acid Fractionator (distillation column)			
Purpose: Recover HNO ₃ from evaporator overheads Phases: Gas, liquid Primary Species: HNO ₃ , HCl, HF, H ₂ O, Hg, HgCl ₂ , H ₂ SO ₄ , SO ₂ , SO ₃ Key Outputs: Gas and liquid output composition and temperature Op Range: 90 -- 115°C, 10 -- 12 psia			
Vapor/liquid equilibrium HNO ₃ , HCl, HF, H ₂ O, Hg, HgCl ₂ , H ₂ SO ₄ , SO ₂ , SO ₃	C. (Black Box)	White or Gray Box	Stack emission standards for NO _x Chloride and fluoride concerns for downstream MOCs and possibly grout quality

Phenomena	Current INEEL Approach (refer to Table II)	Planned SRS Approach For FY-2001 (refer to Table II)	Constraints/Targets
24. Thermal Catalytic Oxidizer Purpose: Burn off hydrocarbons (HCs) generated from upstream operations (e.g., melter) Phases: Gas Primary Species: Gas - N ₂ , O ₂ , CO ₂ , CO, H ₂ , Hg, HgCl, HgCl ₂ , HgO, various HCs [set of plausible species includes: methane, ethane, ethylene, propane, butane, formaldehyde, acetone, benzene, toluene, butadiene, naphthalene Ref 7], H ₂ S, SO ₂ , and SO ₃ Key Outputs: Gas output composition going to stack Op Range: 800-1100°C, 5 – 12 psia			
Finite-rate heterogeneous (or catalytic) chemical reaction OR Gas phase chemical equilibrium HC/CO oxidation reactions	C. (Black Box)	White or Black Box	Stack emission standards for HCs

Notes: 1 - “O” is the default designation for “not modeled” - there is no “O” modeling approach entry in any of the phenomena listed in Table II; 2 - The changeout frequency of a HEPA depends on the PSD of the gas, and the impact of the PSD increases dramatically if it includes the submicron range. Consequently, we will not attempt to theoretically determine the PSD of gas streams until there is evidence that the melter off gas includes significant quantities of solid particles or liquid droplets in the submicron range; 3 - only one of unit operations #8 and #11 will be used, not both.

References: 1 - Barnes (2000a); 2 - Barnes (2000b); 3 - Patterson (1999); 4 - Welland (1997); 5 - Langowski, Darab, and Smith (1996); 6 - Schindler (1998); 7 - Soelberg (2001).

TABLE II: PHENOMENA MODELING APPROACHES

Approaches	Important Parameters
Adsorption	
This involves physical (reversible) and chemical (usually irreversible) adsorption.	
<p>B. (Gray Box 1)</p> <ul style="list-style-type: none"> - An isotherm (such as Freundlich or Langmuir) is used to correlate the solid phase mass ratio (solute/sorbent) to the equilibrium solute concentration - The Thomas kinetic equation is developed from the isotherm to estimate effluent solute concentration based upon influent solute concentration, rate constant, maximum solid phase mass ratio, mass of sorbent, throughput volume, and the flow rate. 	(parameters): Parameters for the Thomas equation
<p>C. (Gray Box 2)</p> <ul style="list-style-type: none"> - A semi-empirical partition coefficient dependent upon several parameters is used to determine effluent solute concentration 	$f_i(\text{param1, param2, ...})$ Partition coefficient dependent upon parameters 1, 2, and
<p>D. (Black Box)</p> <ul style="list-style-type: none"> - Vendor data provides column design parameters based upon INEEL's designated throughputs and removal efficiency 	
Aerosol growth by condensation and agglomeration	
<p>This involves the coupling of three fundamental phenomena:</p> <ul style="list-style-type: none"> - Homogeneous nucleation of particles (liquid or solid) from a supersaturated gas - Heterogeneous nucleation/condensation of vapor from a supersaturated gas on an existing aerosol - Agglomeration growth of an aerosol under the influences of shear and Brownian diffusion <p>An aerosol containing a condensable vapor is cooled to a saturation ratio above 1.0. The vapor changes phase to liquid or solid, either through homogeneous nucleation or through condensation on pre-existing particles. All particles grow by collision and agglomeration through the mechanisms listed above. As a result of the particles' growth, their collectability and/or deposition tendency change.</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - The aerosol PSD is represented as a discrete function of spatial position, time, and particle size, $n(x_i, t, d_p)$ - A general dynamic equation (GDE) for the discrete function 'n' is written with terms to account for diffusion, advection, condensation growth, agglomeration growth diffusion account, and particle body forces - Suitable functions are used to represent source terms in the GDE - The GDE is solved numerically for n 	TBD
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Approximate the GDE by retaining only the terms for coagulation and condensation - Assume a similarity solution ("self-preserving" PSD) and develop estimates the required terms in the GDE - Solve the resulting equation for N_{∞}(total particle concentration) and hence for $n(d_p)$ via the assumed self-preserving functional form 	TBD
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Assume that aerosol growth dynamics result in a PSD of known form (e.g., log-normal, bi-modal 	d_m, σ : Parameters which describe a standard PSD (mean particle diameter and standard deviation of a log-normal distribution)

Approaches	Important Parameters
log-normal, etc.) - Obtain key parameters in the assumed PSD from measurements, assumption, etc. (e.g., mean particle diameter and standard deviation of a log-normal distribution) - Assume that aerosol growth ceases after the above form is reached	
Finite-rate heterogeneous (or catalytic) chemical reaction	
Chemical species present in a fluid (gas or liquid) diffuse to the surface of a second phase (liquid or solid), react at a finite rate, and are consumed to form other chemical species. Concentrations of all affected species change in the mixture with time as they are produced or consumed and diffuse to and from the bulk fluid at finite rates. The multi-dimensional (continuum) aspects of the underlying fundamental phenomena are collapsed into a lumped-parameter form that is assumed applicable throughout the reaction region.	
A. (White Box) - Use approach A. (White Box 1) under <i>Viscous single-phase flow with volumetric sources</i> to simulate advective diffusion within the fluid. - Represent the phase interface(s) as boundaries in the computational mesh with appropriate boundary conditions representing heterogeneous/catalytic rate expressions appropriate for the interfaces. - Calculate overall reaction rates and average outflow compositions and flow rates by numerical integration over appropriate surfaces in the computational mesh.	CFD param: (see “Important Parameters” for <i>Viscous single-phase flow with volumetric sources</i> , approach A. (White Box 1)) $k_i(T, c_i, A)$: Heterogeneous kinetic rate expressions as functions of (temperature), (reactant concentration at reaction surface), and (reaction surface area per unit volume) for reactions deemed important
B. (Gray Box) - Estimate diffusion rates and heterogeneous reaction rates from macroscopic parameters (bulk concentrations, pressure, temperature, Reynolds numbers, Peclet numbers, etc.) based on transport theory (e.g., Chapman-Enskog, correlations (e.g., Thiele modulus), etc. - Determine whether heterogeneous reaction rate is transport or kinetically limited - Assume less-limiting step to be infinitely fast and calculate reaction rates using lumped-parameter equations. - Calculate exit concentrations of all species based on (a) residence times, (b) calculated effective reaction rates, and (c) quasi-equilibrium in fast reactions	$k_i(T, c_i, A)$: Heterogeneous kinetic rate expressions as functions of (temperature), (reactant concentration at reaction surface), and (reaction surface area per unit volume) for reactions deemed important D_i : Effective diffusion coefficients for individual species in fluid
Finite-rate homogeneous chemical reaction	
This involves the same phenomena listed under <i>Viscous single-phase flow with volumetric sources</i> ; however, the continuum aspects of the phenomena are simplified. Chemically reacting species present in a fluid (gas or liquid) mix by convection and diffusion, react at a finite rate, and are consumed to form other chemical species. Concentrations of all affected species change in the mixture with time as they are produced or consumed and diffuse to and from the bulk fluid at finite rates. The multi-dimensional (continuum) aspects of the underlying fundamental phenomena are collapsed into a lumped-parameter form that is assumed applicable throughout the reaction region.	
A. (White Box) - Use approach A. (White Box 1) under <i>Viscous single-phase flow with volumetric sources</i> to simulate advective diffusion within the fluid. - Represent the homogeneous reactions as volumetric sources terms with appropriate homogeneous rate expressions. - Calculate overall reaction rates and average outflow compositions and flow rates by numerical integration over appropriate surfaces in the computational mesh.	CFD param: (see “Important Parameters” for <i>Viscous single-phase flow with volumetric sources</i> , approach A. (White Box 1)) $k_i(T, c_i)$: Homogeneous kinetic rate expressions as functions of (temperature) and (reactant concentration) for all reactions deemed important

Approaches	Important Parameters
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Estimate diffusion and kinetic rates of all reactions deemed important - Partition reaction set into (a) fast reactions which can be assumed to be equilibrated, (b) slow reactions which must be treated as non-equilibrated (i.e., rate limited) - Use approach A. (White Box) under <i>Liquid phase chemical equilibrium</i> or approach A. (White Box) under <i>Gas phase chemical equilibrium</i> for the equilibrium calculations as appropriate - Determine whether reaction rate is transport or kinetically limited - Assume less-limiting step to be infinitely fast and calculate effective reaction rates using lumped-parameter equations. - Determine a suitable computational timestep (should not exceed the time scale of the fastest processes being treated as being rate limited) - Calculate exit concentrations of all species based on (a) residence times, (b) calculated effective reaction rates, and (c) quasi-equilibrium in fast reactions 	<p>$k_i(T)$: Kinetic rate constants for reactions deemed to be important</p> <p>D_i: Effective diffusion coefficient for individual species in fluid</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Use stoichiometric ratios, empirical reaction extent factors, and/or product conversion ratios to calculate the conversion of reactants to products in the mixture (e.g., in oxidation of NO_x to NO₃- the fractions of NO and NO₂ in the initial mixture which are converted to NO₃- are specified and the resulting final mixture composition is calculated from this). 	<p>f_i: Empirical fractional conversion of species i or extent of reaction i</p>
Gas/liquid/solid equilibrium	
<p>This involves coupling several phenomena:</p> <ul style="list-style-type: none"> - Vapor/liquid equilibrium - Solid/liquid equilibrium - Chemical equilibrium in each of the three phases <p>All species in the three phases reach thermodynamic equilibrium at the temperature and pressure of the mixture quickly relative to the time step of the simulation. The interphase transfer of species and the intraphase equilibria are solved simultaneously. The activities of all solid species are assumed to have a value of one.</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients and gas phase fugacity coefficients using appropriate models (e.g., NRTL for aqueous phase, equation of state for gas phase). - Equilibrium constants (solid solubility, VLE, and intraphase chemical reactions) are based upon activities and fugacities - Equilibrium constants are determined from Gibbs free energies of formation. Temperature dependence is determined from ideal heats of reaction. Pressure dependence of constants involving gaseous species is determined from the ideal volume changes of reaction. 	<p>ω, B_{ij}: Accentric factor, virial coefficients for bimolecular interactions between gas species present</p> <p>γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest</p> <p>$K_i(T, P)$: Proportionality constant relating fugacity of specie i to activity of specie i in the liquid phase at temperatures and pressures of interest</p> <p>$K_{sp,i}(T)$: Solubility constant for solid specie i at temperatures of interest</p> <p>$K_{j,m}(T, P)$: Equilibrium constant for reaction j in phase m at temperatures of interest (and pressures of interest for constants involving gaseous species)</p> <p>$\Delta G_o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest</p> <p>ΔH_o: Ideal heat of reaction - the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant.</p> <p>ΔV_o: Ideal volume change of reaction - the volume change in the reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This</p>

Approaches	Important Parameters
	parameter pertains only to equilibrium constants involving gaseous species. (species): List of all species that are likely to be present in the 3-phase system
B. (Gray Box) <ul style="list-style-type: none"> - Assume the vapor is a perfect gas, so fugacity coefficients are equal to one - Calculate non-ideal solution aqueous phase activity coefficients using appropriate models (e.g., NRTL). - Equilibrium constants (solid solubility, VLE, and intraphase chemical reactions) are based upon activities and partial pressures - Equilibrium constants are determined from Gibbs free energies of formation. Temperature dependence is empirically derived. Pressure dependence of constants involving gaseous species is empirically derived or ignored. 	γ_i : Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest $K_i(T, P?)$: Proportionality constant relating partial pressure of specie <i>i</i> to mole fraction of specie <i>i</i> in the liquid phase at temperatures of interest (modified Raoult's and Henry Laws) $K_{sp,i}(T)$: Solubility constant for solid specie <i>i</i> at temperatures of interest $K_{j,m}(T, P?)$: Equilibrium constant for reaction <i>j</i> in phase <i>m</i> at temperatures of interest $\Delta G_o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest (species): List of all species that are likely to be present in the 3-phase system
C. (Black Box 1) <ul style="list-style-type: none"> - Assume liquid solution is ideal and the vapor is a perfect gas, so all fugacity coefficients and activity coefficients have a value of one - Equilibrium constants (solid solubility, VLE, and intraphase chemical reactions) are based upon concentrations and partial pressures - Equilibrium constants are determined empirically or found in the literature. Temperature dependence is accounted for. 	$K_i(T)$: Proportionality constant relating partial pressure of specie <i>i</i> to mole fraction of specie <i>i</i> in the liquid phase at temperatures of interest (Raoult's Law for solvent and Henry Law for solutes) $K_{sp,i}(T)$: Solubility constant for solid specie <i>i</i> at temperatures of interest $K_{j,m}(T)$: Equilibrium constant for reaction <i>j</i> in phase <i>m</i> at temperatures of interest (species): List of all species that are likely to be present in the 3-phase system
D. (Black Box 2) <ul style="list-style-type: none"> - Use specie-specific removal fractions to partition components to the three phases 	f_i : Phase partition fractions for all species assumed to be present (species): List of all species that are likely to be present in the 3-phase system
Gas phase chemical equilibrium	
A gas mixture has had sufficient time for all species in the mixture to reach thermodynamic equilibrium at the temperature and pressure of the mixture.	
A. (White Box) <ul style="list-style-type: none"> - Calculate non-ideal solution gas phase fugacity coefficients using an appropriate model (e.g., generalized non-ideal gas equation of state). - Identify chemical reactions likely to occur and products likely to be formed - Calculate species partial pressures by minimization of Gibbs free energy subject to stoichiometric constraints for reactions and products identified as likely to occur 	ω, B_{ij} : Accentric factor, virial coefficients for bimolecular interreactions between gas species present $\Delta G^o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest (species): List of all species that are likely to be present in gas & liquid phases
B. (Black Box) <ul style="list-style-type: none"> - (same as approach A, except ideal gas mixture is assumed; mixture fugacity coefficients assumed equal to unity for all species) 	$\Delta G^o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest (species): List of all species that are likely to be present in gas & liquid phases
Generation of melter offgas particulates	
C. (Black Box) <ul style="list-style-type: none"> - (TBD) 	
Heat transfer between two nondisperse phases	
Two phases are present in a region with neither phase disperse. A geometrically definable interface exists between the phases and heat flows across the interface from the higher-temperature to the lower-temperature region. Phase change may occur at the interface resulting in mass transfer between phases. Intrapphase mass transport between the interface and the bulk of any fluid phases present may occur.	

Approaches	Important Parameters
Heat may also be exchanged between the two phases and the boundary of the mixing volume.	
C. (Black Box) - (TBD)	
Interphase heat transfer with one phase disperse	
A liquid and a gas phase flow into a finite mixing volume at different temperatures and intermingle. Heat flows from the higher-temperature phase to the lower-temperature phase causing each phase to exit at a different temperature from its inlet. If water is present in either the liquid or the gas phase, condensation and/or evaporation may occur resulting in changes to the mass flow rates of the two phases. The impact on mass flow rates from phase change of species other than water are assumed negligible. Heat may be exchanged with the mixture at the boundary of the mixing volume.	
A. (White Box) - Use a full 5- or 6-equation model (e.g., RELAP5) to simulate the 2-phase flow mixture with heat transfer and phase change of water, neglecting interphase mass transfer of all other species, and heat transfer at the boundary - With this model calculate the outlet temperatures and flow rates of each phase.	C_{pg}, C_{pl} : Specific heats of gas and liquid mixtures Δh_{fg} : Latent heat of water at pressure of mixture $T_{sat}(P)$: Saturation temperature of water at pressure of mixture H : Wall heat transfer coefficient correlation (based on macroscopic parameters)
B. (Gray Box) - Assume each phase is well-mixed and that a single length scale can be used to characterize the temperature gradient between phases. - Use the HTU method to calculate the overall heat transfer rate between the gas and liquid. Estimate gas-side and liquid-side H values using correlations from the literature which relate these parameters to other dimensionless groups calculated from macroscopic operating parameters (e.g., liquid and gas flow rates, gas and liquid phase transport properties, geometric ratios, etc.) - Calculate the heat exchange with the wall based on the local phase temperatures and the heat transfer coefficient - Limit phase temperatures so that metastable states are not allowed (i.e., subcooled vapor or superheated liquid) if water is present. When appropriate assume a saturated interface separates the phases. - Assume 1-D flows of each phase (co- or countercurrent). Then use the calculated local interphase and wall heat transfer rates, and a simple energy balance to calculate changes of temperatures and mass flow rates of gas and liquid with position in the mixing volume.	H_g, H_l : Heights of transfer unit for gas and liquid phases K_g, k_l : Gas and liquid phase thermal conductivities μ_g, μ_l : Gas and liquid phase viscosities D_p : Characteristic length for heat transfer (e.g., bubble diameter, packing unit size, etc.) ρ_g, ρ_l : Gas and liquid phase densities C_{pg}, C_{pl} : Specific heats of gas and liquid mixtures Δh_{fg} : Latent heat of water at pressure of mixture $T_{sat}(P)$: Saturation temperature of water at pressure of mixture H : Wall heat transfer coefficient correlation (based on macroscopic parameters)
C. (Black Box) - Assume complete thermal equilibration is achieved between gas and liquid (including the effect of heat transfer at the boundary) as they exit the mixing volume. - Using an appropriate wall heat transfer coefficient, a simple energy balance, the latent heat of water, and the specific heats of the liquid and gas phases calculate the exit temperatures and mass flow rates of each phase.	C_{pg}, C_{pl} : Specific heats of gas and liquid mixtures Δh_{fg} : Latent heat of water at pressure of mixture $T_{sat}(P)$: Saturation temperature of water at pressure of mixture H : Wall heat transfer coefficient correlation (based on macroscopic parameters)
Interphase mass transfer with one phase disperse	
A liquid and a gas phase flow into a finite mixing volume at different compositions and intermingle. Species diffuse at finite rates between the liquid and gas phases. Intrapphase transport is driven by concentration gradients between the bulk and the interface. Concentrations at the interface are thermodynamically limited	
A. (White Box) - Define a representative relative velocity between phases using 2-phase flow correlations from the	V_{gl} : Relative velocity between bulk liquid and gas CFD param: (see "Important Parameters" for <i>Viscous single-phase flow with volumetric sources</i> ,

Approaches	Important Parameters
literature, - Use a full 3-D CFD model in each phase together with suitably-defined diffusion coefficients to calculate local diffusion rates in each phase. - Calculate limiting species concentrations based on VLE. - Assume 1-D flows of each phase (co- or countercurrent). Using calculated local interphase diffusion rates and thermodynamic limits on phase concentrations calculate the 1-D variation of species concentrations in each phase.	approach A. (White Box 1) VLE param: Required thermodynamic parameters for VLE calculation for pressure and temperature range of mixture <i>zzz</i>
B. (Gray Box) - Assume each phase is well-mixed and that a single length scale can be used to characterize the concentration gradient between phases. - Use the HTU method to calculate the overall mass transfer rate between the gas and liquid. Estimate gas-side and liquid-side H values using correlations from the literature which relate these parameters to other dimensionless groups calculated from macroscopic operating parameters (e.g., liquid and gas flow rates, gas and liquid phase transport properties, geometric ratios, etc.) - Calculate limiting species concentrations based on VLE. - Assume 1-D flows of each phase (co- or countercurrent). Using calculated local interphase diffusion rates and thermodynamic limits on phase concentrations calculate the 1-D variation of species concentrations in each phase.	H_g, H_l : Heights of transfer unit for gas and liquid phases D_{gi}, D_{li} : Effective intraphase diffusion coefficients for individual species in gas and liquid D_p : Characteristic length for heat transfer (e.g., bubble diameter, packing unit size, etc.) VLE param: Required thermodynamic parameters for VLE calculation for pressure and temperature range of mixture
C. (Black Box) - Assume complete thermodynamic equilibration between gas and liquid as they exit the mixing volume. - Calculate exit temperatures and mass flow rates for gas and liquid using suitable interphase heat transfer model. - Calculate species concentrations in separate phases using vapor/liquid equilibrium model.	(see “Important Parameters” for referenced models)
D. (Black Box) - Use empirical partition factors to distribute each specie between liquid and gas phases	f_i : Gas partition fractions for all solid species present
Liquid droplet entrainment in a gas stream	
Gas flowing alongside (or through) a liquid in a mixing region entrains a portion of the liquid as droplets in the gas. The particle loading in the gas phase is thus increased and the mass flow rate of the liquid stream is reduced.	
B. (Gray Box) - Use entrainment correlation relating the entrainment to the macroscopic parameters which characterize the interaction of the gas and liquid streams (e.g., relative velocity, liquid surface tension, etc.) - Calculate entrainment rate of liquid from the prevailing conditions in the gas/liquid mixing region and the entrainment correlation	$\epsilon_i(V_r, \sigma)$: Liquid entrainment fraction correlation to macroscopic parameters (relative velocity, liquid surface tension, etc.)
C. (Black Box) - Use empirical entrainment fraction applied to the liquid stream to calculate liquid loading in gas phase	ϵ_i : Liquid entrainment fraction
Liquid filtration	
A colloidal mixture of a liquid with suspended particules undergoes solid/liquid separation by passing through a filter medium. Particles are trapped by the filter medium and thus removed from the liquid	

Approaches	Important Parameters
<p>by one or more of the following mechanisms:</p> <ul style="list-style-type: none"> - Sieve effect of filter medium - Sieve effect of accumulated filter cake <p>The second mechanism results in increasing particle collection efficiency as solids accumulate in or on the filter. It also results in increasing pressure drop across the filter due to increased flow resistance. In the cross-flow variant of liquid filtration the filter cake is continually scoured from the filter surface by the liquid, which flows parallel to the surface of the filter. In this case the liquid flow parallel to the filtering surface is generally many times greater than the flow of filtrate through the filter.</p> <p>Typically, the details of the fundamental processes described are not modeled. Particle collection efficiencies as functions of particle size are provided by the filter medium vendors or by testing with standard colloidal solutions.</p>	
A. (White Box)	
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Use particle removal efficiency correlation appropriate for the type of filter used - From the initial size distribution of particles in the liquid and the removal efficiencies obtained from the correlation calculate the size distribution and overall mass loading of particulate in the filtrate 	<p>PSD_p: Initial droplet size distribution in the inlet gas</p> <p>$\epsilon(d_p, \dots)$: Correlation of particle collection efficiency with particle size and macroscopic parameters</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Apply an empirically derived overall mass removal efficiency to the gas stream to determine total solids loading as filtrate exits the filter 	<p>f_i: Overall removal fraction for particles from the liquid</p>
Liquid phase chemical equilibrium	
A liquid mixture has had sufficient time for all species in the mixture to reach thermodynamic equilibrium at the temperature and pressure of the mixture.	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients using an appropriate model (e.g., NRTL, Pitzer, etc.). - Identify chemical reactions likely to occur and products likely to be formed - Calculate species concentrations by minimization of Gibbs free energy subject to stoichiometric constraints for reactions and products identified as likely to occur 	<p>γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest</p> <p>$\Delta G^\circ(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest</p> <p>ΔH_o: Ideal heat of reaction - the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant.</p> <p>(<i>species</i>): List of all species that are likely to be present</p>
<p>B. (Black Box)</p> <ul style="list-style-type: none"> - (same as approach A. (White Box), except no activity coefficient model is utilized; activity coefficients assumed equal to unity for all species) 	<p>γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest</p> <p>$\Delta G^\circ(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest</p> <p>(<i>species</i>): List of all species that are likely to be present</p>
Mist removal	
<p>A gas laden with liquid droplets forced to flow tangentially into a cylindrical vessel and then parallel to the cylindrical axis through a fine mesh structure (usually constructed of woven metal or an inert material such as fiberglass, Kevlar, etc.). Larger liquid droplets impinge on the cylindrical wall due to centrifugal force. Smaller droplets follow the gas flow through the mesh structure where most are collected by one or more of the following mechanisms:</p> <ul style="list-style-type: none"> - Sieve effect - Brownian diffusion within gas phase to liquid boundary 	

Approaches	Important Parameters
<p>The second mechanism occurs by virtue of the mesh structure being coated with a layer of liquid. The gas bubbles through the liquid layer after being dispersed into tiny bubbles as it passes through the mesh. As the gas bubbles pass through the liquid layer the finest particles can diffuse to the spherical surfaces of the bubbles and be collected by the HEME, despite their size being below what would be collected by the sieve effect.</p> <p>Typically, the details of the fundamental processes described may not all be modeled. Overall particle collection efficiencies may typically be provided by HEME mesh vendors as a function of particle size, mesh fineness, and gas/liquid and flow ratio.</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - (TBD, if deemed appropriate) 	
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Use particle removal efficiency correlation appropriate for the type of mesh used - From the initial size distribution of particles in the gas and the removal efficiencies obtained from the correlation calculate the size distribution and overall mass loading of particulate in the exit gas 	<p>PSD_p: Initial droplet size distribution in the inlet gas</p> <p>$\epsilon(d_p, G/L)$: Correlation of particle collection efficiency with particle size and gas/liquid flow ratio</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Apply an empirically derived overall mass removal efficiency to the gas stream to determine total solids loading as gas exits the collection device 	<p>f_i: Overall removal fraction for particles from the gas stream</p>
Particle collection by wet electrostatic precipitation	
<p>A gas laden with particles is mixed with a water mist and then flows through an electrical corona discharge region resulting in charging of the particles (liquid and solid) through contact with ions produced in the corona. The gas and particles then flow into a vessel parallel to electrically charged collection plates. The particles migrate toward those plates having a charge opposite that on the particles and are collected on the plates. The effect of the deposition of liquid particles on the plates is to provide a continuous washing film of water flowing down the plates and resulting in the deposited solid particles moving down in the liquid film to a collection tank. The tank is also periodically emptied.</p> <p>Typically, the details of the fundamental processes involved in this unit operation may not all be modeled. Overall particle collection efficiencies may typically be provided as functions of the macroscopic operating parameters (e.g., solids loading in the inlet gas, corona charging current and voltage, collection plate charging voltage, gas flow rate, plate washing frequency, etc.).</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate electric field strength between collection plates based on applied voltage and dielectric properties of gas - Calculate migration velocities of particles in collection region, based on particle size, composition, charging voltage, residence time in charging region, electric field strength, etc. - Calculate particle collection efficiencies as a function of particle using migration velocity and gas residence time in collection region - Calculate overall fraction of solids in gas which are removed and exit concentration of particles 	<p>PSD_s: Size distribution of solid particles</p> <p>ϵ: Dielectric properties of gas</p> <p>μ: Gas viscosity</p>
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Use vendor-supplied correlation of particle removal efficiency as a function of WESP operating parameters such as gas velocity, particle characteristics (mean size, composition, etc.), gas velocity, applied voltages to corona and plate regions, etc. - Calculate the fraction of particles that are removed and the resulting exit particle loading in the gas. 	<p>$f(d_p, V, Q, \dots)$: Vendor-supplied correlation of particle removal efficiency as function of operating parameters (d_p, V, Q, etc.)</p>

Approaches	Important Parameters
C. (Black Box) - Apply an empirically derived or vendor-supplied overall mass removal efficiency to the gas stream to determine total solids loading as gas exits the collection device	f_i : Overall removal fraction for solids from the gas stream
Particle collection by sedimentation	
Solid particles suspended in a fluid (gas or liquid) migrate through the fluid under the action of a body force (e.g., gravity, centrifugal force, etc.) in a collecting device (e.g., a settling tank, packed bed scrubber tank, cyclone, centrifuge, etc.) onto a collecting surface. (In a packed bed gas scrubber the surface would be the liquid on the surface of the packing material). The particle concentration in the fluid decreases as the fluid passes through the collecting device.	
A. (White Box)	
B. (Gray Box) - Estimate a characteristic distance through which a particle must migrate to be collected - Calculate the velocity of migration as a function of particle size - Calculate the fraction of particles of each size that are removed from the collection height, migration velocity, and residence time in the collecting device assuming that all particles are initially uniformly distributed through the fluid and the fluid moves uniformly through the device	PSD_s : Size distribution of solid particles (aerodynamic diameters) L_c : Characteristic migration distance for particles to be collected ρ_p : Particle density
C. (Black Box) - Apply empirical removal factors to individual species present in the solid phase	f_i : Removal fractions for all solid species present
Particle impingement due to inertia	
Particles (solid or liquid) in a flowing fluid move under the influence of the fluid viscous force and inertia of the particles themselves. When the flow path of the fluid is not straight the particle trajectories may result in impingement on a flowfield boundary. Extraction of the particles from the fluid and material deposition on the boundary result.	
A. (White Box) - Use approach A. (White Box 1) under <i>Viscous single-phase flow with volumetric sources</i> to calculate the 3-D flowfield of the fluid alone - Using the calculated fluid flowfield calculate trajectories of individual particles of different sizes starting from different locations in the inlet flowfield boundary. Particle trajectories are calculated from Newton's second law using the particle position, inertia, and fluid-particle viscous forces calculated from the flowfield - Assuming particles are uniformly distributed through the inlet boundary, calculate the fraction of particles deposited on the boundary as a function of particle size - Using the particle size distribution calculate the mass deposition rate on the boundary and the final particle loading the fluid stream	PSD : Size distribution of particles CFD param: (see "Important Parameters" for approach A under <i>Viscous single-phase flow with volumetric sources</i>)
B. (Gray Box) - Use approximate correlations of particle deposition efficiency vs macroscopic flowfield and particle parameters (e.g., characteristic flowfield dimension, "slip" velocity, particle size, particle density) - Using the particle size distribution calculate the mass deposition rate on the boundary and the final particle loading the fluid stream	PSD : Size distribution of particles $f(L,V,D,\rho)$: Correlation for particle deposition fraction
C. (Black Box) - Apply empirical removal factors to individual species present in the solid phase	f_i : Removal fractions for all solid species present

Approaches	Important Parameters
<p>Particle removal from gas by HEPA filtration</p> <p>This involves the coupling of three fundamental phenomena:</p> <ul style="list-style-type: none"> - Viscous single-phase flow with volumetric sources - Brownian diffusion of particles from bulk gas to a sink - Particulate removal by sieve action <p>A gas containing an aerosol is forced through a fibrous medium. Particles in the gas move with the gas by advection and within the gas by Brownian diffusion. The surface of the fibrous medium is assumed to be a sink for particles (i.e., zero particle concentration in the gas exists at the surface) and the particles diffuse toward the medium by virtue of the concentration gradient. As the gas move through the medium the concentration of particles is depleted according to the total residence time and diffusion behavior of the gas.</p> <p>Typically, the details of the fundamental processes above are not all modeled. Overall particle collection efficiencies are typically provided by filter medium vendors as a function of particle size (and sometimes pressure drop through the fiber).</p>	
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Use particle removal efficiency correlation appropriate for the type of filter medium being used - From the initial size distribution of particles in the gas and the removal efficiencies obtained from the correlation calculate the size distribution and overall mass loading of particulate in the exit gas 	<p>PSD_p: Initial particle size distribution in the inlet gas</p> <p>$\epsilon(d_p, \Delta p)$: Correlation of particle collection efficiency with particle size and pressure drop</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Apply an empirically derived overall mass removal efficiency to the gas stream to determine total solids loading as gas exits the collection device 	<p>f_i: Overall removal fraction for solids from the gas stream</p>
<p>Solid/liquid equilibrium</p>	
<p>Dissolved species in a liquid remain in solution if it is thermodynamically favorable to do so. Otherwise, separate solid phases precipitate, each composed of the pure molecular or ionic forms of the constituent species (molecular or ionic) in solution. Such precipitation proceeds until the species in the solid and liquid phases reach thermodynamic phase equilibrium at the temperature and pressure of the mixture.</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients using appropriate models (e.g., NRTL for aqueous phase, generalized correlations for aqueous phase). - Assume each precipitated solid is a pure substance at the temperature and pressure of the mixture. - Calculate species concentrations in solid and liquid phases by equating fugacities of each specie in solid and liquid phases. 	<p>$f_i^S(P, T)$: Fugacity of each solid specie at temperature(s) pressure(s) of the mixture.</p> <p>γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest</p> <p>$f_i(P, T)$: Standard state fugacity of each liquid phase specie at temperature(s) pressure(s) of the mixture.</p> <p>ΔH_c: Ideal heat of reaction – the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant.</p> <p>(<i>species</i>): List of all species that are likely to be present in solid & liquid phases</p>
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Assume ideal solution in aqueous phase (activity coefficients are unity) - Proceed as in “White Box” approach (above) 	<p>$f_i^S(P, T)$: Fugacity of each solid specie at temperature(s) pressure(s) of the mixture.</p> <p>$\Delta G^o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest</p> <p>ΔH_c: Ideal heat of reaction - the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant.</p> <p>(<i>species</i>): List of all species that are likely to be present in solid & liquid phases</p>

Approaches	Important Parameters
C. (Black Box) - Use species-specific removal factors to partition gas phase components to solid and liquid phases	f_i : Liquid phase partition fractions for all species assumed to precipitate
Solid/liquid chemical equilibrium	
<p>In a liquid mixture all species present in the liquid phase react to form compounds as a result of a specified set of reactions. In addition, electrolytes dissociate into their component ionic species. The species within the liquid phase reach thermodynamic chemical equilibrium at the temperature and pressure of the mixture (this assumes that sufficient time is provided for full equilibration of all reactions).</p> <p>Dissolved species in the liquid remain in solution if it is thermodynamically favorable to do so. Otherwise, separate solid phases precipitate, each composed of the pure molecular or ionic forms of the corresponding species (molecular or ionic) in solution. Such precipitation continues until the species in the solid and liquid phases reach thermodynamic phase equilibrium at the temperature and pressure of the mixture.</p>	
A. (White Box) - Calculate non-ideal solution aqueous phase activity coefficients using appropriate models (e.g., NRTL for aqueous phase, generalized correlations for aqueous phase). - Assume each precipitated solid is a pure substance at the temperature and pressure of the mixture. - Calculate species concentrations in the liquid phase by minimization of the mixture Gibbs free energy subject to the following constraints: <ul style="list-style-type: none"> · Changes in species amounts are related by the stoichiometric coefficients in a set of linearly independent reactions which represent all reactions that can occur between the species which are present · The total amount of each specie present (in both phases) is the amount initially present plus the changes in the amount of that specie that occur by virtue of all the reactions and their corresponding extents · The chemical potentials (partial molar Gibbs energy) of each specie in gas and solid phases are equal. 	$f_i^S(P,T)$: Fugacity of each solid specie at temperature(s) pressure(s) of the mixture. γ_i : Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest $\Delta G^o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest ΔH_o : Ideal heat of reaction - the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant. <i>(species)</i> : List of all species that are likely to be present in solid & liquid phases
B. (Gray Box) - Assume ideal solution in aqueous phase (activity coefficients are unity) - Proceed as in “White Box” approach (above)	$f_i^S(P,T)$: Fugacity of each solid specie at temperature(s) pressure(s) of the mixture. $\Delta G^o(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest ΔH_o : Ideal heat of reaction - the heat of reaction when each of the reactants and products is in the limiting state where it approaches ideal behavior. This parameter is needed for each chemical reaction and each phase change – i.e., each equilibrium constant. <i>(species)</i> : List of all species that are likely to be present in solid & liquid phases
C. (Black Box) - Use species-specific removal factors to partition gas phase components to solid and liquid phases	f_i : Liquid phase partition fractions for all species assumed to precipitate
Steady state heat exchange between a fluid and its boundary	
<p>This involves the coupling of two fundamental phenomena:</p> <ul style="list-style-type: none"> - Viscous single-phase flow with volumetric sources - Heat transfer at a fluid boundary <p>A moving fluid at one temperature flows next to a solid boundary at a different temperature. Heat flows between the fluid and the boundary by two paths: (a) via direct radiation between the bulk fluid and the boundary, and (b) via conduction between the viscous sublayer and the boundary. The fluid</p>	

Approaches	Important Parameters
<p>temperature in the sublayer is determined by heat transport within the bulk fluid to the region near the boundary. This intrafluid transport is driven by velocity and thermal gradients. The boundary is assumed to have sufficiently high thermal mass and conductivity that it can be treated as an infinite sink at constant temperature.</p> <p>Typically, the details of the fundamental processes above are not all modeled. Macroscopic models have been developed which correlate the heat transfer rate between the fluid and the wall with macroscopic parameters (e.g., Re, Pr, etc.)</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Use approach A under <i>Viscous single-phase flow with volumetric sources</i> to calculate the temperatures and velocities throughout the flowfield - Calculate local heat transfer coefficient between fluid and wall in each computation grid cell based on standard correlations and generate the boundary condition to be applied - Integrate the heat flow over the boundary to obtain the overall heat exchange rate - Calculate the mass average exit fluid temperature by integrating over the exit boundary 	<p>CFD param: (see “Important Parameters” for <i>Viscous single-phase fluid flow</i>, approach A)</p> <p>H: Heat transfer coefficient correlation (based on macroscopic parameters)</p> <p>C_p: Fluid specific heat</p> <p>K: Fluid thermal conductivity</p> <p>ρ: Fluid density</p> <p>μ: Fluid viscosity</p>
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Estimate a heat transfer coefficient between the fluid and wall based on standard correlations and calculate the rate of heat flow between the two - Using a simple energy balance, the calculated heat flow, and the volumetric heat source in the fluid calculate its exit temperature 	<p>H: Heat transfer coefficient correlation (based on macroscopic parameters)</p> <p>C_p: Fluid specific heat</p> <p>K: Fluid thermal conductivity</p> <p>ρ: Fluid density</p> <p>μ: Fluid viscosity</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Assume complete temperature equilibration between fluid and wall 	
Steady state heat exchange between two fluids in a heat exchanger	
<p>This involves the coupling of three fundamental phenomena:</p> <ul style="list-style-type: none"> - Viscous single-phase flow with volumetric sources - Heat transfer at a fluid boundary - Conduction heat transfer through a solid wall <p>Two moving fluids at two different temperatures flow through passageways which are separated by a solid boundary. By virtue of the temperature gradient between the fluids heat flows from the warmer to the colder through the solid wall which separates them. Heat flows between the bulk fluids and the wall via radiation and at the wall/fluid interface via conduction. Velocity and thermal gradients within the fluids are established and heat is transported from the bulk fluids to the viscous sublayers next to the wall by conduction and convection.</p> <p>Typically, the details of the fundamental processes above are not all modeled. Macroscopic models have been developed which correlate the heat transfer rate between the fluids with macroscopic flow parameters (e.g., Re, Pr, etc.)</p>	
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Estimate heat transfer coefficients between each fluid and the wall based on standard correlations - Calculate conductance through the wall based on Fourier’s law of conduction - Calculate the rate of heat flow between the two fluids using a simple electrical circuit analogy - Using a simple energy balance and the calculated overall heat flow between the fluids, calculate the exit temperature of each 	<p>h: Heat transfer coefficient correlation (based on macroscopic parameters)</p> <p>C_p: Fluid specific heat</p> <p>k_i: Thermal conductivities of two fluids</p> <p>ρ_i: Densities of two fluids</p> <p>μ_i: Viscosities of two fluids</p> <p>k_w: Thermal conductivity of the wall separating the fluids</p>

Approaches	Important Parameters
C. (Black Box)	
Steady state single-phase mixing with volumetric sources	
Chemical species present in one or more homogeneous streams flow into a mixing volume and mix before leaving in a single, blended stream. Mixing occurs at both macro and micro scales at finite rates. Chemical species diffuse through the mixture and are produced or consumed by volumetric sources (e.g., chemical reactions). The composition of the exit stream varies spatially and temporally according to the mixing and volumetric sources within the mixing volume.	
A. (White Box) - (same as “A. (White Box 1)” under <i>Viscous single-phase flow with volumetric sources</i>)	(see referenced approach)
B. (Gray Box) - Develop correlation for mixing rate as explicit function of key macroscopic parameters (e.g., mass-specific power input). - Compare mixing rate (at infinite reaction rate) with reaction rate (at infinite mixing rate) to determine which mechanism is limiting. - Calculate outlet concentrations on basis of step determined to be rate-limiting	Mixing rate: Correlation of mixing rate with macroscopic parameters $k_i(T)$: Kinetic rate constants for reactions deemed to be important
C. (Black Box) - Assume perfect mixing of all streams and calculate composition of exit stream by simple mass balance	
Submicron particle collection by steam condensation	
This involves the coupling of three fundamental phenomena: - Viscous single-phase flow with volumetric sources - Nucleation and growth of droplets from subcooled steam - Particle impingement due to inertia A gas containing an aerosol is accelerated through a venturi. A high-pressure jet of steam is throttled into the flowing gas. The expanding steam cools to below the saturation limit and condenses preferentially on the surfaces of the particles in the gas stream causing them to grow in size. Intense mixing of the supersaturated steam, droplets, and particles enhances their growth and coalesce. The growth of the smallest particles results in their being collectible by inertial methods downstream of the condensation region (e.g., by cyclonic action or by passage through a high-efficiency mist eliminator). Typically, the details of the fundamental processes above are not all modeled. Overall particle collection efficiencies have been correlated to macroscopic parameters such as mass specific energy input of the steam jet.	
B. (Gray Box) - Use vendor- or EPA-supplied correlations of particle collection efficiency with operating parameters: particle size, mass-specific energy input, etc. - From the initial size distribution of particles in the gas and the removal efficiencies obtained from the correlations calculate the size distribution and overall mass loading of particulates in the exit gas	PSD_s : Particle size distribution and overall solids loading the inlet gas $\epsilon(d_p, e)$: Particle removal efficiency correlation with particle size and mass-specific energy input
C. (Black Box) - Apply an empirically derived overall mass removal efficiency to the gas stream to determine total solids loading as gas exits the collection device	f_i : Overall removal fraction for solids from the gas stream
Transient thermal conduction	
A solid body at one temperature is immersed in a fluid (liquid or gas) at a different temperature. Heat	

Approaches	Important Parameters
flows to or from the solid across the its boundary by virtue of the temperature gradient. As heat flows to/from the solid the temperature inside the solid body changes with time until thermal equilibration between the solid and fluid is achieved.	
Two-phase flow with heat transfer	
Liquid flow and vapor flow in the same space and undergo phase change with water the principal specie moving between the phases. Heat transfer between the wall and the liquid and/or the gas may influence the evaporation or condensation of water. The dynamics of the flow (e.g., the effective friction factor and pressure drop in pipe flow, the effective liquid and vapor wall heat transfer coefficients, etc.) are influenced by the presence of the second phase and by the phase changes.	
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Treat the flow as strictly one-dimensional pipe flow and use a “drift flux” approach to solve the conservation equations for the liquid and vapor phases - Use published flow regime maps and correlations for wall heat transfer coefficients, and friction coefficients - Solve the 1-D conservation equations numerically (e.g., using a 1-D two-phase flow code such as RELAP-5) to obtain temperatures and mass flow rates of liquid an vapor leaving the pipe 	<p>$H(\alpha)$: Heat transfer coefficient correlations for two-phase flow</p> <p>$f_w(\alpha)$: Wall friction coefficient correlations for two-phase flow</p> <p>C_p: Liquid specific heat</p> <p>K: Effective liquid thermal conductivity</p> <p>ρ_v, ρ_l: Vapor and liquid densities</p> <p>μ: Liquid viscosity</p> <p>Steam tables: Thermodynamic properties of water</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Use lumped parameter mass & energy conservation equations for the region - Use simplifying assumptions about the two-phase flow (e.g., liquid and vapor are saturated; all heat to/from the wall goes to phase change) to allocate heat flow from the wall to the fluid, to calculate phase change, and to solve the conservation equations 	<p>Steam tables: Thermodynamic properties of water</p> <p>$f_w(\alpha)$: Overall wall friction coefficient correlation for two-phase flow as a function of void fraction (or quality)</p>
Vapor/liquid equilibrium	
In a liquid and gas mixture all species present reach a state of thermodynamic equilibrium between its gaseous and liquid forms is also achieved for each specie between its liquid and gaseous forms (this assumes that sufficient time is provided for full equilibration of all species between the liquid and gas phases).	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients and gas phase fugacity coefficients using appropriate models (e.g., NRTL for aqueous phase, generalized correlations for aqueous phase). - Calculate species concentrations in gas and liquid phases by equating chemical potentials (partial molar Gibbs energy) of each specie in gas and liquid phases. 	<p>σ_i: Fugacity coefficients for gaseous phase species at temperature(s) pressure(s) and composition of the mixture</p> <p>γ_i: Activity coefficients for aqueous phase species at temperature(s) pressure(s) and composition of the mixture</p> <p>$f_i(P, T)$: Standard state fugacities of all species assumed present at temperature(s) and pressure(s) of interest</p> <p>(<i>species</i>): List of all species that are likely to be present in gas & liquid phases</p>
<p>B. (Gray Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients using appropriate model (e.g., NRTL). Assume ideal solution behavior in gas phase - Calculate species concentrations in gas & liquid phases by equating chemical potentials (partial molar Gibbs energy) of each specie in gas and liquid phases are equal. 	<p>γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest</p> <p>$\Delta G^{\circ}(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest</p> <p>(<i>species</i>): List of all species that are likely to be present in gas & liquid phases</p>
<p>C. (Black Box)</p> <ul style="list-style-type: none"> - Use species-specific factors to partition species between gas and liquid phases 	<p>f_i: Phase partition fractions for all species assumed to be present</p>
Vapor/liquid chemical equilibrium	

Approaches	Important Parameters
<p>In a liquid/gas mixture all species present react to form a specified set of compounds as a result of a specified set of reactions. In addition, electrolytes dissociate into component ionic species. The species within the liquid and gas phases reach thermodynamic equilibrium at the temperature and pressure of the mixture (this assumes that sufficient time is provided for full equilibration of all reactions). Equilibrium is also achieved for each specie between its liquid and gaseous forms, and (in the case of an electrolyte) between its molecular and dissociated forms.</p>	
<p>A. (White Box)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients and gas phase fugacity coefficients using appropriate models (e.g., NRTL for aqueous phase, generalized correlations for aqueous phase). - Calculate species concentrations in gas and liquid phases by minimization of the mixture Gibbs free energy in the gas or the liquid phase subject to the following constraints: <ul style="list-style-type: none"> · Changes in species amounts are related by the stoichiometric coefficients in a set of linearly independent reactions which represent all reactions that can occur between the species which are present · The total amount of each specie present (in both phases) is the amount initially present plus the changes in the amount of that specie that occur by virtue of all the reactions and their corresponding extents · The chemical potentials (partial molar Gibbs energy) of each specie in gas and liquid phases are equal. 	<ul style="list-style-type: none"> σ_i: Fugacity coefficients for gaseous phase species at temperature(s) pressure(s) and composition of the mixture γ_i: Activity coefficients for aqueous phase species at temperature(s) pressure(s) and composition of the mixture $\Delta G^\circ(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest ΔH_o: Ideal heat of reaction - the heat of reaction when each of the reactants and products is in its standard state. This parameter is needed for each chemical reaction and each phase change. (<i>species</i>): List of all species that are likely to be present in gas & liquid phases
<p>B. (Gray Box 1)</p> <ul style="list-style-type: none"> - Calculate non-ideal solution aqueous phase activity coefficients using appropriate model (e.g., NRTL). Assume ideal solution behavior in gas phase - Calculate species concentrations in gas & liquid phases by minimization of the mixture Gibbs free energy in the gas or the liquid phase subject to the following constraints: <ul style="list-style-type: none"> · Changes in species amounts are related by the stoichiometric coefficients in a set of linearly independent reactions which represent all reactions that can occur between the species which are present · The amount of each specie present is the amount initially present plus the changes in the amount of that specie that occur by virtue of all the reactions and their corresponding extents · The chemical potentials (partial molar Gibbs energy) of each specie in gas and liquid phases are equal. 	<ul style="list-style-type: none"> γ_i: Activity coefficients for aqueous phase species at temperature(s) and pressure(s) of interest $\Delta G^\circ(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest (<i>species</i>): List of all species that are likely to be present in gas & liquid phases
<p>C. (Gray Box 2)</p> <ul style="list-style-type: none"> - Assume ideal solutions in aqueous and gas phases, and apply Raoult's Law and Henry's Law to relate gas and liquid phase concentrations of individual species. - Calculate species concentrations in gas & liquid phases by minimization of the mixture Gibbs free energy in the gas or the liquid phase subject to the following constraints: <ul style="list-style-type: none"> · Changes in species amounts are related by the stoichiometric coefficients in a set of linearly independent reactions which represent all reactions that can occur between the species which are present · The amount of each specie present is the amount initially present plus the changes in the amount of that specie that occur by virtue of all the reactions and their corresponding extents · The chemical potentials (partial molar Gibbs energy) of each specie in gas and liquid phases are 	<ul style="list-style-type: none"> $\Delta G^\circ(T)$: Standard free energies of formation of all species assumed present at temperature(s) of interest (<i>species</i>): List of all species that are likely to be present in gas & liquid phases

Approaches	Important Parameters
equal.	
D. (Black Box) <ul style="list-style-type: none"> - Assume no intraphase chemical reaction (or equilibration) occurs - Use species-specific factors to partition species between gas and liquid phases 	f_i : Phase partition fractions for all species assumed to be present
Venturi scrubber particle collection	
This involves the coupling of five fundamental phenomena: <ul style="list-style-type: none"> - Viscous single-phase flow with volumetric sources - Particle motion in a moving fluid - Liquid atomization and droplet breakup under shear - Aerosol agglomeration - Particle impingement due to inertia Two streams, a gas stream containing solid particles, and a liquid stream which is broken into a stream of liquid droplets, flow together through a constriction (venturi) in the flowfield. The only significant effect of the particles on the gas is to slightly increase its effective density and the gas behaves essentially like a single phase fluid. The liquid droplets are generally much larger than the solid particles in the gas. Because of their larger size the liquid particles accelerate and decelerate more slowly than the smaller, solid particles which are swept along with the gas. A significant fraction of the solid particles collide and coalesce with the larger, liquid droplets because of the difference in their velocities. The droplets containing the solid particles are eventually swept downstream and are collected by passage of the gas through a knock-out drum and mist eliminator. <p>Typically, the details of the fundamental processes listed above are not all modeled. Macroscopic models have been developed which correlate solid particle collection efficiencies to particle size and scrubber operating parameters such as the pressure drop through the venturi.</p>	
B. (Gray Box 1) <ul style="list-style-type: none"> - Calculate a representative velocity difference between particles and droplets, a particle diffusion coefficient, and a characteristic time for agglomeration - Calculate the rate of particle deposition on droplets as a function of particle size from inertial and Brownian diffusion mechanisms - Calculate the fraction of particles of each size that are removed and overall DF for VS. 	PSD_w : Size distribution of water droplets PSD_s : Size distribution of solid particles ΔV : Velocity difference between large & small particles $D(d_p)$: Particle diffusion coefficient as function of particle size
C. (Gray Box 2) <ul style="list-style-type: none"> - Use a textbook correlation of particle removal efficiency as a function of d_p and VS operating parameters such as Δp - Calculate the fraction of particles of each size that are removed and overall DF for VS. 	μ_g : Gas viscosity ρ_p, ρ_l : Particle, liquid densities σ_l : Liquid surface tension P : Pressure T : Temperature
D. (Black Box) <ul style="list-style-type: none"> - Apply empirical removal factors to individual species present in the solid phase 	f_i : Removal fractions for all solid species present
Viscous single-phase flow with volumetric sources	
A single-phase real fluid flows through a region under the influences of pressure gradients, viscous stresses, fluid inertia, and flowfield boundaries, obstructions, etc. Species and heat within the fluid diffuse through the flowfield according to concentration and temperature gradients, local diffusivities, and volumetric sources of heat and chemical species.	
A. (White Box 1)	(Note): Most transport parameters will in general be functions of local fluid conditions—temperature, pressure, velocities, gradients, etc.—because of the effects of turbulence.

Approaches	Important Parameters
<ul style="list-style-type: none"> - Use a transient 3-D Navier-Stokes computational model (CFD model) to calculate velocity, temperature, and species concentration fields throughout the flowfield defined by the boundaries of the model. - Continuum conservation equations for mass, momentum, energy, and species conservation are typically solved. 	<p>The term ‘effective’ used below is meant to include the effects of both molecular level fundamental processes (e.g., Fickian diffusion) and macroscopic turbulence.</p> <p>D_i: Effective intraphase diffusion coefficients for individual species in fluid</p> <p>μ: Effective viscosity</p> <p>k: Effective thermal conductivity</p> <p>C_p: Specific heat of fluid</p> <p>ρ_f: Fluid density</p> <p>(paths): Reaction paths for all volumetric source terms</p> <p>$k_i(T)$: Rate constants for determining species (or heat) volumetric source terms as functions of local fluid conditions</p>
<p>B. (White Box 2)</p> <ul style="list-style-type: none"> - (same as approach A except a steady-state model is used) 	<p>CFD param: (see “Important Parameters” for approach A)</p>
<p>Waste form properties as functions of processing parameters</p>	
<p>A waste feed is transformed into a waste form (e.g., glass, grout, etc.) by a process (e.g., a glass melter, a grout mixing/casting/curing operation, etc.). The properties of the waste form (e.g., leaching rate of hazardous constituents, liquidus temperature, phases present, compressive strength, etc.) are completely determined by (a) the composition of the feed, and (b) the processing parameters. Because of this determinism the quantitative measures of the waste form properties can be predicted by some function of the composition variables and the processing parameters (e.g., through multivariate linear regression of measured data, through thermodynamic equations, etc.).</p>	
<p>B. (Gray Box)</p>	

LIST OF ACRONYMS AND ABBREVIATIONS FOR TABLES I & II:

dp	Particle diameter
Δp	Pressure drop
VS	Venturi Scrubber
DF	Decontamination factor
p	Particle property
g	Gas property
l	Liquid property
μ	Viscosity
ρ	Density
P	Pressure
T	Temperature
VLE	Vapor/Liquid Equilibrium
MOC	Materials of Construction
PCDD	Polychlorinated di-benzodioxin
PCDF	Polychlorinated di-benzofuran
PSD	Particle Size Distribution

TABLE III: REPRESENTATIVE COMPOSITIONS OF DILUTE SBW FEED

		<u>Units</u>	<u>WM-181</u>	<u>WM-184</u>	<u>WM-186</u>
<i>Physical Characteristics</i>					
Volume	Vol.	US gallons	275900	262600	281500
Specific Gravity	SpGr	g/ml	1.150518583	1.218753333	1.15832
Undissolved Solids	UDS	g/l	8.965714286	<visible	#N/A
<i>Elements</i>					
Acid	H+	Normal Acid	1.643	1.673333333	1.363333333
Aluminum	Al	Molar	0.211375	0.507033333	0.2637
Antimony	Sb	Molar	3.28561E-08	2.04119E-08	9.19611E-10
Arsenic	As	Molar	<3.82E-5 M	7.62954E-10	3.43731E-11
Barium	Ba	Molar	3.69058E-05	No Est.	No Est.
Beryllium	Be	Molar	8.43401E-12	5.23964E-12	2.3606E-13
Boron	B	Molar	0.016074344	< 1.39E-02 M	<1.39E-02 M
Bromine	Br	Molar	1.55204E-07	9.64208E-08	4.34401E-09
Cadmium	Cd	Molar	0.005014523	< 4.7E-03 M	<4.70E-03 M
Calcium	Ca	Molar	0.04457752	0.016033333	0.0498
Cerium	Ce	Molar	9.13642E-06	5.67601E-06	2.55719E-07
Chloride	Cl	Molar	0.010143797	0.02753904	0.018014613
Chromium	Cr	Molar	0.0027228	<4.0E-3 M	0.004133333
Dysprosium	Dy	Molar	3.20037E-10	1.98823E-10	8.95753E-12
Erbium	Er	Molar	5.26188E-12	3.26895E-12	1.47275E-13
Fluoride	F	Molar	0.088557909	0.023159841	0.039827909
Gadolinium	Gd	Molar	1.32289E-07	8.21846E-08	3.70263E-09
Gallium	Ga	Molar	9.75402E-15	6.05969E-15	2.73005E-16
Germanium	Ge	Molar	4.51781E-09	2.80669E-09	1.26449E-10
Holmium	Ho	Molar	1.35831E-11	8.4385E-12	3.80177E-13
Iodine	I	Molar	0.000182836	0.000113587	5.1174E-06
Iron	Fe	Molar	0.01168553	0.014566667	0.015633333
Lanthanum	La	Molar	4.60799E-06	2.86271E-06	1.28973E-07
Lead	Pb	Molar	0.000994553	0.000283102	0.000417849
Lithium	Li	Molar	2.01724E-11	1.25321E-11	5.64604E-13
Manganese	Mn	Molar	0.012952771	No Est.	No Est.
Mercury	Hg	Molar	0.000480369	0.000686309	0.00094222
Molybdenum	Mo	Molar	0.000521159	1.1398E-05	5.13513E-07
Neodymium	Nd	Molar	1.52541E-05	9.47664E-06	4.26948E-07
Nickel	Ni	Molar	0.001152972	<4.14E-3 M	<4.14E-03 M
Nitrate	NO3	Molar	3.388	3.99	2.945
Palladium	Pd	Molar	1.80438E-06	1.12097E-06	5.05029E-08
Phosphorus	P	Molar	0.006134224	0.010499607	0.000494051
Plutonium	Pu	Molar	1.9837E-06	1.23238E-06	5.55219E-08
Potassium	K	Molar	0.121087848	0.084658412	0.139136484
Praseodymium	Pr	Molar	4.2586E-06	2.64566E-06	1.19194E-07
Rhodium	Rh	Molar	1.86601E-06	1.15926E-06	5.22277E-08
Rubidium	Rb	Molar	2.85521E-06	1.7738E-06	7.99145E-08
Ruthenium	Ru	Molar	8.70785E-06	5.40976E-06	2.43724E-07
Samarium	Sm	Molar	2.92665E-06	1.81818E-06	8.19141E-08
Selenium	Se	Molar	<1.25E-5 M	2.5495E-07	1.14862E-08

Silver	Ag	Molar	3.38608E-05	2.02753E-08	9.13455E-10
Sodium	Na	Molar	0.859915477	1.284629464	0.840953825
Sulfate	SO4	Molar	0.03826369	0.027366667	0.029077958
Technetium	Tc	Molar	3.01066E-06	1.87037E-06	8.42654E-08
Tellurium	Te	Molar	1.47353E-06	9.15429E-07	4.12425E-08
Terbium	Tb	Molar	1.0824E-09	6.72439E-10	3.02952E-11
Thulium	Tm	Molar	2.60487E-15	1.61828E-15	7.29077E-17
Tin	Sn	Molar	1.68497E-07	1.04679E-07	4.71608E-09
Uranium	U	Molar	0.000318727	0.000180953	0.000382231
Ytterbium	Yb	Molar	4.39256E-16	2.72888E-16	1.22943E-17
Yttrium	Y	Molar	3.50974E-06	2.18043E-06	9.82341E-08
Zirconium	Zr	Molar	0.006062829	< 1.21E-02 M	< 1.2e-2 M

Actinides and Daughters

Thallium	Tl-207	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Thallium	Tl-208	mCi/l	1.12013E-06	6.95882E-07	3.13513E-08
Lead	Pb-209	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Lead	Pb-210	mCi/l	1.08013E-09	6.71029E-10	3.02317E-11
Lead	Pb-211	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Lead	Pb-212	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Lead	Pb-214	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Bismuth	Bi-210m	mCi/l	1.08013E-22	6.71029E-23	3.02317E-24
Bismuth	Bi-210	mCi/l	1.08013E-09	6.71029E-10	3.02317E-11
Bismuth	Bi-211	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Bismuth	Bi-212	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Bismuth	Bi-213	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Bismuth	Bi-214	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Polonium	Po-210	mCi/l	1.04012E-09	6.46176E-10	2.9112E-11
Polonium	Po-213	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Polonium	Po-214	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Polonium	Po-215	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Polonium	Po-216	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Polonium	Po-218	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Astatine	At-217	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Radon	Rn-219	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Radon	Rn-220	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Radon	Rn-222	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Francium	Fr-221	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Francium	Fr-223	mCi/l	2.24026E-10	1.39176E-10	6.27027E-12
Radium	Ra-223	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Radium	Ra-224	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Radium	Ra-225	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Radium	Ra-226	mCi/l	3.4404E-09	2.13735E-09	9.62934E-11
Radium	Ra-228	mCi/l	2.28027E-13	1.41662E-13	6.38224E-15
Actinium	Ac-225	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Actinium	Ac-227	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Actinium	Ac-228	mCi/l	2.28027E-13	1.41662E-13	6.38224E-15
Thorium	Th-227	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Thorium	Th-228	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Thorium	Th-229	mCi/l	8.40098E-11	5.21911E-11	2.35135E-12
Thorium	Th-230	mCi/l	3.96046E-07	2.46044E-07	1.10849E-08
Thorium	Th-231	mCi/l	1.04012E-05	6.46176E-06	2.9112E-07

Thorium	Th-232	mCi/l	3.48041E-13	2.1622E-13	9.74131E-15
Thorium	Th-234	mCi/l	1.04012E-05	6.46176E-06	2.9112E-07
Protactinium	Pa-231	mCi/l	4.40051E-08	2.73382E-08	1.23166E-09
Protactinium	Pa-233	mCi/l	0.001440168	0.000894705	4.03089E-05
Protactinium	Pa-234m	mCi/l	1.04012E-05	6.46176E-06	2.9112E-07
Protactinium	Pa-234	mCi/l	1.32015E-08	8.20147E-09	3.69498E-10
Uranium	U-232	mCi/l	9.60112E-07	5.9647E-07	2.68726E-08
Uranium	U-233	mCi/l	1.60019E-08	9.94117E-09	4.47876E-10
Uranium	U-234	mCi/l	0.000400047	0.001074804	2.11479E-09
Uranium	U-235	mCi/l	1.04012E-05	2.81214E-05	1.53625E-07
Uranium	U-236	mCi/l	1.64019E-05	5.51244E-05	1.48493E-08
Uranium	U-237	mCi/l	3.76044E-06	2.33618E-06	1.05251E-07
Uranium	U-238	mCi/l	1.04012E-05	9.75972E-06	1.95203E-06
Uranium	U-240	mCi/l	3.36039E-13	2.08765E-13	9.4054E-15
Neptunium	Np-237	mCi/l	0.000832851	0.000894705	4.03089E-05
Neptunium	Np-238	mCi/l	3.84045E-08	2.38588E-08	1.0749E-09
Neptunium	Np-239	mCi/l	1.08013E-05	6.71029E-06	3.02317E-07
Neptunium	Np-240m	mCi/l	3.36039E-13	2.08765E-13	9.4054E-15
Plutonium	Pu-236	mCi/l	3.16037E-06	1.96338E-06	8.84556E-08
Plutonium	Pu-238	mCi/l	0.593343756	0.336306306	0.005374516
Plutonium	Pu-239	mCi/l	0.015315081	0.062972973	0.000750193
Plutonium	Pu-240	mCi/l	0.003698017	0.00323088	0.00014556
Plutonium	Pu-241	mCi/l	0.442087294	0.094441117	0.004254825
Plutonium	Pu-242	mCi/l	8.73507E-06	2.43559E-06	1.0973E-07
Plutonium	Pu-244	mCi/l	3.36039E-13	2.08765E-13	9.4054E-15
Americium	Am-241	mCi/l	0.036199679	0.075945946	0.000671814
Americium	Am-242m	mCi/l	7.60089E-06	4.72206E-06	2.12741E-07
Americium	Am-242	mCi/l	7.60089E-06	4.72206E-06	2.12741E-07
Americium	Am-243	mCi/l	1.08013E-05	6.71029E-06	3.02317E-07
Curium	Cm-242	mCi/l	1.08013E-05	6.71029E-06	3.02317E-07
Curium	Cm-243	mCi/l	1.52018E-05	9.44411E-06	4.25483E-07
Curium	Cm-244	mCi/l	0.001000117	0.000621323	2.79923E-05
Curium	Cm-245	mCi/l	1.48017E-07	9.19558E-08	4.14286E-09
Curium	Cm-246	mCi/l	9.60112E-09	5.9647E-09	2.68726E-10
Curium	Cm-247	mCi/l	1.08013E-14	6.71029E-15	3.02317E-16
Curium	Cm-248	mCi/l	1.16014E-14	7.20735E-15	3.2471E-16
Californium	Cf-249	mCi/l	8.80103E-15	5.46764E-15	2.46332E-16
Californium	Cf-250	mCi/l	8.40098E-15	5.21911E-15	2.35135E-16
Californium	Cf-251	mCi/l	1.36016E-16	8.44999E-17	3.80695E-18

Fission Products

Tritium	H-3	mCi/l	0.028656685	0.004224997	0.000190347
Beryllium	Be-10	mCi/l	1.48017E-09	9.19558E-10	4.14286E-11
Carbon	C-14	mCi/l	6.0007E-08	3.72794E-08	1.67954E-09
Selenium	Se-79	mCi/l	0.000216025	0.000134206	6.04633E-06
Rubidium	Rb-87	mCi/l	1.44017E-08	8.94705E-09	4.03089E-10
Strontium	Sr-90	mCi/l	25.07736436	13.44260157	20.38024919
Yttrium	Y-90	mCi/l	27.60321652	17.14851862	0.772586656
Zirconium	Zr-93	mCi/l	0.001080126	0.000671029	3.02317E-05
Niobium	Nb-93m	mCi/l	0.000800093	0.000497059	2.23938E-05
Niobium	Nb-94	mCi/l	0.000560065	0.000347941	1.56757E-05
Zirconium	Zr-95	mCi/l	0.02972973		

Technetium	Tc-98	mCi/l	1.28015E-09	7.95294E-10	3.58301E-11
Technetium	Tc-99	mCi/l	0.004800559	0.002982351	0.000134363
Ruthenium	Ru-106	mCi/l	0.001871889	0.00323088	0.00014556
Rhodium	Rh-102	mCi/l	1.00012E-06	6.21323E-07	2.79923E-08
Rhodium	Rh-106	mCi/l	0.005200606	0.00323088	0.00014556
Palladium	Pd-107	mCi/l	8.00093E-06	4.97059E-06	2.23938E-07
Cadmium	Cd-113m	mCi/l	0.001960228	0.001217793	5.48648E-05
Indium	In-115	mCi/l	4.80056E-14	2.98235E-14	1.34363E-15
Tin	Sn-121m	mCi/l	3.48041E-05	2.1622E-05	9.74131E-07
Tin	Sn-126	mCi/l	0.000204024	0.00012675	5.71042E-06
Antimony	Sb-125	mCi/l	0.06694425	0.009444112	0.000425483
Antimony	Sb-126m	mCi/l	0.000204024	0.00012675	5.71042E-06
Antimony	Sb-126	mCi/l	2.84033E-05	1.76456E-05	7.9498E-07
Tellurium	Te-123	mCi/l	1.88022E-16	1.16809E-16	5.26255E-18
Tellurium	Te-125m	mCi/l	0.003720434	0.002311322	0.000104131
Iodine	I-129	mCi/l	< check logs	6.64865E-05	7.38996E-07
Cesium	Cs-134	mCi/l	0.158675081	0.008917964	0.630229045
Cesium	Cs-135	mCi/l	0.000440051	0.000273382	1.23166E-05
Cesium	Cs-137	mCi/l	27.05515266	16.80803354	0.757246892
Barium	Ba-137m	mCi/l	25.60298344	15.90587234	0.716602116
Lanthanum	La-138	mCi/l	9.60112E-14	5.9647E-14	2.68726E-15
Cerium	Ce-142	mCi/l	1.48017E-08	9.19558E-09	4.14286E-10
Cerium	Ce-144	mCi/l	0.000532123	0.004473527	0.000201544
Praseodymium	Pr-144	mCi/l	8.40098E-05	5.21911E-05	2.35135E-06
Neodymium	Nd-144	mCi/l	8.00093E-13	4.97059E-13	2.23938E-14
Promethium	Pm-146	mCi/l	3.92046E-05	2.43559E-05	1.0973E-06
Promethium	Pm-147	mCi/l	0.212024707	0.131720505	0.005934361
Samarium	Sm-146	mCi/l	1.36016E-10	8.44999E-11	3.80695E-12
Samarium	Sm-147	mCi/l	3.64042E-09	2.26162E-09	1.01892E-10
Samarium	Sm-148	mCi/l	1.88022E-14	1.16809E-14	5.26255E-16
Samarium	Sm-149	mCi/l	1.6802E-15	1.04382E-15	4.7027E-17
Samarium	Sm-151	mCi/l	0.172020045	0.10686758	0.00481467
Europium	Eu-150	mCi/l	7.60089E-09	4.72206E-09	2.12741E-10
Europium	Eu-152	mCi/l	0.001480172	0.000919558	4.14286E-05
Europium	Eu-154	mCi/l	0.266571307	0.032576432	0.108363634
Europium	Eu-155	mCi/l	0.087507027	0.082014654	0.043578989
Gadolinium	Gd-152	mCi/l	6.80079E-16	4.225E-16	1.90347E-17
Holmium	Ho-166m	mCi/l	2.28027E-08	1.41662E-08	6.38224E-10
Thulium	Tm-171	mCi/l	8.80103E-13	5.46764E-13	2.46332E-14

Activation Products

Cobalt	Co-60	mCi/l	0.099614336	0.025282202	0.767567568
Nickel	Ni-63	mCi/l	0.058870944	0.00994117	0.000447876

TABLE IV: REPRESENTATIVE COMPOSITIONS IN SBW TANK

-Taken From Table 9 of Barnes (2000b)–

Radionuclides decayed to 7/1/99		WM-180	WM-188	WM-189	Total or Average
Earliest date composition valid		Jun-00	Jun-05	Apr-05	
	Volume, gallons	284,550	288,000	296,000	868,550
	Density, g/cm ³	1.26	1.28	1.35	1.30
	UDS, g/liter	0.62	2.56	1.94	1.72
	TOC, g/liter		0.60	10.40	3.74
	pH	-0.05	-0.41	-0.37	-0.28
		Moles/liter	Moles/liter	Moles/liter	Moles/liter
H+	Acid	1.13E+00	2.56E+00	2.35E+00	2.02E+00
Ac+3	Actinium	9.53E-16	1.93E-15	2.40E-15	1.77E-15
Al+3	Aluminum	5.82E-01	5.40E-01	9.99E-01	7.10E-01
Am+4	Americium	7.52E-08	1.34E-07	1.33E-07	1.14E-07
Sb+5	Antimony	3.19E-08	1.20E-06	2.50E-06	1.26E-06
As+5	Arsenic	4.67E-05	1.31E-04	2.30E-05	6.67E-05
At	Astatine	2.36E-28	4.76E-28	5.93E-28	4.37E-28
Ba+2	Barium	5.04E-05	7.68E-05	6.53E-05	6.43E-05
Be+2	Beryllium	4.76E-09	3.34E-07	1.26E-06	5.41E-07
Bi+5	Bismuth	4.53E-18	1.04E-17	1.10E-17	8.67E-18
B+3	Boron	1.01E-02	2.64E-02	1.91E-02	1.86E-02
Br-1	Bromine	1.52E-07	9.57E-05	4.26E-07	3.19E-05
Cd+2	Cadmium	7.64E-04	8.59E-03	7.23E-03	5.56E-03
Ca+2	Calcium	3.35E-02	8.98E-02	7.13E-02	6.50E-02
Cf+3	Californium	9.08E-21	1.83E-20	2.28E-20	1.68E-20
Ce+4	Cerium	8.92E-06	2.06E-05	2.09E-05	1.69E-05
Cs+1	Cesium	9.49E-06	2.18E-05	2.30E-05	1.82E-05
Cl-1	Chloride	3.07E-02	2.70E-02	3.13E-02	2.97E-02
Cr+3	Chromium	3.25E-03	1.55E-02	6.41E-03	8.40E-03
Co+2	Cobalt		4.92E-06	7.74E-06	4.27E-06
Cu+2	Copper		6.65E-06	9.37E-05	3.41E-05
Cm+3	Curium	4.77E-12	9.65E-12	1.20E-11	8.85E-12
Dy+3	Dysprosium	3.14E-10	7.26E-10	7.64E-10	6.04E-10
Er+3	Erbium	5.16E-12	1.19E-11	1.26E-11	9.93E-12
Eu+3	Europium	2.57E-07	5.91E-07	6.22E-07	4.92E-07
F-1	Fluoride	4.13E-02	9.41E-02	1.11E-01	8.26E-02
Fr+1	Francium	2.76E-23	5.57E-23	6.93E-23	5.11E-23
Gd+3	Gadolinium	3.29E-07	3.20E-06	3.11E-05	1.18E-05
Ga+3	Gallium	9.56E-15	2.21E-14	2.33E-14	1.84E-14
Ge+4	Germanium	4.43E-09	2.24E-07	1.09E-08	7.95E-08
Ho+3	Holmium	1.33E-11	3.08E-11	3.24E-11	2.56E-11
In+3	Indium	6.70E-07	1.35E-06	1.69E-06	1.24E-06
I-1	Iodine	1.18E-03	4.26E-04	4.36E-04	6.76E-04
Fe+3	Iron	1.73E-02	2.72E-02	2.60E-02	2.36E-02
La+3	Lanthanum	4.52E-06	1.04E-05	1.10E-05	8.69E-06
Pb+2	Lead	1.22E-03	1.13E-03	9.66E-04	1.10E-03
Li+1	Lithium	1.91E-07	1.23E-06	1.29E-05	4.86E-06
Mg+2	Magnesium			3.43E-04	1.17E-04
Mn+4	Manganese		2.24E-02	1.97E-02	1.41E-02

Hg+2	Mercury	9.60E-04	2.00E-03	2.48E-03	1.82E-03
Mo+6	Molybdenum	1.80E-05	3.52E-04	3.16E-04	2.30E-04
Nd+3	Neodymium	1.49E-05	3.46E-05	3.64E-05	2.88E-05
Np+4	Neptunium	1.64E-05	9.87E-06	1.72E-05	1.45E-05
Ni+2	Nickel	1.46E-03	5.55E-03	4.35E-03	3.80E-03
Nb+5	Niobium	3.18E-08	1.86E-06	2.19E-06	1.37E-06
NO3-1	Nitrate	5.05E+00	6.34E+00	7.44E+00	6.29E+00
Pd+4	Palladium	1.77E-06	4.09E-06	4.26E-06	3.39E-06
PO4-3	Phosphate		5.82E-03	1.37E-02	6.58E-03
Pu+4	Plutonium	5.47E-06	6.36E-06	6.82E-06	6.22E-06
Po+4	Polonium	1.08E-18	2.18E-18	2.71E-18	2.00E-18
K+1	Potassium	1.81E-01	2.29E-01	1.59E-01	1.90E-01
Pr+4	Praseodymium	4.17E-06	9.66E-06	1.02E-05	8.03E-06
Pm+3	Promethium	1.53E-09	3.08E-09	3.84E-09	2.83E-09
Pa+4	Protactinium	4.25E-12	8.59E-12	1.07E-11	7.89E-12
Ra+2	Radium	1.52E-14	3.07E-14	3.82E-14	2.81E-14
Rn	Radon	1.14E-19	2.30E-19	2.87E-19	2.11E-19
Rh+4	Rhodium	1.83E-06	4.23E-06	4.45E-06	3.52E-06
Rb+1	Rubidium	2.80E-06	6.47E-06	6.81E-06	5.39E-06
Ru+3	Ruthenium	8.54E-06	2.63E-05	2.32E-05	1.94E-05
Sm+3	Samarium	2.87E-06	6.64E-06	6.98E-06	5.52E-06
Se+2	Selenium	1.02E-05	1.27E-04	8.84E-06	4.85E-05
Si+4	Silicon		1.58E-03	1.53E-04	5.77E-04
Ag+1	Silver	4.37E-06	1.17E-04	2.51E-05	4.88E-05
Na+1	Sodium	1.97E+00	1.59E+00	1.70E+00	1.75E+00
Sr+2	Strontium	4.95E-06	1.14E-05	1.20E-05	9.48E-06
SO4-2	Sulfate	4.22E-02	5.88E-02	4.58E-02	4.90E-02
Tc+7	Technetium	2.80E-06	6.80E-06	7.30E-06	5.66E-06
Te+6	Tellurium	1.44E-06	3.34E-06	3.52E-06	2.78E-06
Tb+4	Terbium	1.06E-09	2.45E-09	2.58E-09	2.04E-09
Tl+3	Thallium	2.89E-20	4.15E-07	1.43E-06	6.24E-07
Th+4	Thorium	9.34E-11	1.89E-10	2.35E-10	1.73E-10
Tm+3	Thulium	2.55E-15	5.91E-15	6.22E-15	4.91E-15
Sn+4	Tin	1.78E-07	4.39E-07	9.94E-07	5.43E-07
Ti+4	Titanium			2.34E-06	7.97E-07
U+4	Uranium	1.48E-04	3.31E-04	4.04E-04	2.96E-04
V+5	Vanadium		2.12E-06	8.38E-06	3.56E-06
Yb+3	Ytterbium	4.30E-16	9.96E-16	1.05E-15	8.29E-16
Y+3	Yttrium	3.44E-06	7.96E-06	8.38E-06	6.62E-06
Zn+2	Zinc		4.96E-05	1.19E-04	5.71E-05
Zr+2	Zirconium	1.10E-03	1.87E-02	2.03E-02	1.35E-02

TABLE V: REPRESENTATIVE GLASS COMPOSITIONWaste Species

		Oxide form (Anion form in Glass)	Mass Fraction Oxides in Glass
Aluminum	Al	Al ₂ O ₃	0.083890392
Arsenic	As	As ₂ O ₃	6.10428E-05
Barium	Ba	BaO	2.11297E-05
Beryllium	Be	BeO	4.8017E-07
Boron	B	B ₂ O ₃	0.001058636
Cadmium	Cd	CdO	0.00023939
Calcium	Ca	CaO	0.006652719
Cerium	Ce	CeO ₂	1.00551E-05
Chromium	Cr	Cr ₂ O ₃	0.000629842
Cobalt	Co	Co ₃ O ₄	5.73356E-06
Copper	Cu	CuO	0.000137062
Gadolinium	Gd	Gd ₂ O ₃	7.94293E-05
Iron	Fe	Fe ₂ O ₃	0.004287623
Lead	Pb	PbO	0.000720884
Lithium	Li	Li ₂ O	1.25314E-05
Magnesium	Mg	MgO	0.001199333
Manganese	Mn	MnO ₂	0.003031035
Mercury	Hg	HgO	0
Molybdenum	Mo	MoO ₃	6.85832E-05
Nickel	Ni	NiO	0.000271763
Potassium	K	K ₂ O	0.022844955
Ruthenium	Ru	RuO ₂	2.04957E-05
Sodium	Na	Na ₂ O	0.157642155
Strontium	Sr	SrO	3.05082E-05
Titanium	Ti	TiO ₂	1.14118E-05
Uranium	U	U ₃ O ₈	0.000699675
Zinc	Zn	ZnO	0.000211106
Zirconium	Zr	ZrO ₂	1.92664E-05
Chloride	Cl	Cl	0.002584381
Fluoride	F	F	0.000403192
Iodide	I	I	4.2051E-05
Nitrate	NO ₃	NO ₃	0
Phosphate	P ₂ O ₅	P ₂ O ₅	0.002403788
Sulfate	SO ₃	SO ₃	0.010698003
Radionuclides			
Cesium	Cs	Cs ₂ O	2.85457E-06
Europium	Eu	Eu ₂ O ₃	1.43948E-08
Americium(III)	Am	Am ₂ O ₃	7.53245E-08
Tecneium-99	Tc	TcO ₂	2.0004E-06
Plutonium (IV)	Pu	PuO ₂	<u>6.40331E-06</u>
Sum of Waste in Glass			0.3

Frit

		Oxide form	Weight Percentage (as % of Frit)	Mass Fraction Oxides in Glass
Boron	B	B ₂ O ₃	15%	0.105
Calcium	Ca	CaO	5%	0.035
Iron	Fe	Fe ₂ O ₃	10%	0.07
Lithium	Li	Li ₂ O	5%	0.035
Silicon	Si	SiO ₂	65%	<u>0.455</u>
Sum of Frit in Glass				0.7

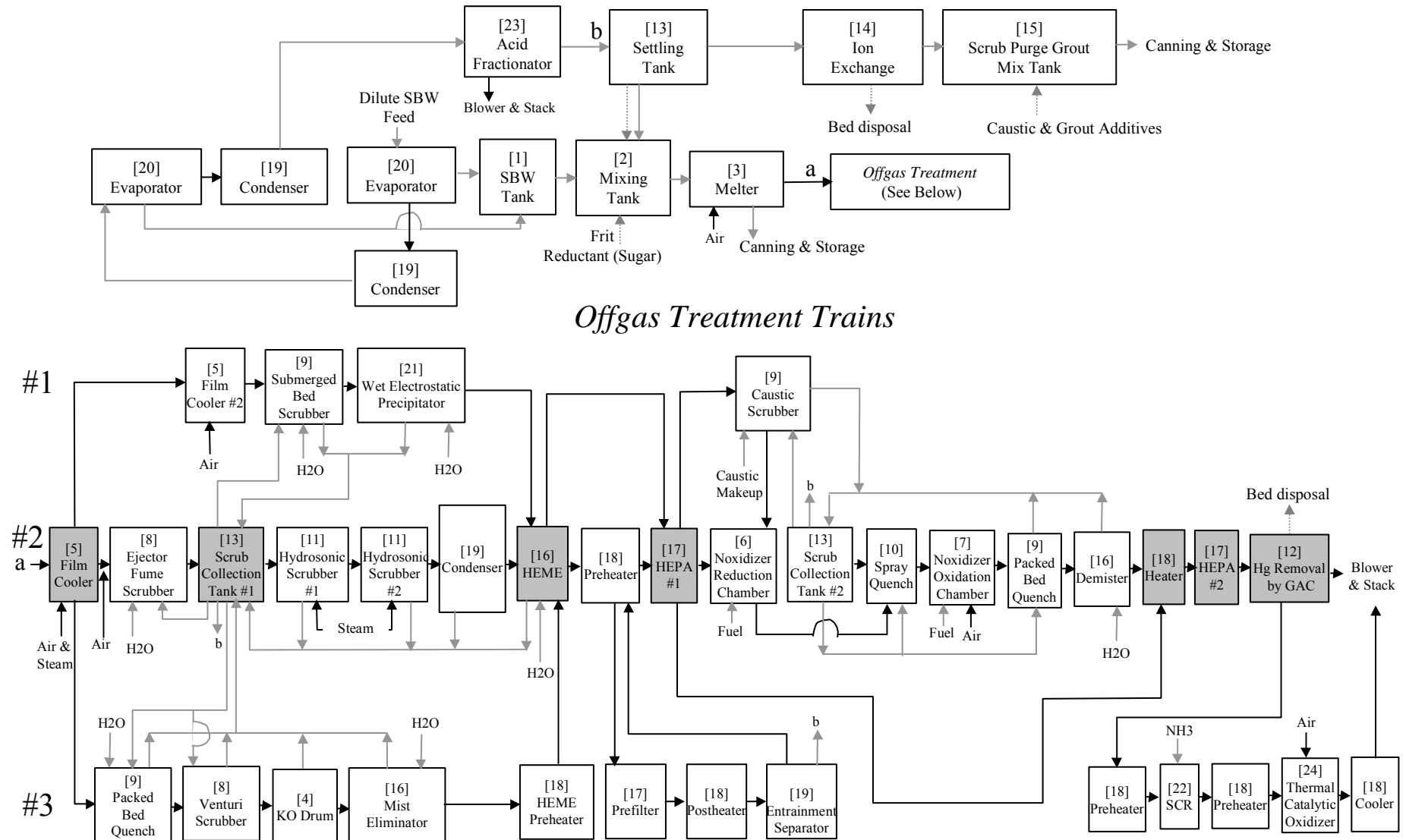
TABLE VI: MISCELLANEOUS MASS BALANCE ASSUMPTIONS

Evaporator	<ul style="list-style-type: none"> • Batch process terminates when solution reaches a specific gravity of 1.33
Acid Fractionator	<ul style="list-style-type: none"> • Bottoms stream is 10 M nitric acid
Melter	<ul style="list-style-type: none"> • Steady-state glass production rate of 127 kg/hr • Glass waste loading - 30% wt. of the glass is composed of nonvolatile species in the waste on an oxide basis (a representative glass composition is shown in Table V) • A limit of 33% Fe+3 to Fe+2 reduction determines the amount of sugar [C6H12O6] added (this corresponds to about 141 g sugar per liter of waste) • Frit will comprise 70% wt. of the glass, and its composition is as shown in Table V. • 45 SCM/Hr of input air
Ejector Fume Scrubber	<ul style="list-style-type: none"> • 145 SCM/Hr of air (pressure control) added to input gas stream
Caustic Scrubber	<ul style="list-style-type: none"> • Caustic makeup is 10 M NaOH • Maintain pH of 7.0
Noxidizer	<ul style="list-style-type: none"> • Fuel is kerosene • NOx conversion in denoxidizer complies with MACT • O2 in effluent is 2% on a dry basis • heat loss to the environment is ~10%
SCR	<ul style="list-style-type: none"> • Ammonia feed is pure NH3 gas
Settling Tank	<ul style="list-style-type: none"> • 2% of liquid passes to ion exchange
Scrub Purge Grout Mix Tank	<ul style="list-style-type: none"> • Grout waste loading – 42.5 % wt • 50% wt. NaOH solution added to maintain pH 12.0 • Representative recipe is as follows: 101 kg NaOH solution, 117 kg solid Ca(OH)2, 693 kg liquid waste, 72 kg portland cement, and 647 kg blast furnace slag

FIGURES

Figure I: Process Configurations

FIGURE I: PROCESS CONFIGURATIONS



Notes: 1) Offgas trains were constructed to envelope the unit operations of Hanford, Savannah River, and West Valley. To visualize a given train (#1, 2, or 3) follow the dark arrows which trace the sequence of unit operations treating the offgas for that train. Cross-connections between trains indicate common components.

2) Shaded boxes represent unit operations common to all three offgas trains.

3) Numbers in brackets refer to unit operation descriptions in Table I.

4) \longrightarrow represents gas stream; \rightarrow represents liquid stream; $\cdots\rightarrow$ represents solid stream.

REFERENCES

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