DEVELOPMENT OF A MULTIPLE LIQUID COMPONENT CAPABILITY IN GOTHIC TO BETTER SUPPORT BORIC ACID, RADIOLOGICAL, AND GSI-191 ANALYSES

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ABSTRACT

GOTHIC™ is a versatile and generally applicable software package that solves complex thermal hydraulics problems. GOTHIC solves the conservation equations for mass, momentum and energy for multicomponent, multi-phase flow in lumped parameter and/or multi-dimensional geometries. A distinctive feature of GOTHIC is the ability to track different types of components in the continuous liquid field, including **SOLID PARTICLES** and **DISSOLVED GAS**. Each component type provides a unique capability. For example, **SOLID PARTICLE** components occupy volume within the continuous liquid fields and impact the bulk liquid mass and energy conservation equations (via volume fraction occupied and effective values for the fluid density and heat capacity). As the name implies, a **SOLID PARTICLE** component is intended to model solid particles, but by using appropriate input parameters, aqueous solutions such as boric acid can be modeled. The convective transport and diffusion is calculated for each component type along with appropriate source terms (e.g., for **SOLID PARTICLES** these include gravitational settling or buoyancy, resuspension and bed load transport). A component can be included in the initial conditions and added at a boundary condition.

Given the different types of components and the fundamental physics included in GOTHIC (e.g., viscous shear and diffusion), the component tracking capability substantially extends its range of applications. Example applications include: boron tracking and mixing in the primary system, effects of gas release on water hammer events, and debris tracking related to GSI-191. Current versions of GOTHIC restrict users to a single liquid component per simulation. The current development effort removes this restriction and allows multiple components (both number and type) to be tracked in a single simulation. This new capability allows: multiple dissolved gases, soluble boron and dissolved gases to co-exist, and multiple debris fields with different characteristic sizes/properties to be considered. In this paper, the assumptions, impact on the other conservation equations, and the solution scheme are discussed for each type of tracked component. Results from simple canonical problems used to verify this new feature are also presented.

GOTHIC™ incorporates technology developed for the electric power industry under the sponsorship of EPRI, the Electric Power Research Institute.

KEYWORDS
GOTHIC, GSI-191, Boron Transport & Mixing, Dissolved Gas

1. INTRODUCTION

GOTHIC [1] is a general-purpose thermal-hydraulics software package for design, licensing, safety and operating analysis of nuclear power plant systems, containments, and confinement buildings. Conservation equations are solved for three (or more) primary fields, including continuous liquid, steam, N non-condensing gases, and any number of M interacting droplet fields. Optional secondary fields are also available to represent ice, mist, and liquid components. GOTHIC can also track radioactive nuclides in the vapor, including decay and formation of daughter products. Other phenomena include models for commonly available safety equipment, heat transfer to structures and hydrogen burn.

GOTHIC provides a 3-dimensional treatment for multiphase flow, including the full treatment of the momentum transport terms in multidimensional models, with optional models for turbulent shear and turbulent mass and energy diffusion. A two-equation turbulence model is used to calculate the turbulent diffusion coefficients. Both first- and second-order accurate spatial schemes are available for the convection terms in the mass, energy and momentum balances.

In addition to multidimensional modeling, GOTHIC can be used in a 1D or lumped modeling mode that is typical for codes used in the nuclear power industry. These modeling modes can be combined in a single model, as shown in Figure 1, which makes GOTHIC a very useful tool that bridges the gap between CFD and lumped parameter modeling. It can solve entire classes of problems that cannot be adequately addressed by traditional system, or even subchannel, codes.

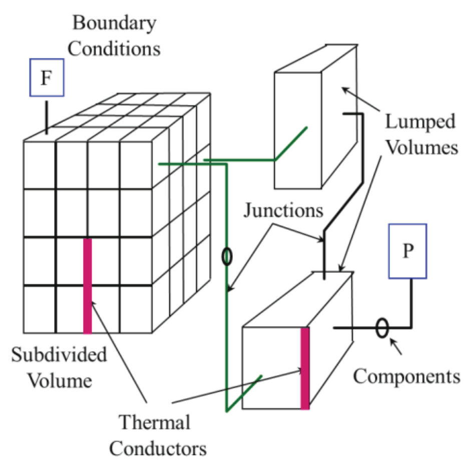

Figure 1. Schematic representation of Modeling Flexibility provided by GOTHIC.

2. LIQUID COMPONENTS

A liquid component in GOTHIC refers to a substance that is tracked in the continuous liquid field. The substance could be solid particles, another liquid or a gas subject to the modeling assumptions described here. The user defines the type of the substance and provides values for parameters that influence its behavior. **SOLID PARTICLE** components occupy volume within the liquid phase and impact the bulk liquid conservation equations (via volume fraction occupied and effective values for the fluid density and heat capacity) while the **DISSOLVED GAS** components do not occupy volume and therefore do not impact the bulk liquid conservation equations.

Current versions of GOTHIC (version 8.1 and earlier) restrict users to a single liquid component per simulation. The current development effort removes this restriction and allows multiple components (both number and type) to be tracked in a single simulation. This new capability allows: multiple dissolved gases, soluble boron and dissolved gases to co-exist, and multiple debris fields with different characteristic sizes/properties to be considered.

2.1. Solid Particles

For a **SOLID PARTICLE** component, GOTHIC models the convective transport, settling, bed load (motion of the settled material), resuspension of settled particles, and diffusion (both molecular and turbulent) of suspended particles. The amount of a **SOLID PARTICLE** component is quantified using the volume fraction (fraction of the total liquid volume that is occupied by the liquid component). Additionally, the fraction of each **SOLID PARTICLE** component that is suspended versus settled is tracked separately in each computational volume. The liquid component is characterized by user defined values for the material density, specific heat, characteristic diameter, a shape factor that influences the settling rate, a maximum allowable packing fraction for the component, and shear limits that control the resuspension and sliding of the deposited material.

The momentum and energy equations for the continuous liquid field use effective density and heat capacity values that are calculated based on the volume occupied by the component(s). However, the user-specified density and specific heat for the component(s) is constant (temperature independent). Additionally, it is assumed that the viscosity and thermal conductivity of the continuous liquid field are not affected by the presence of the component(s). Since momentum and energy balances are solved for the liquid/component mixture, the components are assumed to be in mechanical and thermal equilibrium with the continuous liquid field. The one exception is the relative motion in the vertical direction due to gravitational settling. A settling velocity, which can be positive or negative, is calculated individually for each component using a force balance that accounts for buoyancy effects.

Settled particles will continue to fall until they reach the bottom of a cell that is blocked, at which point a sediment layer will be formed. Resuspension of the settled material due to shear and turbulence mechanisms is considered. The migration of the settled material to adjacent cells due to shear imposed by the liquid flow, which is referred to as the bed load, is also considered. For the purposes of modeling the bed load, particle deposition and resuspension, it is assumed that the particles for a particular component are uniformly sized and non-cohesive; however, the effects of particle non-uniformity and cohesion can be accounted for in user specified multipliers.

If a **SOLID PARTICLE** component is defined with a characteristic particle size less than or equal to zero then the settling contribution is ignored and the suspended fraction is always equal to one. The convective transport and diffusion are still calculated. This approach can be used to model trace amounts of another liquid in the continuous liquid field (e.g., boric acid). However, this model assumes the continuous liquid field and aqueous solution are well-mixed, but do not interact, react, or separate/stratify (e.g., miscible fluids). The model also does not currently account for precipitation or evaporation effects (the entirety of the component remains in the continuous liquid field). In this approach the aqueous solution will occupy volume and will affect the conservations equations for the continuous liquid field.

2.2. Dissolved Gas

GOTHIC models the convective transport, diffusion, release and absorption of a **DISSOLVED GAS** component. Unlike **SOLID PARTICLE** Components, the **DISSOLVED GAS** Components do not occupy volume or impact the characteristics of the continuous liquid field. The mass and energy of these components is ignored in the continuous liquid balance equations. Gas release due to bubble nucleation and diffusion at the nucleation sites, diffusion to bubbles and surfaces, boiling and evaporation and bubble sweeping are calculated. It is assumed the released gas enters the vapor phase at the liquid temperature, while the energy associated with absorbed gas is neglected.

3. APPLICATIONS

Given the different types of components and the fundamental physics included in GOTHIC (e.g., viscous shear and diffusion), the component tracking capability substantially extends its range of applications. Example applications include:

- Boron tracking in the primary system.
- Account for the impact of gas release on water hammer events. When the pressure in the liquid is reduced, some of the dissolved gas may be released from the water, forming bubbles or added to the vapor space above the liquid.
- Debris tracking related to GSI-191.

Extending this capability to allow for multiple liquid components will allow for:

- Multiple dissolved gases to be considered.
- Both soluble boron and dissolved gases to be considered in the same simulation.
- Multiple debris fields with different characteristic sizes/properties to be considered.

The following sections provide additional details about three specific applications that can leverage the liquid component capability available in GOTHIC.

3.1. Boron Tracking, Concentration, and Precipitation

Boron transport and mixing can be important for neutron kinetics and determining if boron precipitation can occur. Particular concerns are boron dilution transients and the potential for recriticality to occur when a un-borated slug of water is transported to the core. The transport and mixing phenomena determine the localized boron concentrations for this event and determine whether recriticality is possible. The inclusion of second-order accurate spatial schemes for the convection terms in the mass, energy and momentum balances allows GOTHIC to better model boron transport by reducing the amount of numerical diffusion relative to the first-order upwind schemes that are traditionally applied in thermal-hydraulic codes within the nuclear industry. GOTHIC also includes molecular and turbulent diffusion of mass, momentum, and energy, which better captures the fluid mixing that occurs in the downcomer, lower plenum, and core regions. This mixing is important for determining the localized boron concentration throughout the system.

Boron precipitation is primarily a concern for accident conditions, specifically during cold leg injection following a large cold leg break. In this scenario the water in the core would be boiling and the net flow entering the core would be equivalent to the decay heat boil-off rate. As the water boils the boron concentration increases and eventually can reach the solubility limit and begin to precipitate. To prevent boron precipitation in these scenarios, the safety injection flow is switched from cold leg injection to hot leg injection. The required switchover timing is dependent on the concentration of boron in the various systems (RCS, RWST, accumulators), the decay heat level, and mixing processes within the reactor vessel. Therefore, the boron transport and mixing models are important for establishing this timing.

Although boron precipitation is not explicitly modeled in the current version of GOTHIC, the localized concentrations can be compared to solubility limits to evaluate the potential for precipitation to occur. If precipitation is found to occur, it could be assumed that precipitate will deposit locally. The additional resistance to decay heat removal due to the precipitate deposit on the surface of fuel rods can be included using heat transfer surface options. Meanwhile, the impact of reduced volume and flow area at that location can be considered using the variable porosity feature available in GOTHIC. This treatment could be refined in future versions of GOTHIC to allow for the precipitated material to be converted to a **SOLID PARTICLE** component and be transported downstream.

3.2. Radiological Analyses

Tracking of radioactive isotopes (fission products) released during an accident that involves severe core damage is another application that can utilize this capability. GOTHIC already includes a multi-field drop capability as well as the capability of modeling radioactive elements. GOTHIC solves individual mass, energy and momentum balances for each droplet field. Each droplet field is assumed to have a log normal distribution. Agglomeration and deposition are calculated by integrating the effect over the entire size range of the distribution. Agglomeration within each field is modeled as well as agglomeration between interacting fields.

Meanwhile, the radioactive isotope model accounts for decay and daughtering. In existing versions of GOTHIC the radioactive material is assumed to move with the vapor phase. However, leveraging the liquid component capability will allow the radioactive isotopes to be extended to the liquid fields. This will allow GOTHIC to be applied to accident conditions where interaction with the water and drop phases is an important mechanism for the retention of radioactive material in the containment. This same capability could also be used to model the removal of particulates or harmful toxins from exhaust gases using a spray scrubber.

3.3. Debris Transport for GSI-191

Debris transport is an important aspect of the risk-informed evaluation of Generic Safety Issue (GSI)-191 because it determines the total volume of debris transported to the sump strainer surface as a function of time throughout the transient. This impacts both the structural integrity of the strainer and the ability to maintain recirculation flow between the sump and reactor vessel. The transport of debris during the recirculation phase is dependent on the break location, water level, and flow rate.

NEI -04-07, Volume 2 [2] allows the transport fractions to be refined using CFD modeling of the recirculation pool. The guidance in Ref. [2] states: "*Once the containment recirculation pumps are activated and the ECCS flow is drawn from the recirculation sump, detailed flow patterns in the containment pool can be obtained using state-of the-art 3D computational fluid dynamics (CFD). Thus, fully three-dimensional (3D) flow patterns can be obtained, which in turn can be used to predict the various flow paths to the recirculation sump(s).*" However, the current approaches do not explicitly model the debris. Instead, the CFD calculated velocities and turbulent kinetic energy profiles are post-processed and compared to the debris-specific settling velocities, incipient and bulk transport velocities to determine the percentage of debris expected to transport to the sump strainer. Applying GOTHIC and the liquid component capability can explicitly model the debris and therefore directly consider the influence of debris laden water and settling on flow profiles. This will provide a more efficient approach than the current two-step process.

Various types of debris within containment must be considered in GSI-191 analyses, including:

- Insulation → low-density fiberglass (LDFG), reflective metal insulation (RMI), Nukon, Thermal-Wrap, Microtherm, *etc*.
- Qualified and unqualified coatings → epoxy, inorganic zinc silicate primer (IOZ), enamel, *etc*.

- Latent debris → fiber and other particulates (dirt/dust)
- Miscellaneous debris → tags, labels, plastic signs, tie wraps, *etc*.

The corresponding properties (e.g., density, characteristic size, *etc*.) for these different types of debris cover a wide range of values. Therefore, it is advantageous to have the ability to model multiple debris fields within a given simulation.

In the event that the sump strainer fails, the debris transport and in-vessel effects on long term cooling can also be evaluated with GOTHIC. Based on the amount of debris that has been transported to the strainer, GOTHIC can then model the transport of that debris through the recirculation lines and determine the amount of debris that ultimately enters the vessel and if that debris will reach the core inlet. This resulting potential core blockage represents a long term cooling concern. Additionally, if a significant debris bed builds up on the bottom of the core it could disrupt the mixing processes and accelerate the onset of boron precipitation.

GOTHIC includes the necessary modeling capabilities to predict the flow fields in containment, sump, piping and reactor vessel. The 3D geometry is modeled using geometric blockage forms to represent walls and obstructions in the flow field. A 3D model of the lower containment can be created, including any equipment or obstructions (including curbs) that would impact the flow patterns and debris transport to the sump strainer. A multidimensional core model can be used to consider the effects of core blockage on both the fuel thermal performance and local boron concentration. Local core blockage can be simulated by using the variable porosity feature available in GOTHIC.

4. GOVERNING EQUATIONS

This section presents the mass balance associated with the liquid components and the impact the liquid components has on the other governing equations.

4.1. Mass Balance for each Individual Component

The mass balance for the k[th] tracked liquid component in the continuous liquid field is:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\int_V \mathrm{H}\alpha_l(\chi_c\rho_c)_k dV \\
&= -\underbrace{\int_{A_f}[\mathrm{H}\alpha_l(\chi_c\zeta_c\rho_c)_k\vec{u_l}\cdot\vec{n}]dA_f}_{convective\ transport} + \underbrace{\int_{A_f}\left[\mathrm{H}\alpha_l(\rho_c D_c)_k\vec{\nabla}(\chi_c\zeta_c)_k\cdot\vec{n}\right]dA_f}_{diffusion} \\
&+\Upsilon\left[-\underbrace{\int_{l_y}\left[\mathrm{H}\rho_{c,k}\overrightarrow{q_{b_x,k}}\cdot\overrightarrow{n_x}\right]dy}_{\substack{bed\ load\ transport\\ in\ the\ x\ direction}} - \underbrace{\int_{l_x}\left[\mathrm{H}\rho_{c,k}\overrightarrow{q_{b_y,k}}\cdot\overrightarrow{n_y}\right]dx}_{\substack{bed\ load\ transport\\ in\ the\ y\ direction}} + \dot{s}_{c,k}\right] + \dot{s}_{c,k,BC}
\end{aligned}
\tag{1}
$$

where a generalized Heaviside function is used to define volume and area porosities:

$$H(x) = \begin{cases} 1 \text{ if x is in the fluid} \\ 0 \text{ if x is in an obstacle} \end{cases} \tag{2}$$

Meanwhile, V is the volume bounded by flow area A_f, α_l is the bulk liquid volume fraction, χ_c is the volume fraction of a specific liquid component relative to the bulk liquid volume, ζ_c is the fraction of the tracked liquid component that is in solution (suspended particles), ρ_c is the material density of the tracked component, $\overrightarrow{u_l}$, is the liquid velocity, $\vec{n}$ is the outward facing unit normal vector, D_c is the mass diffusion coefficient for the tracked component, q_{b_x} and q_{b_y} are the volumetric bed load transport rates per unit width, l_{x} and l_{y} are the effective bed load transport widths, $\dot{s}_c$ is a generalized source term, and $\dot{s}_{c,BC}$ is a source term that includes boundary condition contributions. For **SOLID PARTICLE** components the generalized source term includes settling and resuspension at the top and bottom of the volume. In Equation (1), ϒ is set to 0 if the user-defined characteristic diameter is less than or equal to zero for a particular **SOLID PARTICLE** component and ϒ is set to 1 if the user-defined characteristic diameter is greater than to zero.

For **DISSOLVED GAS** components the molar density is tracked rather than the volume fraction. Therefore, mass balance is modified as follows:

1) $\chi_{c,k}$ is replaced with $\chi_{g,k}$ which represents the molar density (moles/ft^3)
2) $\rho_{c,k}$ is replaced with $\mathcal{M}_{g,k}$ which represents the molecular weight
3) $\zeta_{c,k}$ is always unity **(**all suspended since these components do not settle).
4) q_{b_x} and q_{b_y} are always zero (no bed transport because these components do not settle).
5) $\dot{s}_{c,k}$ is replaced with $\dot{s}_{g,k}$ which includes the release and absorption of gas instead of settling and resuspension.

No inter-field exchange terms are needed in the component mass balances for either **SOLID PARTICLE** or **DISSOLVED GAS** since all liquid components are assumed to be non-interacting.

4.2. Impact on Continuous Liquid Mass Equation

The continuous liquid phase mass balance is altered only for **SOLID PARTICLE** components. **DISSOLVED GAS** components are assumed to have a negligible amount of mass relative to the continuous liquid field and are therefore neglected in the liquid phase mass balance. The mass balance for the continuous liquid field is:

$$\begin{aligned} \frac{\partial}{\partial t}\int_V \mathrm{H}\alpha_l\left(1-\chi_{c,tot}\right)\rho_l dV = -\int_A \left[\mathrm{H}\alpha_l(1-\chi_{c.tot})\rho_l\overrightarrow{u_l}\cdot\vec{n}\right]dA \\ -\sum_{k=1}^{N_{solid}}\left[\int_{A_f}\left[\mathrm{H}\alpha_l\rho_l D_{c,k}\vec{\nabla}(\chi_c\zeta_c)_k\cdot\vec{n}\right]dA_f\right] + \int_{A_{I_l}} S_l^m dA_{I_l} + E_l^m + \dot{s}_{l,BC} \end{aligned} \tag{3}$$

where S_l is the rate of phase change over interface area A_{I_l}, E_l is the source of liquid due to equipment (e.g., nozzles) and $\dot{s}_{l,BC}$ is the mass source rate from other sources (e.g., boundary conditions).

The diffusion term in this expression represents the liquid mass that replaces **SOLID PARTICLE** components that have diffused to a neighboring cell.

4.6. Impact on Continuous Liquid Energy Equation

The energy balance for the continuous liquid field is:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\int_V \mathrm{H}\alpha_l\left[\left(1-\chi_{c,tot}\right)\rho_l(h+ke)_l - P\right]dV + \sum_{k=1}^{N_{solid}}\left[\frac{\partial}{\partial t}\int_V \mathrm{H}\alpha_l\left[\chi_{c,k}\rho_{c,k}\left(h_{c,k}+ke_l\right)\right]dV\right] \\
&= -\int_{A_f}\left\{\mathrm{H}\alpha_l\left[\left(1-\chi_{c,tot}\right)\rho_l(h+ke)_l\right]\overrightarrow{u_l}\cdot\vec{n}\right\}dA_f \\
&-\sum_{k=1}^{N_{solid}}\left[\int_{A_f}\left\{\mathrm{H}\alpha_l\left[\chi_{c,k}\zeta_{c,k}\rho_{c,k}\left(h_{c,k}+ke_l\right)\right]\overrightarrow{u_l}\cdot\vec{n}\right\}dA_f\right] \\
&-\int_V P\frac{\partial}{\partial t}\left[\mathrm{H}\alpha_l\right]dV \\
&+\int_{A_f}\left[\mathrm{H}\alpha_l\left(1-\chi_{c,tot}\right)\rho_l c_{p_l} D_l^e\vec{\nabla}T_l\cdot\vec{n}\right]dA_f \\
&+\sum_{k=1}^{N_{solid}}\left[\int_{A_f}\left\{\mathrm{H}\alpha_l\rho_{c,k}D_{c,k}\left[\vec{\nabla}\left(\chi_{c,k}\zeta_{c,k}\left(h_{c,k}+ke_l\right)\right)\cdot\vec{n}\right]\right\}dA_f\right] \\
&-\sum_{j=1}^{N_{solid}}\left[\int_{A_f}\left\{\mathrm{H}\alpha_l\rho_l D_{c,k}\left[\vec{\nabla}\left(\chi_{c,k}\zeta_{c,k}\left(h_l+ke_l\right)\right)\cdot\vec{n}\right]\right\}dA_f\right] \\
&+\sum_{k=1}^{N_{solid}}\left[-\int_{l_y}\left[(\rho_c h_c)_k\overrightarrow{q_{b_x,k}}\cdot\overrightarrow{n_x}\right]dy-\int_{l_x}\left[(\rho_c h_c)_k\overrightarrow{q_{b_y,k}}\cdot\overrightarrow{n_y}\right]dx\right] \\
&+\int_{A_{w_l}} s_l^e\,dA_{w_l}+\int_{A_{I_l}} s_l^e\,dA_{I_l}+E_l^e
\end{aligned}
\tag{4}
$$

where h is the enthalpy, ke is the kinetic energy, P is the pressure, c_p is the specific heat, D_l^e is the thermal diffusion coefficient, T_l is the liquid temperature, s_l^e is the energy source rate from walls, S_l^e is the energy source rate due to phase change, and E_l^e is the energy source rate due to equipment and boundary conditions.

Again, this only includes the contributions of **SOLID PARTICLE** Components. The energy of the **DISSOLVED GAS** components, and their impact on the bulk liquid energy, is neglected.

It is assumed that the enthalpy of the liquid component is given by:

$$h_{c,k} = \left(c_p\right)_{c,k}[T_l - T_o] \tag{5}$$

where the specific heat of the liquid component is user specified and assumed to be constant (temperature independent). The reference temperature is assumed $T_o = 0\ °F$. Again, the bulk liquid and liquid components are assumed to be in thermal equilibrium.

4.4. Impact on Continuous Liquid Momentum Equation

For the liquid momentum balance the pure liquid density will be replaced by the mixture density, which is defined as:

$$\rho_{lt} = \left(1 - \chi_{c,tot}\right)\rho_l + \sum_{k=1}^{N_{solid}} (\chi_c \zeta_c \rho_c)_k \tag{6}$$

DISSOLVED GAS components do not impact the vapor energy balance.

4.5. Impact on Non-Condensing Gas Mass Equation

An additional source term is included in the non-condensing mass balances to represent the dissolved gas that is absorbed or released.

4.6. Impact on Vapor Energy Equation

An additional source term is included in the vapor energy balance to represent the dissolved gas that is absorbed or released. **SOLID PARTICLE** components do not impact the vapor energy balance.

4.7. Closure Relationships

The following sections summarize the closure relationships applied for the liquid component capability.

4.7.1. Settling

Settling is only considered for **SOLID PARTICLE** components and if the user specified characteristic diameter of particles is greater than zero. Settling is estimated using a series of explicit calculations. The settling velocity is the velocity of the particles in quiescent water due to gravity (calculated from a balance between drag and gravitational forces). Therefore this velocity it can be positive or negative, where positive represents falling/settling particles and negative represents buoyant particles.

4.7.2. Resuspension

Resuspension is only considered for **SOLID PARTICLE** components and if the user specified characteristic diameter of particles is greater than zero. It is assumed particles within a bed are uniformly mixed (i.e., particles do not preferentially settle within the bed and layering that could occur due to one component settling before another type of component is not considered). Each component type contained within a given cell has an equal probability of being resuspended, but depends on shear force imparted by the liquid flowing over the bed and particle density.

4.7.3. Bed Load Transport

Bed load transport refers to the sliding, rolling and jumping motion of particles near the upper surface of the sediment layer and therefore is only considered for **SOLID PARTICLE** components. This motion is related to drag and lift forces imposed by the flowing stream on the sediment layer. Some of the horizontal momentum may be converted to vertical momentum when the particle hits a large obstacle. The particle then rises into the fluid stream and is transported a distance downstream that is determined by the initial vertical momentum, stream velocity, drag on the particle and the settling velocity. Again, it is assumed particles with a bed are uniformly mixed and therefore each component type contained within a given cell has an equal probability of being transported.

4.7.4. Gas Absorption/Release

The mass source term for **DISSOLVED GAS** components has the form:

$$\dot{S}^{m}_{g,k} = a_k\left(\chi_{sat,k} - \chi_{g,k}\right) \tag{7}$$

where $\dot{S}^{m}_{g,k}$ is the mass flow rate that the kth tracked dissolved gas is released or absorbed from the continuous liquid field, a_k is a generalized release coefficient, $\chi_{g,k}$ is the molar density of the kth tracked dissolved gas in the continuous liquid field and $\chi_{sat,k}$ is the saturated dissolved gas molar density at the existing water temperature and partial pressure of the corresponding free gas.

Henry's Law, which states the solubility of a gas in a solvent is directly proportional to the partial pressure of that gas above the solvent, is used to quantify the gas solubility. This source is applied to the mass balance equations for both the dissolved gas and the corresponding non-condensable gas. As mentioned previously, the dissolved gas is assumed to not occupy any volume in the liquid phase and therefore the impact on the continuous liquid mass is neglected.

Meanwhile, the associated energy source is:

$$\dot{S}^{e}_{g,k} = \dot{S}^{m}_{g,k} h^{*}_{g,k} \tag{8}$$

where $\dot{S}^{e}_{g,k}$ is the rate of energy that accompanies the released/absorbed gas and $h^{*}_{g,k}$ is a characteristic enthalpy of the dissolved gas. This source is only applied to the vapor energy balance equation. The impact of the dissolved gas on the continuous liquid energy is neglected.

The rapid nature of the gas release process necessitates treating these source terms implicitly to ensure numerical stability.

4.8. Source Terms

A liquid component can be included in the initial conditions and/or added at a boundary condition. For the **SOLID PARTICLE** components both the suspended and settled volume fraction can be specified as part of the initial condition and a suspended volume fraction can be specified as part of a boundary condition. For the **DISSOLVED GAS** the relative saturation can be specified for both the initial and boundary conditions.

5. SOLUTION ALGORITHM

The cell balance equations can be expressed in the following form:

$$[J]\delta\{Y\} = -\{E\} \tag{9}$$

where $[J]$ is a matrix of partial derivatives known as the Jacobian, $\{Y\}$ is a vector of solution variables, and $\{E\}$ is a vector of residuals. The equation shown above can be written as a series of contributions that, when super-imposed, govern the interdependency of the different constituents. This approach allows the number of primary solution variables to be minimized and maintains matrices that are reasonable to solve in a computationally efficient manner.

The series of mass balance equations for **SOLID PARTICLE** components can be written in the following form:

$$[J^{cc}]\delta\{Y^c\} + [J^{cw}]\delta\{Y^w\} = -\{E^c\} \tag{10}$$

where:

> $[J^{cc}]$ is the Jacobian for the liquid component equations with respect to the liquid component solution variables $\{Y^c\}$
>
> $[J^{cw}]$ is the Jacobian for the liquid component equations with respect to the primary solution variables $\{Y^w\}$
>
> $\{E^c\}$ is the vector of residuals for the solid particles in the continuous liquid field

Equation (10) can be solved for the change in the liquid component solution vector.

Then the contributions from the **SOLID PARTICLE** components in the continuous liquid field can be super-imposed on the primary balance equations.

A similar set of equations can be derived for the **DISSOLVED GAS** component contributions.

6. VERIFICATION PROBLEMS

A series of test problems were generated to verify the liquid component capability has been properly implemented in GOTHIC. This suite include problems that confirm proper code mechanical, compare results to analytic solutions, and several canonical problems to check expected response.

6.1. Code Mechanics

Null, restart, and backup testing were performed to ensure the code mechanics were working properly. Null testing ensures the simulation results are unaffected for cases without liquid components. Restart testing confirms identical results are obtained if a simulation is run from start to finish or restarted from some intermediate point. Lastly, backup testing confirms all quantities are properly restored if a time step is artificially failed and then repeated with the same time step size.

6.2. Convective Transport

Two separate but similar models were set up. One models the transport of the liquid component while the other traces the temperature rise through a similar model. The liquid component volume fraction from the model with the solid component should be identical to the normalized temperature rise from the thermal model. This testing was conducted for all flow orientations. This testing was also repeated for each differencing scheme available in GOTHIC.

Convective transport testing was also conducted for multiple components. The total amount of component was preserved, but non-uniformly distributed between 5 components fields. It was confirmed that the mixture result is identical to the single component result and that the steady-state volume fraction for each component reaches the specified value. Also, time dependent ramps were applied to each individual component and the volume fraction of each component responded as expected. This result is shown in Fig. 1.

6.3. Diffusion

The calculated transient liquid component concentration is compared to an analytic result, which is shown in Fig. 2. This problem focused on 1D diffusion, but a multi-dimensional variant was also created to verify the diffusion transport was calculated properly in all directions.

6.4. Particle Settling/Buoyancy

A 1D vertical column is initialized with three **SOLID PARTICLE** components, of negative, positive and neutral buoyancy. It is confirmed that the particles separate as expected and that the specified packing fraction for each component is not exceeded. The settling velocity associated with each component is also compared to the hand calculated value.

6.5. Volume Heating

In this case heat is added to a volume that includes a mixture of liquid and component. The calculated heatup rate is compared to a hand calculated result. This problem is repeated with multiple components, preserving total amount of component and total heat capacity, but varying the material density and heat capacity specified for each individual component. The results for these two models should be identical.

6.6. Evaporation

This test model evaporates the liquid from a volume. The results are qualitatively correct, with the volume fraction of the liquid component in the liquid phase reaching 1.0. This result is shown in Fig. 3. The simulation terminated just after all liquid evaporated because the specific heat and density of the liquid component is input as zero so the temperature rise becomes infinite when all liquid is removed.

6.7. Integral Effects Test

This test includes the effect of flow blockages, settling, bed load, and resuspension. Liquid with 2% particles is horizontally injected at a velocity of 2 ft/s for 0-800 seconds and then vertical injection of liquid with increasing velocity over time occurs starting at 800 seconds. A summary diagram is provided in Fig. 4 and several snapshots of the particle volume fractions and velocity vectors throughout the simulation are provided in Fig. 5. The results demonstrate the sediment layer being created during the first part of the simulation. Then the sediment is carried further from the injection location as the vertical velocity increases, which demonstrates the bed load transport. Finally particles in certain regions are swept away entirely by higher velocity flow later in the simulation, but particles are left behind in lower velocity regions created by the flow obstructions. Qualitatively these results align with expectations.

7. CONCLUSIONS

This paper describes the versatile liquid component capability that is available in GOTHIC and was recently expanded to allow the user to define many different fields within a single simulation. This capability, when leveraged with other existing features in GOTHIC, substantially extends the range of applications that can be evaluated. Several of these applications were presented and discussed. The assumptions, impact on the other conservation equations, and the solution scheme were discussed for each type of tracked component. Results from simple canonical problems used to verify the implementation of this feature were also presented.

REFERENCES

1. *GOTHIC Thermal Hydraulic Analysis Package, Version 8.1(QA)*. EPRI, Palo Alto, CA: 2014.
2. NEI 04-07, Vol. 2, "Pressurized Water Reactor Sump Performance Evaluation Methodology" (2004).

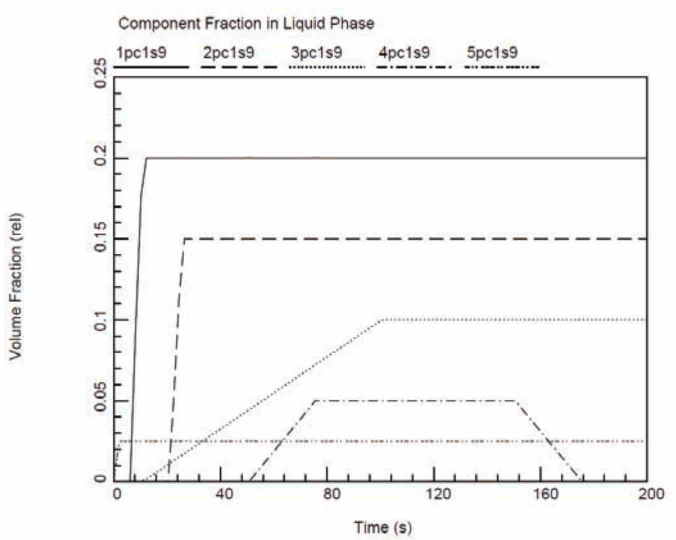

Figure 1. Convection of Multiple SOLID PARTICLE Components.

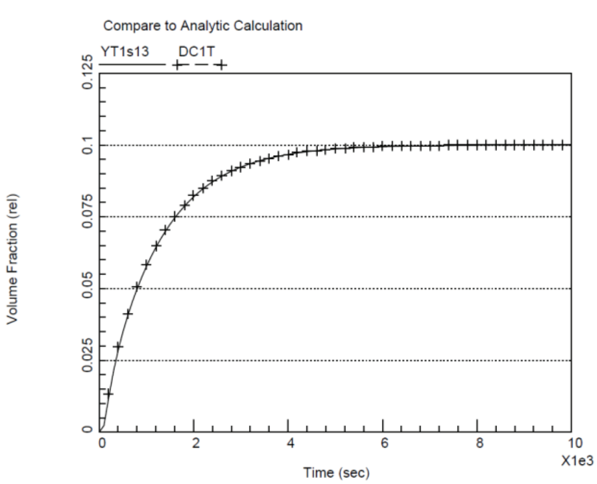

Figure 2. Diffusion.

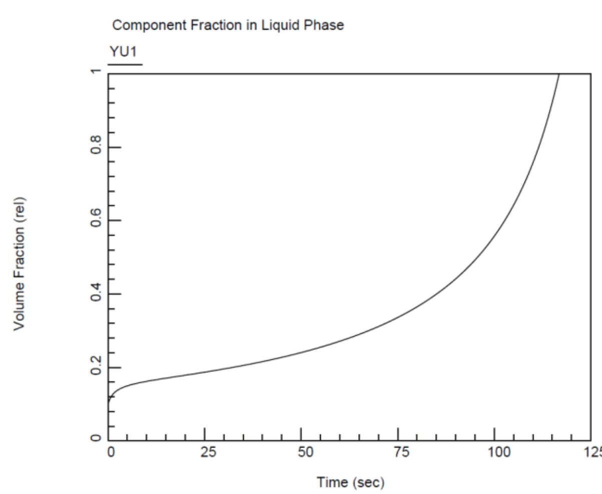

Figure 3. Evaporation.

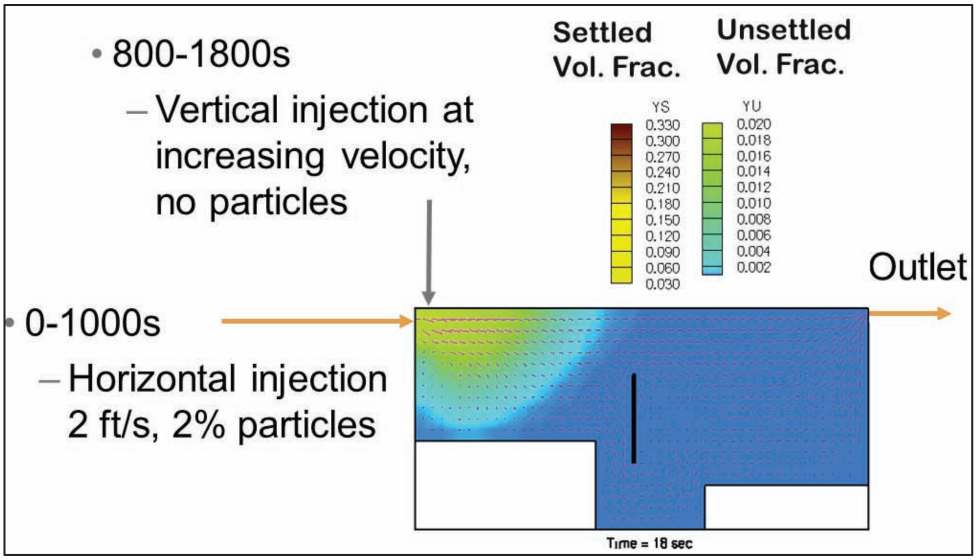

Figure 4. Integral Effects Test of SOLID PARTICLE Component Capability.

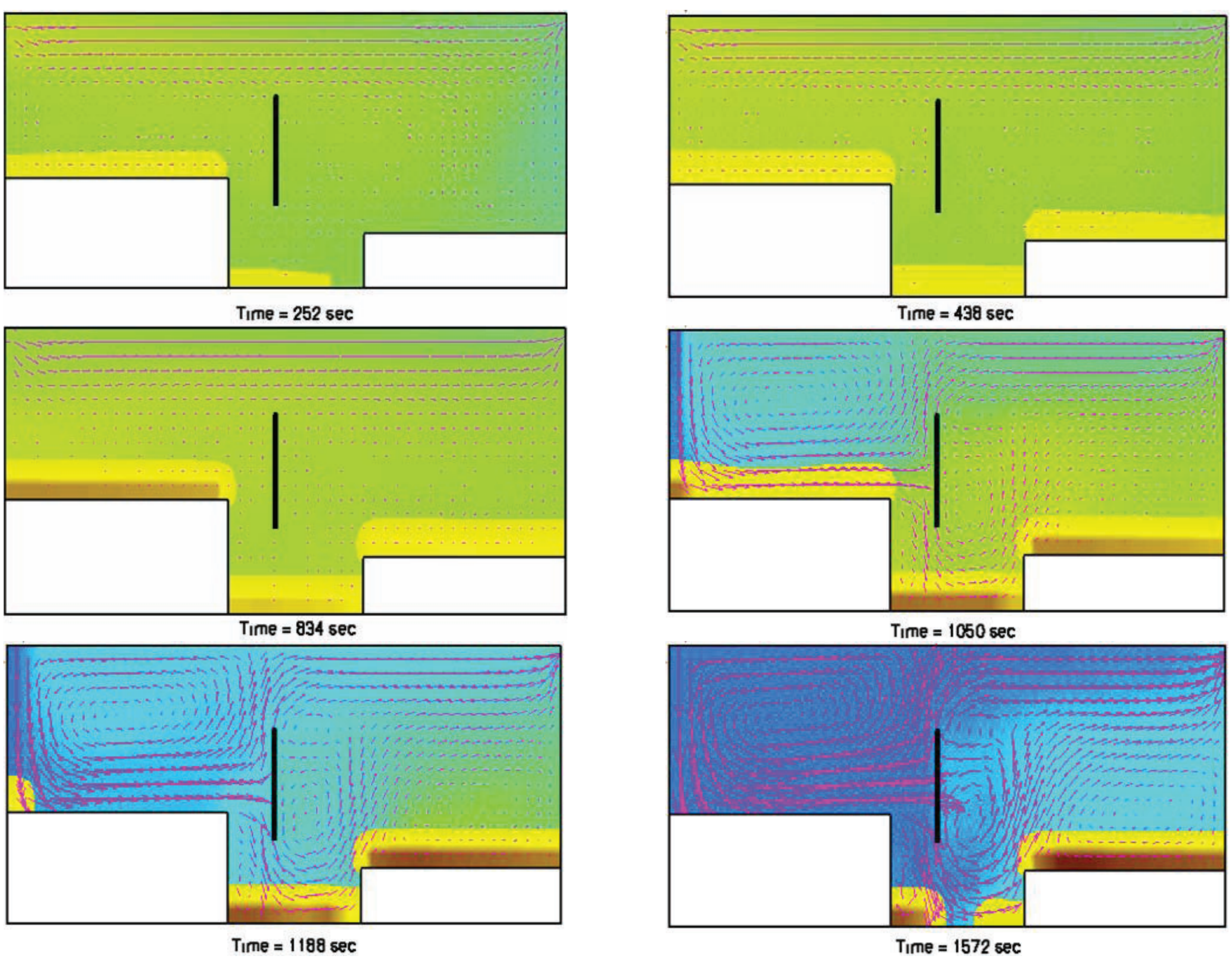

Figure 5. Snapshots of results for Integral Effects Test of SOLID PARTICLE Component Capability.