APPLICABILITY OF GOTHIC 8.3(QA) FOR NON-LWR SIMULATION, AEROSOL MODELING & HYDROGEN MANAGEMENT

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ABSTRACT

GOTHIC™ is a versatile, general purpose thermal-hydraulics software package that includes a graphical user interface (GUI) for constructing analysis models, a numerical solver that includes parallel processing capabilities and a post-processor for evaluating simulation results. It solves the conservation equations for mass, momentum and energy for multicomponent, multi-phase flow in lumped parameter and multi-dimensional geometries (1, 2, or full 3D), including the effects of turbulence, diffusion and buoyancy. The diverse equation set allows GOTHIC to solve multi-physics problems and the flexible nodalization options allows GOTHIC to provide computationally efficient solutions for multi-scale applications.

GOTHIC 8.3(QA), which represents the latest release of the software, includes a variety of new features and capabilities that allow the software GOTHIC to support the advanced modeling and simulation (M&S) requirements of the nuclear industry. The features in GOTHIC 8.3(QA) allow for the software to be used to simulate: 1) advanced, non-LWR concepts currently being developed such as sodium, molten salt and gas cooled designs, 2) dry aerosol applications such as fuel debris retrieval from the Fukushima units or to track particulates for dose, radiological or air quality assessments and 3) hydrogen management, including hydrogen burn and optimized placement of igniters or passive autocatalytic recombiners (PAR) to promote mixing and disrupt stratification. These applications will be highlighted in this paper along with a brief description of other new features included in GOTHIC 8.3(QA).

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

KEYWORDS
GOTHIC, Advanced Reactors, Aerosol Modeling, Hydrogen Management

INTRODUCTION

GOTHIC has been developed over 30+ years, with lineage tracing back to FATHOMS, COBRA-NC [1] and COBRA-TF. It can perform transient analysis including compressibility effects with heat and mass transfer. Many enhancements and capabilities have been added over that period to expand the code's applicability beyond the original sub-channel formulation from COBRA-TF. Conservation equations are solved for three (or more) primary fields, including continuous liquid, steam, non-condensing gases, and any number of interacting droplet fields. Optional secondary fields are also available to represent ice, mist/fog as well as any number of solid particle components, dissolved gases and tracers (including decay and formation of daughter products) that can be tracked in the vapor, liquid and drop fields.

GOTHIC has become a hybrid tool that bridges the gap between traditional system level thermal hydraulics analysis tools (*e.g.*, RELAP, TRAC, TRACE, *etc.*) and computational fluid dynamics (CFD) analysis tools. For example, traditional system level codes are generally limited to confined geometries and wall-drag dominated flows. Meanwhile, GOTHIC includes a full treatment of the fluid-fluid shear as well as molecular and turbulent diffusion, which is consistent with what would be found in a CFD type code. GOTHIC also considers conduction within the fluid and includes 2nd order accurate advection schemes to minimize numerical diffusion. These elements allow GOTHIC to accurately simulate mixing, stratification and buoyancy-driven natural circulation of liquid or vapor in large open regions (*e.g.*, containments, rooms, pools). This has allowed GOTHIC to be used for not only containment analysis, but other applications like thermal stratification in a boiling water reactor (BWR) suppression pool, various spent fuel pool (SFP) applications including cooling and hydrodynamic loads, tracking concentration of hazardous gases and chemicals as well as room heat-up (FLEX/ELAP), equipment qualification (EQ), and hydrogen management. Examples of GOTHIC's validation for mixing and stratification can be found in References [2] and [3]; however, the complete GOTHIC Qualification Report [4], which documents verification & validation (V&V) for a wide range of single and two-phase flow situations, is updated and released with each version of the software.

There are three primary differences between GOTHIC and typical CFD codes:

1. GOTHIC uses a rectangular computational grid with volume and area porosity factors to account for complex 3D geometries while most CFD codes use a computational grid that conforms to the bounding surface (body fitted grid).
2. GOTHIC relies on empirical correlations for near wall boundary layer effects (*e.g.*, heat transfer coefficient and friction factors) while CFD codes may use a much denser grid to resolve the boundary layer behavior.
3. GOTHIC uses a multi-volume modeling approach that makes it easy to model system and loop behavior with a small number of computational nodes. This modeling flexibility is not typically available in a CFD code.

Taken together, these differences make GOTHIC an efficient tool for many thermal hydraulic analyses that is typically much more computationally efficient than CFD due to the lower mesh density requirements. Still, GOTHIC includes the same types of features and capabilities provided by traditional system level codes, including:

- Ability to model all facets of a nuclear plant, including primary side, secondary side and safety systems.
- Models for components such as pumps/fans, valves/doors, heat exchangers, fan coolers, vacuum breakers, pressure relief valves, spray nozzles, coolers and heaters, hydrogen recombiners and ignitors, filters and sump strainer, and dryer/demisters
- Point neutron kinetics model
- Control system capability and trips

Additionally, GOTHIC has been developed within a nuclear quality assurance (NQA) program that complies with 10CFR50, Appendix B and applicable parts of ASME NQA-1. Ongoing support and error reporting complies with 10CFR Part 21 requirements

GOTHIC has been used for design & licensing of existing plants, small modular reactors (SMR) and next generation plant designs. The remainder of this paper focuses on enhancements that have been included in the latest release of the software, GOTHIC 8.3(QA) [4], and corresponding applications for the software.

GENERIC FLUID PROPERTY FRAMEWORK

Like most modeling and simulation tools used in the nuclear industry, the original working fluid in GOTHIC was water. The original water property functions in GOTHIC are implemented as curve fits of data from the ASME steam tables [5] and other sources [6]. These functions provide water property data for the complete range of conditions for which GOTHIC has been validated, including subcooled liquid, saturated liquid and vapor, and superheated vapor regions. Pressures, enthalpies and temperatures from below freezing to near the critical point are covered. These built-in water property functions have proven to be robust, but did present some limitations. This led to the development of a generic framework in GOTHIC for table-based fluid properties that can accommodate a two-phase, compressible flow representation of any fluid.

A process has been developed to generate the Generalized Fluid Property (GFP) tables for GOTHIC using the fluid Equation of State (EOS) from the NIST RefProp [7] computer code or some other generic source. The fluid (.FLD) files from RefProp provide the fluid specific coefficients to evaluate the EOS. RefProp's flash (FLSH) routines provide a general interface for calculating fluid properties for specified X-Y state points defined by two properties (*e.g.,* temperature and pressure). This is the approach for generating the required fluid property tables for water or any other fluids included in RefProp, such as heavy water, refrigerants, *etc.*

The minimum property table requirements needed for GOTHIC are summarized in Table 1. There are two conditions where the data from RefProp is insufficient for GOTHIC's needs. The first is meta-stable conditions (*e.g.,* superheated liquid and subcooled vapor). Each phase/field in GOTHIC is treated separately. Therefore, there will be situations where the liquid can become slightly superheated before starting to flash or the vapor can become slightly subcooled before starting to condense. As a result, properties for each phase must extend beyond the saturation line and into the steam dome, but such information is not available in RefProp. To compensate for this, GOTHIC approximates properties for the meta-stable states by extrapolating along a constant slope based on the last two values nearest the saturation line. Extrapolation is appropriate since the magnitude of superheating/subcooling represents the driving force for moving back to a thermodynamically stable state. This approach also provides a smooth transition of property values across the saturation line, which is essential for code stability.

The second condition is near the freezing point. Since GOTHIC is often used to analyze conditions with very dry atmospheres, where temperatures corresponding to water vapor saturation pressures well below freezing exist, properties at these low temperatures are needed; however, RefProp is limited to calculating properties for water liquid and vapor that are above the freezing point. If data is not available to GOTHIC for these conditions it would represent a significant restriction on GOTHIC applications using the tabular properties, which is not acceptable. To overcome this limitation, the existing built-in functions in GOTHIC are used to extend the water property data available in RefProp to these lower temperatures.

Table 1. Minimum Property Table Requirements for GOTHIC

Phase	**Property Description**
Saturated Liquid and Vapor	Enthalpy, enthalpy derivative $\left(\frac{dH}{dP}\right)_{sat}$, temperature and temperature derivative $\left(\frac{dT}{dP}\right)_{sat}$ as functions of pressure
Subcooled Liquid and Superheated Vapor	Density, partial density derivatives $\left(\frac{\partial\rho}{\partial P}\right)_H$ and $\left(\frac{\partial\rho}{\partial H}\right)_P$, temperature and entropy as functions of pressure and enthalpy
Subcooled Liquid	Enthalpy, constant pressure specific heat, thermal conductivity, viscosity and surface tension as functions of pressure and temperature
Superheated Vapor	Enthalpy, constant pressure specific heat, thermal conductivity and viscosity as functions of pressure and temperature

For fluids not included in RefProp, such as sodium or molten salts, a stand-alone program can be written to evaluate the fluid EOS. For example, methods for generating thermodynamic and transport properties for sodium liquid and vapor are documented in References [8], [9] and [10]. Because GOTHIC is a two-phase thermal-hydraulic code, property tables to be used with GOTHIC must include information for both liquid and vapor phases. This can be challenging when information on the thermodynamic and transport properties is limited. For example, data for molten salts is generally available only for the liquid phase over a limited temperature range and very little, if any, information is available for the vapor phase [11,12]. As a result, the method to calculate molten salt properties was modified to apply temperature dependent multipliers relative to the sodium properties in order to represent each molten salt being considered.

GOTHIC 8.3(QA) includes property tables for water (as an alternative to the built-in water property functions, which are retained to support legacy analyses) as well as property tables for six molten salts:

- $NaCl-MgCl_2$ (58.5%-41.5%)
- $LiF-BeF_2$ (67%-33%) - also referred to as FLiBe,
- LiF-NaF-KF (46.5%-11.5%-42%) - also referred to as FLiNaK,
- $NaF-ZrF_4$ (59.5%-40.5%)
- $KF-ZrF_4$ (58%-42%)
- $NaBF_4-NaF$ (92%-8%)

Proprietary fluid property tables for sodium (Na) and sodium-potassium (NaK) have also been developed to support design and analysis of TerraPower's Traveling Wave Reactor (TWR) concepts.

The water property tables were verified by comparing data points from the GFP tables with a set of independently created water property tables based on the International Association for the Properties of Water and Steam (IAPWS) Formulation 1995 [13]. These property points range from subcooled, to saturated, to superheated, to supercritical states and covered a wide range of values for liquid water and steam. Furthermore, the standard GOTHIC test suite, which includes over 330 simulations covering a wide range of single and two phase conditions was run using both the legacy water property correlations and the newly created water property tables. As expected, given the differences in the fluid property data from the two sources some minor differences exist, but this testing indicated that there were no significant changes in the overall trends or magnitudes for any of the test cases for the two water property options. Also, all test cases ran to completion, which proves the robustness and self-consistency of the new water property tables. This testing also confirmed that the tabular lookup approach does not adversely impact run time relative to the existing correlations. The robustness and computational efficiency are important aspects from a usability perspective.

It was confirmed that the new water property tables provide improved accuracy relative to the built-in functions, particularly in the calculated subcooled water compressibility, which is important for fluid hammer applications. A valve closure simulation was used to test the compressibility and verify the corresponding speed of sound. The model, shown in Fig. 1, represents a 30.48 m (100 ft) long pipe with a constant inlet pressure applied at the left end and a constant flow drawn from the right end. Once flow is established and steady, the flow is abruptly stopped simulating a sudden valve closure.

Figure 1: GOTHIC Model of Valve Closure Test.

This results in a pressure pulse being initiated at the valve location (right end) that then travels back and forth along the length of the pipe that is dampened over time due to irrecoverable pressure losses (*e.g.*, friction). An example GOTHIC response is shown in Fig. 2 when using the built-in water property functions with water at 37.78 C and 17.24 bar (100°F and 250 psia) initially moving at 0.3048 m/s (1 ft/s).

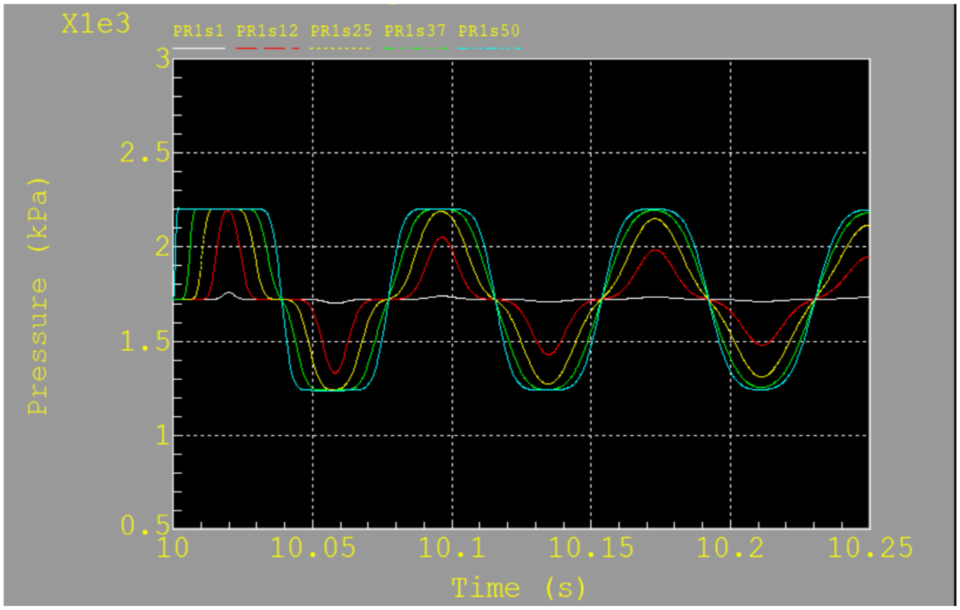

Figure 2: Example Pressure Response to Valve Closure Test using the Built-in Water Property Functions.

The wave propagation speed, which is a measure of the fluid compressibility, can be determined by observing the time that it takes for the pressure wave to traverse the length of the pipe. From Reference [11] the theoretical speed of sound in water for these conditions is 1527.9 m/s (5012.7 ft/s). The corresponding theoretical pressure rise can be calculated using:

$$\Delta P = \rho V c \tag{1}$$

where ρ is fluid density, V is initial velocity, c is speed of sound. It is equal to 4.63 bar (67.12 psi) for these conditions.

A comparison of the results for water (using both the built-in property function and the new water property tables) and sodium are provided in Table 2. These results demonstrates the improved accuracy provided by the new tabular properties, but also the accuracy for both water and sodium.

Table 2. Comparison of Results for Water and Sodium at 17.24 bar initially moving at 0.3048 m/s.

Fluid	Fluid Properties	Metric	Theoretical Result	GOTHIC Prediction	% Relative Error
Water @ 37.78 C	Built-in Functions	Pressure Rise (bar)	4.63	4.83	4.32%
		Speed of Sound (m/s)	1527.9	1562.4	2.26%
	Tabular Properties	Pressure Rise (bar)	4.63	4.65	0.43%
		Speed of Sound (m/s)	1527.9	1527.8	-0.01%
Sodium @ 260 C	Tabular Properties	Pressure Rise (bar)	6.55	6.48	-1.07%
		Speed of Sound (m/s)	2435.4	2426.2	-0.34%

The available experimental data for molten salts is limited and a similar comparison for the speed of sound was not possible; however, a series of verification problems were prepared for each molten salt to confirm the fluid properties were implemented properly. A representative result is shown in Fig. 3, where the GOTHIC predictions are shown as solid lines and the symbols show the underlying data. These figures confirm that the temperature dependent liquid properties implemented in GOTHIC accurately represent the available data.

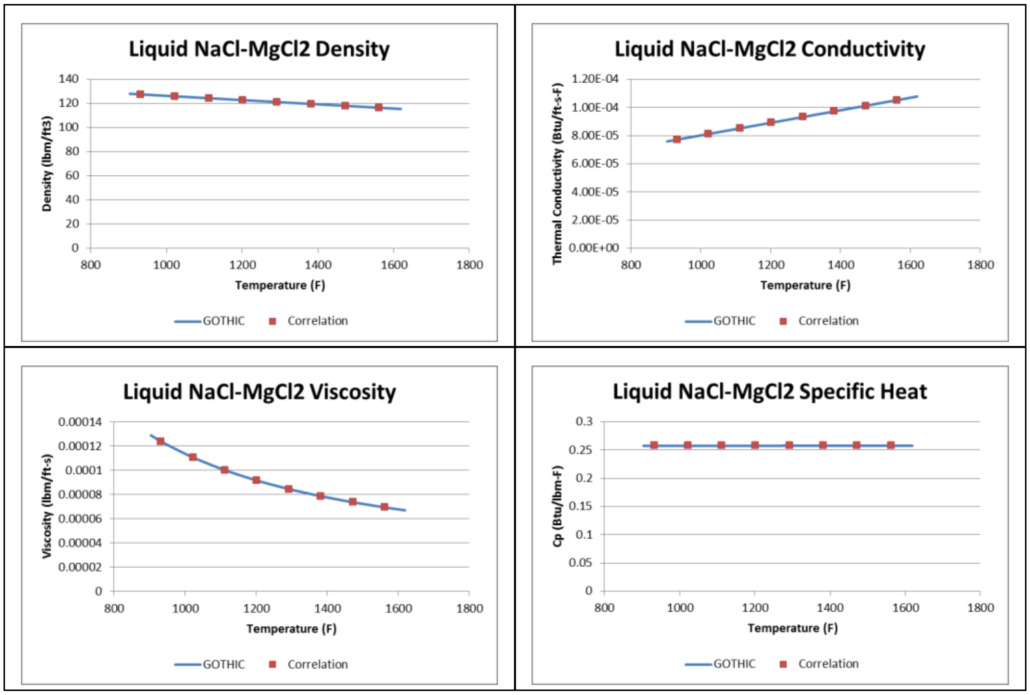

Figure 3: NaCl-MgCl$_2$ Liquid Property Comparisons

AEROSOL MODELING

The COBRA-TF subchannel code provides a three-field representation of two-phase flow, including vapor, continuous liquid and drop fields. This approach of separating the liquid phase into distinct fields allows for the mass and momentum of films and drops to be tracked separately, which is important for accurately capturing the quench front and reflood dynamics for large break loss of coolant accidents. It also allows the code to naturally capture situations of top down reflood, counter-current flow and precursory cooling. Still, COBRA-TF assumes the entrainment/deposition processes result in enough exchange between the liquid film and drop fields such that both fields could be assumed to be in thermal equilibrium and therefore a mixture energy equation was applied. The original COBRA-TF formulation also assumes a uniform drop size distribution characterized by the Sauter Mean Diameter (SMD).

GOTHIC has extended the drop field treatment beyond the original COBRA-TF formulation. Starting with GOTHIC 8.0 the modeling for the drop phase is based on aerosol mechanics, including consideration of the size distribution, agglomeration, entrainment and deposition. A modal approach is used to account for the size distribution of the drops/aerosol using any user specified number of drop/aerosol fields. The drop/aerosol inventory for each field in each computational volume or cell evolves during a simulation based on the transport, phase change and interactions with other drop/aerosol fields and with surfaces. Drop/aerosol interactions within and between fields are modeled, including formation (or entrainment), deposition and agglomeration. Each field is assumed to have a log normal size distribution. A combination of multiple drop/aerosol fields can simulate multi-peaked and non-normal size distributions as shown in Fig. 4, thus allowing a wide range of drop sizes to be tracked in a single application. For each drop/aerosol field, conservation equations for mass, energy, momentum, interfacial area and number density are solved. This allows each field to move with its own velocity, momentum and temperature.

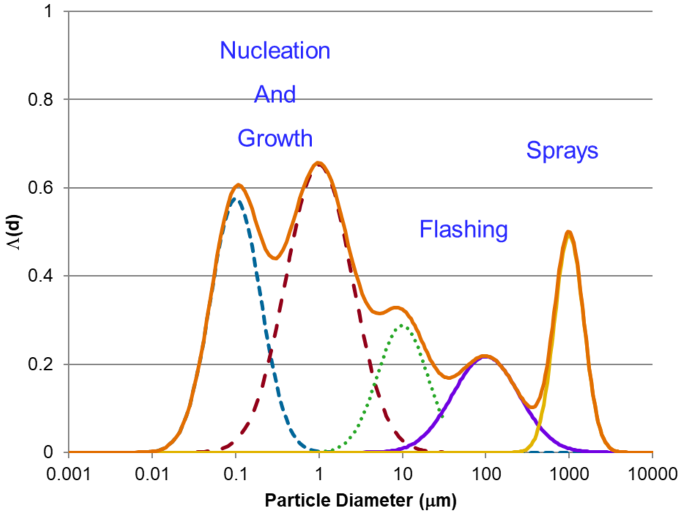

Figure 4: GOTHIC Representation of Multiple Drop/Aerosol Fields

Furthermore, a drop/aerosol field in GOTHIC can represent solid particles surrounded by some amount of water. GOTHIC's capability to track solid particle fields started with GOTHIC 7.2. That version of GOTHIC can model the transport of solid particles in the liquid phase, including deposition, resuspension and the migration of deposited material due to fluid drag (bed load). Then, in GOTHIC 8.2, the solid particle component modeling was extended to allow for multiple solid components to be tracked, each with its own distinct properties, and to model the solid components in the drop/aerosol fields. For a drop/aerosol field with solid components, as the water is depleted, the remaining solid material behaves as a dry aerosol. See References [12] and [13] for details on the solid particle component models, including conservation equations and closure relationships. Further improvements have been made in GOTHIC 8.3(QA) for modeling dry aerosols. For example, GOTHIC 8.2 required a small amount of water to be injected with the solid particles (packing fraction, *i.e.*, solid volume relative to total injected volume, could not be greater than 0.99), but GOTHIC 8.3(QA) allows a packing fraction of 1.0 (100% solid particles) to be injected. Other enhancements for dry aerosol simulations focused on time step control, code robustness and computational efficiency.

In addition to the solid particle capability, GOTHIC is also able to track any number of user defined tracer elements (including radioactive decay and daughtering of nuclides) in the liquid, vapor and droplet fields as well as surfaces and filters. GOTHIC 8.3(QA) includes several improvements to the tracer capability, including options to transfer tracers between phases with condensation or evaporation, convert from one tracer to another on radioactive decay and tracer transport by molecular and turbulent diffusion. This has application for tracking tritium or other materials that can change phase. The tracers can also be used to track concentration of iodine species and other chemicals (including [H+] and [OH-] for pH analysis).

Typical aerosol transport analyses include the phenomena listed in Table 2 and is discussed in Reference [17]. The table also includes fundamental thermal hydraulics phenomena that can affect the migration of drops/aerosols and a brief summary of GOTHIC's current capabilities for each phenomenon.

Table 3. Aerosol Modeling Phenomena and GOTHIC Capabilities.

Phenomena	GOTHIC Modeling Status
Aerosol formation	• Entrainment from films and pools caused by faster moving vapor flow • Specified source • Spray nozzle component • Water to drop conversion at cell faces • Fog formation for water droplets
Growth of aerosol particles	Growth and shrinkage due to condensation and evaporation are included Agglomeration due to: • Thermal Diffusion – Brownian motion • Turbulent Diffusion – relative motion of drops in turbulent eddies • Gravitational Collection – relative motion caused by gravity GOTHIC assumes the periphery of the drop is water when estimating the agglomeration rates.
Shape of particles	Assumes deformable spherical shape for estimating the droplet drag coefficient.
Deposition	Deposition due to: • Impaction - Bulk velocity towards a wall or surface • Gravitational Settling – gravitational forces • Thermal Diffusion – Brownian motion • Turbulent Diffusion – eddy velocity towards a wall or surface • Thermophoresis – motion due to a temperature gradient • Diffusiophoresis – mass diffusion within the vapor phase (Stephan flow for condensation)
Engineered Removal Equipment	• Generalized filter model with size dependent efficiency. • Charcoal filter and dryer/demister models are also available • Spray wash out is automatically included in the agglomeration modeling
Gas phase flow pattern	• 3D flows in complex geometries • Turbulence and jet mixing effects • Buoyancy driven flows • Leakage to adjacent rooms and environment
Liquid phase flow pattern	Transport of deposited aerosol in films and pool – 3D flow in complex geometries
Radioactivity	• Decay and daughter formation • Decay heat • Retention in filters

The drop/aerosol modeling was originally added to GOTHIC to simulate spray cooling in containment following a LOCA. With the addition of solid particles and tracers that can be tracked in the drop/aerosol fields, GOTHIC can be used for fission product tracking/retention as well as debris and dust transport. The fundamental aerosol models have been validated or verified against the referenced correlations. For example, an aerosol subject to only Brownian agglomeration tends to reach a size distribution with a Geometric Standard Deviation (GSD) of about 1.5, regardless of the initial size distribution [18]. Friedlander [19] provides a semi-analytic solution for the aging of an aerosol with agglomeration by thermal diffusion (Brownian agglomeration) alone. For the case considered by Friedlander, the size distribution, approaches a constant shape regardless of the initial GSD or particle concentration. Friedlander [19] also provides a function for the time dependent particle density. A comparison of the analytic solution and GOTHIC results is provided in Fig. 5. These results demonstrate the agglomeration model matches the theoretical self-sustaining size distribution for thermal diffusion agglomeration.

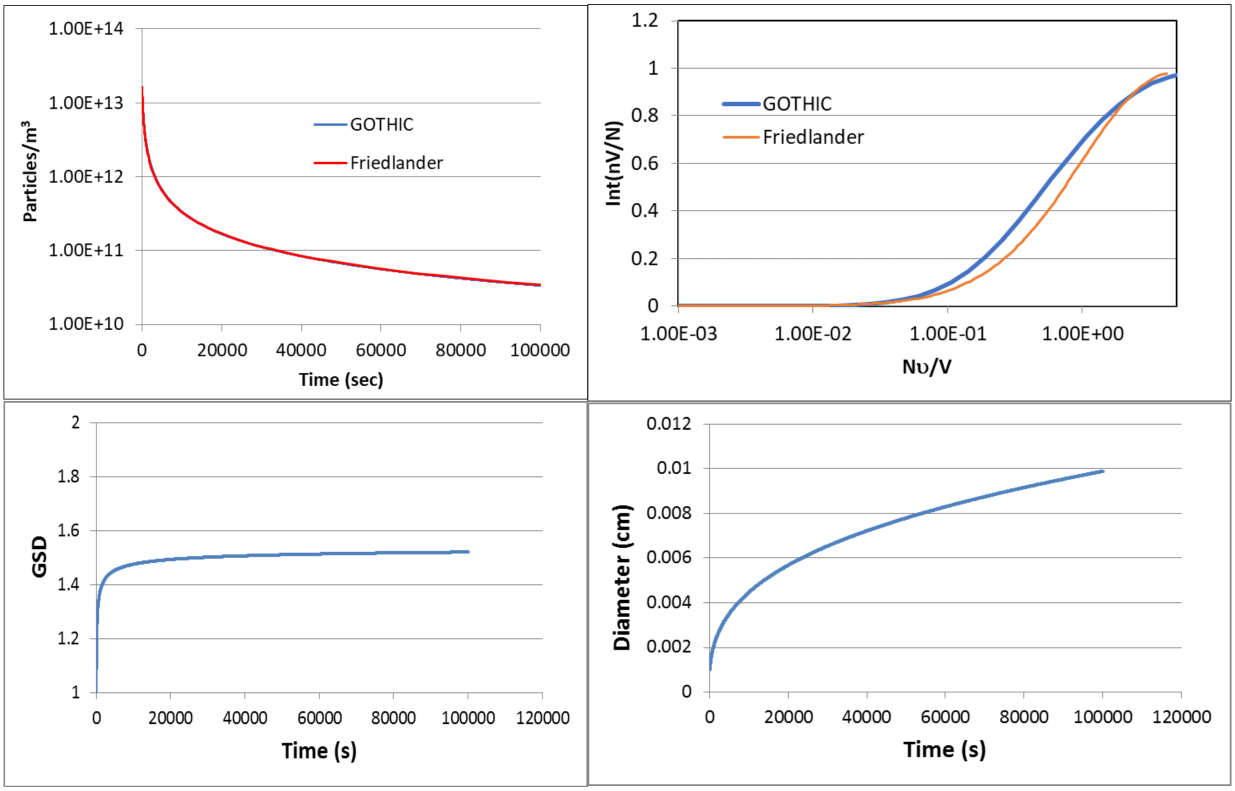

Figure 5: Friedlander Comparisons (Upper Left - Particle Count, Upper Right - Cumulative Normalized Size Distribution, Lower Left – Geometric Standard Deviation with GOTHIC approaching expected result of 1.5, Lower Right – Sauter Mean Diameter from GOTHIC.

Additionally, the Water Aerosol Leakage Experiments (WALE) provide a good basis for evaluation of the overall drop behavior in GOTHIC. In these experiments [20,21], water at high pressure and temperature was injected through a nozzle into a vented containment tank. Aerosol droplets were formed by fragmentation of the liquid jet due to flashing. Various deposition and entrainment mechanisms, as well as evaporation and condensation, influence the relative quantities of droplets deposited in the tank or carried out through the vent line. Both 3D and lumped parameter GOTHIC models have been compared to the experimental data with good agreement. Although not shown here, these results are documented in the GOTHIC Qualification report [4].

The drop/aerosol capabilities have been used extensively since the release of GOTHIC 8.0 in 2012, especially for drop behavior in containments and buildings following a high energy line break and spray effects. For example, Reference [22] is a USNRC Safety Evaluation Report (SER) that accepts the use of GOTHIC to predict mixing rates between sprayed and unsprayed regions inside containment. The overall application is spray removal of iodine from the containment atmosphere in evaluating offsite and control room dose following a Large Break LOCA. Meanwhile, Reference [23] evaluates potential dose consequences due to a LOCA for the ESBWR. GOTHIC was used to demonstrate conservatism in the mixing and transport assumptions in RADTRAD (and Reg. Guide 1.183) for isotope release.

HYDROGEN MANAGEMENT

To assure that containment integrity is maintained in the event of a severe accident with hydrogen generation and release to the containment, it is necessary to show that mitigating devices (igniter, recombiners, mixers, *etc.*) are sufficient and appropriately positioned to avoid large regions with highly combustible or explosive gas mixtures.

The fundamental analysis need is for the hydrogen distribution in a containment building. This is a complex problem involving the building geometry, 3D treatment of the mass, momentum and energy transport, including diffusion and turbulence effects, local heat sources, steam sources, drop behavior (sprays and fog) and heat and mass transfer to walls and equipment, including the formation of films and fog. The operation of the mitigation equipment also affects the hydrogen distribution. For example, a passive autocatalytic recombiner (PAR) creates a local heat source and produces steam leading to buoyancy induced mixing, condensation on walls and equipment and the potential for stratification in the hydrogen concentration. These effects must be included in the distribution analysis. Using a lumped modeling approach is not advised for such studies because it does not consider the potential for localized hydrogen accumulation. For general studies the modeling tool must have predictive capability for complex 3D flow, diffusion (both molecular and turbulent) and possible stratification to assure that adverse combustible situations are avoided. For the wide range of possible conditions, the hydrogen distribution analysis requires a CFD code or a CFD-like code such as GOTHIC.

Although not shown here, GOTHIC has been validated against gas mixing tests in Containment Systems Test Facility at Hanford, mixing tests in the Battelle Model Containment and the NUPEC mixing tests, which provides confidence in GOTHIC's capability to predict the mixing and stratification behavior. Validation has also been performed for recombiner (PAR) performance using test data from AECL. These are all documented in the GOTHIC Qualification report [4].

Fig. 6 demonstrates the results from a GOTHIC 3D PWR containment model used to examine hydrogen mixing following a discharge line small break LOCA in a steam generator compartment. The simulation includes the mixing effects due to the blowdown jet, turbulence, diffusion and buoyancy forces, which are important for capturing the mixing and potential for stratification. For this analysis the hydrogen release from the cladding oxidation (10% of the zirconium inventory) was assumed to be released at a constant rate with the break flow during the first 1500 seconds. Hydrogen from radiolysis and corrosion was assumed to occur at the bottom of the containment at a constant rate throughout the simulation. The break was terminated at 3600 seconds. During the first 1500 seconds the containment is fairly well mixed. From 1500-3600 seconds, the steam flow from the break results in a high steam concentration at high temperature in the upper part of the containment that tends to suppress the mixing of the hydrogen generated at the floor level. After the break is terminated at 3600s, the hydrogen begins to more freely mix with the upper containment. Mixing between the fuel canal and open containment is hampered by the lack of venting, leading to elevated hydrogen concentrations in that region.

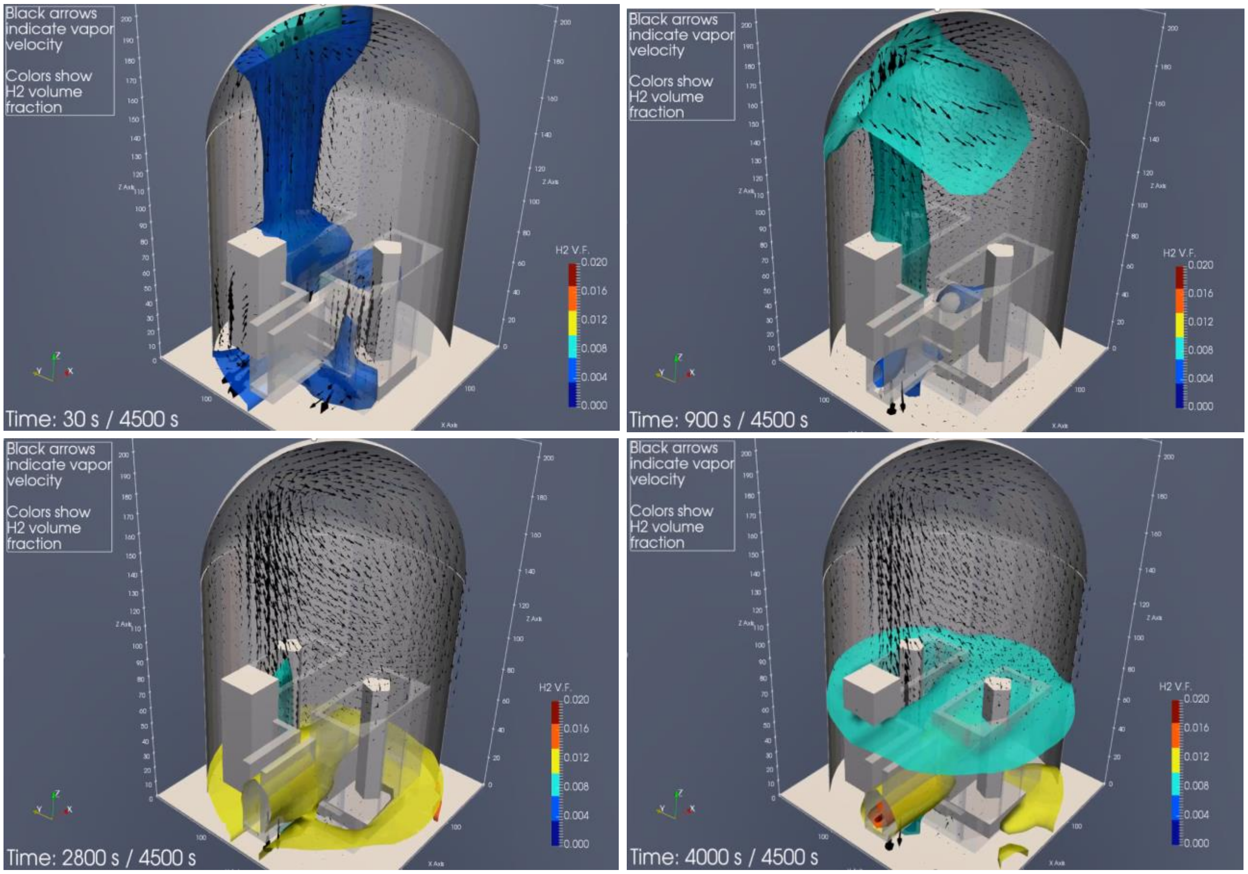

Figure 6: Example of Hydrogen Mixing Analysis using GOTHIC.

GOTHIC has been applied to various issues associated with the accidents at Fukushima, which are documented in Reference [24]. With respect to hydrogen, a 3D GOTHIC model was used to predict combustible gas concentration in the Unit 1 Reactor Building and investigate possible gas contribution from the venting of the suppression pool. Reference [25], by the Committee on the Safety of Nuclear Installations focused on hydrogen generation, transport and mitigation under severe accident conditions as a follow-up to the Fukushima accident, indicates GOTHIC's applicability for analysis of hydrogen gas distribution, combustion, and mitigation. Similarly, Reference [26] poses guidelines for applying single phase CFD codes in nuclear reactor safety problems and GOTHIC is listed as a "*tool for 3D flows*" and "*workhorse for containment safety analysis including hydrogen mixing and dispersal and deposition of radionuclides*."

GOTHIC also includes combustion models for hydrogen in air. The laminar burn model is based on a correlation for the burn velocity. The turbulent burn model uses the turbulence parameters calculated by the two equation turbulence model in GOTHIC and the eddy dissipation concept. Modeling of the propagation of the thin flame front (typically a few mm) through the rather coarse mesh for a containment or building model that is typically on the order of meters represents a significant challenge. The propagation model in GOTHIC examines local gradients in the hydrogen concentration and temperature to determine when the burn is allowed to propagate from one cell to a neighboring cell. The propagation model has been improved in GOTHIC 8.3(QA) to more accurately simulate 3D hydrogen burns. Fig. 7 compares GOTHIC to experimental results to the pressure response from a hydrogen burn test at the Nevada Test Site [27]. The test is for a burn of a 9.9% hydrogen in air mixture in a spherical vessel with ignition at the bottom. A visualization of the calculated flame front 7 seconds is also shown.

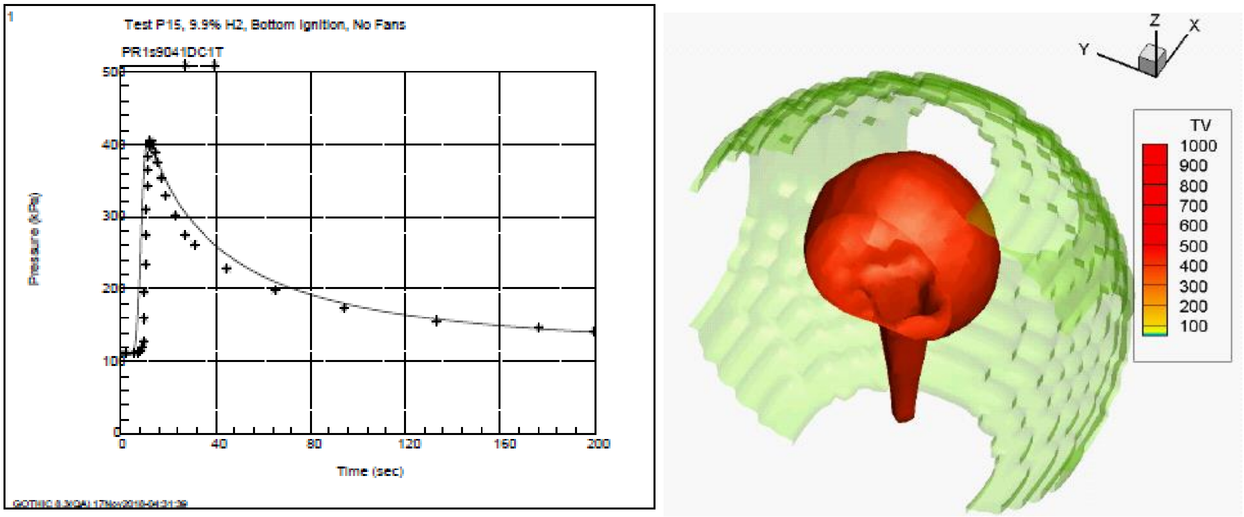

Figure 7: Comparison of GOTHIC results with experimental data from the hydrogen burn test at the Nevada Test Site [27].

OTHER MAJOR ENHANCEMENTS IN GOTHIC 8.3(QA)

Beyond the improvements to extend the capabilities of the software to new applications, GOTHIC 8.3(QA) also includes a variety of improvements to the graphical user interface (GUI). Examples of enhancements include:

- Improved panning, zooming and saved screen states to improve interaction with the drawing pad
- Improvements to copy/paste feature
- Implemented standard keyboard shortcuts (*e.g.*, open, save, print, *etc*.)
- Find/Replace tool for tables
- Ability to toggle between English/Metric units
- Built-in library of material properties that the user can select from and include in their model. Users also have the option of defining and adding their own materials to the library.
- Several features for navigating menu/tables and locating elements from the drawing
- Table peek feature to display details of forcing function or control variable without having to navigate to a different view
- Multiple table display for control variable inputs
- Improvements to reduce time required to generate input and to render the subdivided volume noding diagram

These types of improvements facilitate model construction and review as well as minimize potential for input errors.

CONCLUSIONS

GOTHIC has evolved from the COBRA-TF lineage to become a general-purpose thermal-hydraulic analysis tool that includes both system level and CFD-like attributes. This makes the software applicable to a wide-range of applications. GOTHIC 8.3(QA) represent the latest release of the software and it provides new features that allow the software to now be used for non-LWR analysis as well as for dry aerosol applications.

REFERENCES

1. Wheeler, C.L., et al. *COBRA-NC: A Thermal-Hydraulic Code for Transient Analysis of Nuclear Reactor Components*. Technical report, U.S. Nuclear Regulatory Commission, Washington, D.C., 1986. NUREG/CR-3262, PNL-4710.
2. Skelton, P. and Lane, J.W., *Validating GOTHIC against Rapid Boron Dilution Transients (ISP-43)*, International Congress on Advances in Nuclear Power Plants (ICAPP16), Paper #16503, San Francisco, CA, April 2016.
3. Ozdemir, O.E. and George, T.L., *Thermal Stratification Modeling in Suppression Pool with GOTHIC 8.0*, ANS Winter Meeting, Washington, DC, November 2013.
4. *GOTHIC Thermal Hydraulic Analysis Package, Version 8.3(QA)*. EPRI, Palo Alto, CA: 2019.
5. Meyer C.A., et al., *ASME Steam Tables*, Fifth Edition, 1983.
6. *GOTHIC Thermal Hydraulic Analysis Package Technical Manual*, Version 8.2 (QA), EPRI, Palo Alto, CA, October 2016.
7. Lemmon, E.W., M.L. Huber, and M.O. McLinden, *NIST Reference Fluid Thermodynamic and Transport Properties— RefProp Version 9.0*; Users Guide.
8. Padilla, A., Jr., *High-Temperature Thermodynamic Properties of Sodium,* HEDL-TME 77-27, Hanford Engineering Development Laboratory, Richland, WA, February 1978.
9. Fink, J.K., *Computer Codes Used in the Calculation of High-Temperature Thermodynamic Properties of Sodium*, ANL-CEN-RSD-79-2, Argonne National Laboratory, Argonne, Illinois, December 1979.
10. Fink, J.K., and L. Leibowitz, *Thermodynamic and Transport Properties of Sodium Liquid and Vapor*, ANL/RE-95/2, Argonne National Laboratory, Argonne, Illinois, January 1995.
11. Williams, D.F., *Assessment of Candidate Molten Salt Coolants for the NGNP/NHI Heat-Transfer Loop*, ORNL/TM-2006/69, Oak Ridge National Laboratory, Oak Ridge, Tennessee, June 2006.
12. Williams, D.F., L.M. Toth and K.T. Clarno, *Assessment of Candidate Molten Salt Coolants for the Advanced High-Temperature Reactor (AHTR)*, ORNL/TM-2006/12, March 2006.
13. Linstrom, P.J. and Mallard, W.G., Eds., *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, National Institute of Standards and Technology, Gaithersburg MD, 20899, https://doi.org/10.18434/T4D303, (retrieved June 11, 2019)
14. Lane, J.W. and George, T.L., *Development of a Multiple Liquid Component Capability in GOTHIC to Better Support Boric Acid, Radiological, and GSI-191 Analyses*, NURETH-16, Chicago, IL, August 2015.
15. Carstens, N.A. and George, T.L., *Development of Multiple Solid Components Capability in GOTHIC Droplet Fields*, ANS Meeting, Las Vegas, NV, 2016.
16. Harvey, A.H., Thermodynamic Properties of Water: Tabulation from the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use, NISTIR 5078, NIST, October 1998.
17. *State of the Art Report on Nuclear Aerosols*, NEA/CSNI/R(2009)5, 2009.
18. Hinds, W.C., *Aerosol Technology, Properties, Behavior and Measurement of Airborne Particles*, John Wiley and Sons, New York, 1982.
19. Friedlander, S.K., *Smoke, Dust and Haze, Fundamentals of Aerosol Behavior*, John Wiley and Sons, New York, 1977.
20. Fluke, R.J., Ogram, G.L., Rogers, L.N., and Weaver, K.R., *Aerosol Behavior in the Water Aerosol Leakage Experiments*, Technical report, Proceedings of the 2nd International Conference on Containment Design & Operation, Toronto, October 14-17, 1990.
21. Fluke, R.J., Ogram, G.L., Rogers, L.N, and Forrest, C.F., *The Water Aerosol Leakage Experiments: Programme Description and Preliminary Results*, Technical report, Proceedings of the 2nd International Conference on Containment Design & Operation, Toronto, October 14-17, 1990.
22. ML110800666, *Turkey Point Units 3 and 4 – Issuance of Amendments Regarding Alternative Source Term (TAC NOS. ME1624 AND ME1625)*, June 23, 2011.

23. ML091830154, *Licensing Topical Report: NEDO-33279, Revision 3, "ESBWR Fission Product Removal Evaluation Model"*, June 2009.
24. Fukushima Technical Evaluation: Phase 2--Revised GOTHIC Analysis - https://www.epri.com/#/pages/product/3002005295/?lang=en-US
25. ML15224B463, *Status Report on Hydrogen Management and Related Computer Codes*, June 2014
26. ML071581053, *Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications*, May 15, 2007
27. Ratzel, A.C., *Data Analyses for Nevada Test Site (NTS) Premixed Combustion Tests*, Technical Report, Sandia National Labs, Albuquerque, NM, July 1985.