## Tracking Radioactive Isotopes in HVAC and Application for Hot Cell Analyses – 20155

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#### **ABSTRACT**

In recent years, the surge in the number of isotope production facilities under design has increased the need to analyze isotope migration in facility Heating, Ventilation, and Air Conditioning (HVAC) during normal operations and accident scenarios. These facilities are used to produce isotopes for medical, security, and industrial applications and as such are subject to license and regulatory requirements 10CFR20, 10CFR30, 10CFR50, and 10CFR70. GOTHIC, a general-purpose thermal-hydraulics software package, includes the ability to model isotopic tracers, radioactive decay and isotope migration as well as HEPA and charcoal filters for isotope retention. A GOTHIC model was developed by Zachry Nuclear Engineering (ZNE) to examine the effect of negative room pressure, HEPA filtration, and HVAC fluctuations on radiation areas, hot cells and gloveboxes. Radioactive tracers were used to simulate the concentration of spills within contaminated areas, track the migration of isotopes of interest, and determine the isotopic retention and buildup on facility HEPA filters. A variety of isotopes with concern to dose (e.g., Kr-85, Sr-90, I-131, etc.), including their decay and progeny, are included in the analysis. Negative pressures are maintained in the regions of interest by a representative central HVAC system equipped with a volumetric fan that exhausts to the environment after a series of isolation valves and HEPA filters.

GOTHIC is an industry trusted tool for providing engineering solutions for a variety of applications, including fission product tracking, aerosol and particulate transport and ventilation assessments. The software provides an integrated analysis environment 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. It has been developed and maintained under a Quality Assurance program in compliance with the requirements of 10CFR50 Appendix B and applicable portions of ASME NQA-1 since 1995.

GOTHIC has been used for assessing both forced and natural convection conditions for a wide range of applications, including:

- Tracking concentration of hazardous gases and chemicals for habitability and safety assessments
- Determining ventilation and filtration requirements and optimizing location and arrangement of these systems
- Room heat-up, including diverse and FLEXible coping strategies for Extended Loss of AC Power (FLEX/ELAP)
- Equipment Qualification (EQ)

A distinctive feature of GOTHIC is the ability to track many different fields/substances in a simulation, including user defined tracer elements, in the liquid, vapor and droplet fields as well as surfaces and filters. This capability allows GOTHIC to model fission product transport and release or the removal of particulates or harmful toxins from exhaust gases using a spray scrubber or other types of filtration systems. GOTHIC also includes models for engineered equipment, such as fans, filters, charcoal filters, dryers/demisters, dampers, etc. The aerosols and other filtered material are removed or accumulated in these components.

The range of aerosol and radiological applications that GOTHIC has been used for includes:

- Source Term
  - o Primary Coolant (Equilibrium) Activity
  - o Non-Water Coolant Source/Leakage
- Conditions for Iodine Re-evolution
  - o Sump/Suppression Pool Conditions and pH
  - o RWST Conditions and pH
- Isotope Removal Mechanisms
  - o Containment Sprayed and Unsprayed Region Mixing
  - o Charcoal Filter Heating due to Iodine decay
- Radionuclide Transport and Decay
  - o Post-LOCA Release in containment
  - o Transport between connected Compartments and vent systems
  - o Groundwater transport of radionuclides.
- Non-Newtonian Fluid modeling for sludge, waste tanks, etc.

ADAMS ML071581053 (titled "Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications") poses guidelines for applying single phase CFD codes in nuclear reactor safety problems and GOTHIC is listed as a "tool for 3D flows" and "dispersal and deposition of radionuclides." The Nuclear Quality Assurance (NQA) pedigree of GOTHIC is an important aspect for applications in the nuclear industry. The fundamental tracer models (convective transport, molecular and turbulent diffusion, removal mechanisms, etc.) have been verified using analytical solutions and validated against applicable separate effects tests. Also, GOTHIC has been benchmarked to many integrated effects tests, including Phebus FP (Fission Product). GOTHIC gives good agreement for the buildup and decay of fission products in Phebus Test 3.

The model developed by ZNE demonstrates GOTHIC's applicability and acceptability for use in analyzing the migration and retention of radioactive isotopes and their progeny in normal operation and accident scenario analyses for isotope production facilities, hot cells, and gloveboxes. The tracer activities calculated by GOTHIC can then be used in downstream radiation transport and shielding codes like RADTRADNAI©<sup>a</sup>, MCNP®<sup>b</sup>, and MicroShield®<sup>c</sup> to determine on-site and off-site doses.

#### INTRODUCTION

The recent surge in the number of facilities under design which use and/or produce radioactive isotopes increases the need to analyze isotope migration in facility Heating, Ventilation, and Air Conditioning (HVAC) both during normal operations and accident scenarios. Isotope facilities are used to produce radioactive isotopes for medical, security, and industrial applications. Potential for migration of radioactive isotopes through facility HVAC is also important for new High-Assay Low-Enriched Uranium (HALEU) and existing nuclear fuel fabrication facilities. Particulate and aerosolized isotopes migrate through facility HVAC creating hot spots due to filter accumulation which may increase occupational dose while other radioactive isotopes bypass the filtration systems and are ultimately released to atmosphere in small

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<sup>&</sup>lt;sup>b</sup> MCNP® is a registered trademark of Triad National Security, LLC, manager and operator of LANL, in the United States and/or other countries.

<sup>&</sup>lt;sup>c</sup> MicroShield® is a registered trademark of Grove Software in the United States and/or other countries.

quantities which may impact public dose The facilities mentioned above are subject to license and regulatory requirements under 10CFR20, 10CFR30, 10CFR50, and 10CFR70. Guidance in 10CFR20 defines occupational and public dose limits for such facilities.

GOTHIC, a general-purpose thermal-hydraulics software package, includes the ability to model isotopic tracers, radioactive decay and isotope migration as well as HEPA and charcoal filters for isotope retention. A model was developed by ZNE to examine the effect of negative room pressure, HEPA filtration, and HVAC fluctuations on irradiation containing areas such as irradiation cells, hot cells and gloveboxes. Radioactive tracers within the model are used to simulate the concentration of spills within contaminated areas, track the migration of isotopes of interest, and determine the isotopic retention and buildup on facility HEPA filters. A variety of isotopes with concern to dose (e.g., Kr-85, Sr-90, I-131, etc.), including their decay and progeny, are included in the analysis. Negative pressures are maintained in regions of interest by a representative central HVAC system equipped with a volumetric fan that exhausts to the environment after a series of isolation valves and HEPA filters. Although facility charcoal filters not included in the demonstration model, GOTHIC includes a charcoal filter model for HVAC applications.

The model developed by ZNE demonstrates GOTHIC's applicability and acceptability for use in analyzing the migration and retention of radioactive isotopes and their progeny in normal operation and accident scenario analyses for isotope production facilities, hot cells, and gloveboxes.

#### **BACKGROUND**

GOTHIC is an industry trusted tool for providing engineering solutions for a variety of applications, including fission product tracking, aerosol and particulate transport and ventilation assessments. The software provides an integrated analysis environment that includes a graphical user interface (GUI) for constructing analysis models, a numerical solver with parallel processing capabilities to minimize computational times 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. GOTHIC has been developed and maintained under a Quality Assurance program in compliance with the requirements of 10CFR50 Appendix B and applicable portions of ASME NQA-1 since 1995.

GOTHIC has been used for assessing both forced and natural convection conditions for a wide range of applications, including:

- Tracking concentration of hazardous gases and chemicals for habitability and safety assessments
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A distinctive feature of GOTHIC is the ability to track many different fields/substances in a simulation, including user defined tracer elements, in the liquid, vapor and droplet fields as well as surfaces and filters. This capability allows GOTHIC to model fission product transport and release or the removal of particulates or harmful toxins from exhaust gases using a spray scrubber or other types of filtration system. GOTHIC also includes models for engineered equipment, such as fans, filters, charcoal filters, dryers/demisters, dampers, etc. to simulate buildings with operating HVAC systems.

#### **DESCRIPTION OF MODEL**

The GOTHIC demonstration model includes control volumes for a simple containment building and the surrounding atmosphere. The atmosphere and containment are connected via a leakage path to account for building vents, open external doors, and other points of air ingress. Inside the containment, four control volumes represent an irradiation area, a room adjacent to the irradiation area, a hot cell, and a glovebox. These areas are each connected to the containment building and a common exhaust header through a network of flow paths. The noding diagram for the hot cell demonstration model is shown below in Fig. 1.

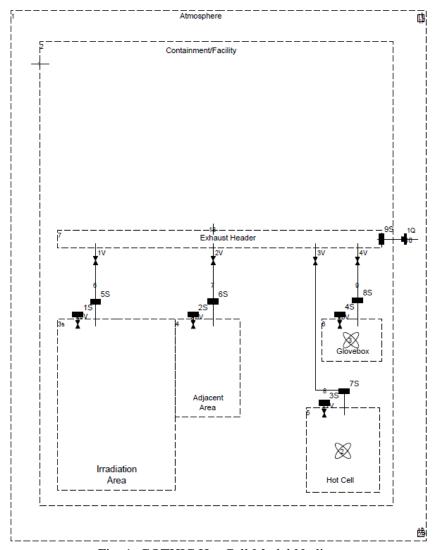


Fig. 1. GOTHIC Hot Cell Model Noding.

Each flow path in and out of the contaminated areas and the common exhaust header is equipped with a HEPA filter with an assumed 95% efficiency for particulate isotopes. Noble gases are assumed to be uninhibited by the HEPA filters with respect to radioactive holdup and migration time. Additionally, the flow paths entering the contaminated areas have built-in control valves placed after the filters and the flow paths exiting the contaminated areas have leakage valves after the filters. This configuration is representative of an expected as-built configuration of a radioactive isotope production facility. The series of filters and valves on each flow path enable GOTHIC to hold the contaminated areas at negative pressures

as would be expected to minimize release of radionuclides and ultimately contamination of surrounding non-radioactive controlled areas. A volumetric fan coupled with a final HEPA filter between the exhaust header and the environment represent the plant stack that maintains the negative pressures in the areas of interest as indicated in TABLE I. The pressure in the adjacent area was set slightly higher as it does not contain a tracer source.

TABLE I.	Vacuum	Pressures	Modeled	for A	Areas of	Interest
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Area of Interest	Vacuum (in w.g.)		
Irradiation Area	-1.0		
Adjacent Area	-0.2		
Hot Cell	-1.0		
Glovebox	-1.0		

Tracer sources in the vapor phase are modeled in the three radioactively contaminated areas (irradiation area, hot cell, and glovebox). Each source has defined isotope activities, progeny and decay fractions, half-lives, and the aforementioned HEPA filter efficiencies for each isotope. Specifically, various isotopes of concern to dose are tracked within the model such as Sr-90, Mo-99, I-131, Xe-133, and Cs-137. The tracer sources are released at one hour into the transient over a one second period. This provides adequate time for the model to establish an equilibrium between the volumes and the HVAC configuration prior to the release. The short release period quickly maximizes the total activity of isotopes introduced into the model similar to the assumption of a "puff" release seen in some accident dose analyses.

The control volume for the irradiation area is subdivided with a three-dimensional computational grid giving sixty-four uniform cells. The tracer source is placed on the lowest z-plane of the volume. The volume is subdivided to observe the air flow vectors created by the facility HVAC system.

#### **DISCUSSION**

GOTHIC includes models to simulate the transport of radioactive isotopes and the performance of filter systems designed to retain fission products inside containment following a severe accident with core damage or other event resulting in the release of radioactive isotopes. These systems typically include one or more of the following components:

- 1. Fan
- 2. Demister
- Dryer
- 4. High Efficiency Particulate Arresting (HEPA) Filter/Generalized Filter
- 5. Charcoal Filter

A fan or pump may be included to force vapor, liquid, entrained drops and aerosols through the system. A demister removes water droplets, as well as fission products carried by the drops from the flow. To maximize the effectiveness of downstream HEPA and charcoal filters, the system may include a dryer that removes moisture and reduces the humidity of the flow by adding heat. HEPA filters trap small particles and charcoal filters remove iodine molecules from the flow.

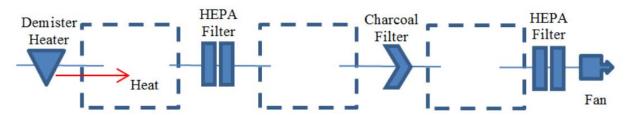


Fig. 2. Emergency Air Filtration System [1].

The tracer transport, HEPA/generalized filter, and charcoal filter models are of particular importance to this hot cell demonstration model and as such are described in the following sections.

## **Tracer Transport**

GOTHIC solves a set of tracer transport equations that track the molar inventory of each tracer in vapor and liquid phases and each drop field in each cell. The user may define a tracer type that is optionally tracked in the vapor, liquid and/or conductor surfaces. If a tracer type is tracked in the liquid, it is automatically tracked in the liquid phase and each drop field.

The tracer inventory is also tracked in filters (both generalized and charcoal filters). The effects of radioactive decay can be optionally included.

Basic assumptions for the tracer conservation equations are:

- 1. Tracers do not have any mass or volume.
- 2. Tracers have no effect on the thermodynamic or thermal hydraulic transport properties of the carrier fluids.
- 3. Aside from diffusion, tracers move at the same speed as the carrier fluid.
- 4. For drop entrainment, deposition and agglomeration, the tracers are transferred with the transferred mass.
- 5. The diffusion of any particular tracer is not affected by the presence of other tracers.

The general form of the tracer conservation [1] is

$$\frac{\partial}{\partial t} \underbrace{\int_{V} \Theta \alpha_{\phi} \Phi_{k\phi} dV}_{storage} = \underbrace{-\int_{V} \Theta \lambda_{k} \alpha_{\phi} \Phi_{k\phi} dV}_{decay} + \underbrace{\sum_{l \neq k} \int_{V} \Theta \lambda_{l} \eta_{lk} \alpha_{\phi} \Phi_{l\phi} dV}_{daughtering} - \underbrace{\int_{A} \Lambda_{f_{k}} \Psi \alpha_{\phi} \overrightarrow{u_{v}} \cdot \overrightarrow{n} \Phi_{k\phi} dA}_{convection} + \underbrace{\int_{A} \Psi \alpha_{\phi} D_{k\phi}^{c} \overrightarrow{\nabla} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{diffusion} + \underbrace{\sum_{k \neq k} \int_{V} \Theta \lambda_{l} \eta_{lk} \alpha_{\phi} \Phi_{l\phi} dV}_{interphase transfer} + \underbrace{\sum_{k \neq k} \int_{V} \Phi_{k\phi} \overrightarrow{u_{v}} \cdot \overrightarrow{n} \Phi_{k\phi} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{u_{v}} \cdot \overrightarrow{n} \Phi_{k\phi} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{u_{v}} \cdot \overrightarrow{n} \Phi_{k\phi} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{n} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} dA}_{specified source} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} \cdot \overrightarrow{v} \Phi_{k\phi} + \underbrace{\sum_{k \neq k} \Phi_{k\phi} + \underbrace{\sum$$

where  $\Phi_{k\phi}$  is the molar desntiy of the tracer k in the carrier phase  $\phi$  (including any solid particle liquid components),  $\lambda_k$  is the decay constant of tracer k,  $\eta_{ik}$  is the fraction of tracer i that decays into tracer k,  $\Lambda_{f_k}$  is the filtering factor for tracer k and  $D_{k\phi}^c$  is the total diffusion coefficient for tracer k in phase  $\phi$ , including molecular and turbulent diffusion effect. The filtering factor takes a value one when flow is out of the cell and one minus the filter efficiency when flow is into the cell, passing through the filter.

Tracers are included in the initial system inventory or can be added to the system via Tracer Sources located in a cell or a boundary condition. Radioactive decay can be modeled with up to three progeny for each tracer. The inventory for each tracer can be tracked in the vapor and liquid phases, each drop field, conductor surfaces and tracer and charcoal filters.

The model shown in Fig. 3a provides verification of tracer transport in GOTHIC. The model includes 3 tracers (A, B and C) although only 2 of the tracers (A and C) had non-zero concentrations. All volumes are lumped parameter representations, except for volume 5, which has a 2wx2dx5h grid. Volumes 3 and 4 are connected to the other volumes by isolated flow networks that can be used in GOTHIC to model HVAC systems. A 3D connector is used to connect the lower 6 cells on the east face of Volume 5 to lumped Volume 6. A constant air flow of 0.003 m³/s is supplied with a nominal tracer mixture concentration of 3.53 mol/m³. (20% Tracer A, 80% Tracer C). With a total system volume of 1.42 m³, the system turn over time is 500 seconds. [2]

The air flow is turned on at 100 seconds and turned off at 3,500 seconds. A forcing function applies a linear ramp to the tracer source concentration from 0 to 3.53 mol/m³ over the first 500 seconds of the air injection. A second forcing function is applied to the source concentration of Tracer C so that it quickly drops to 0 at 2,500 seconds.

After the on trip, the concentration of Tracer A in Volume 1 is governed by

$$V\frac{dc}{dt} = Q\left(Min\left(\frac{t}{500}, 1\right)c_s - c\right)$$
 (Eq. 2)

where V is the cell volume (0.28 m<sup>3</sup>), Q is the volumetric vapor flow rate (0.003 m<sup>3</sup>) and  $c_s$  is the source concentration (2.83 mol/m<sup>3</sup>). [2]

Fig. 3b shows GOTHIC calculated results in good agreement with the results of a spreadsheet-based numerical integration of tracer transport governed by Eq. 2 and represented by curve DC4T. Fig. 4c shows Tracer C in multiple locations appearing and turning off at different times dependent on the flow of the tracer through the system.

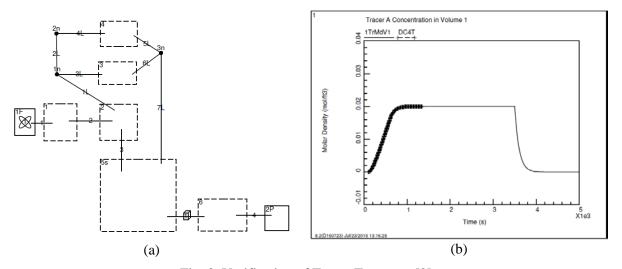


Fig. 3. Verification of Tracer Transport [2].

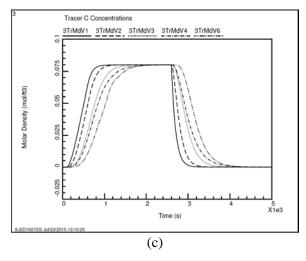


Fig. 4. Verification of Tracer Transport [2].

The tracer diffusion modeling is verified by comparison with an analytic solution for time dependent 1dimensional diffusion. The test geometry is shown in Fig. 5a. [3]

The 1-D diffusion equation with a constant diffusion coefficient is

$$\frac{\partial N'''}{\partial t} = D \frac{\partial^2 N'''}{\partial x^2}$$
 (Eq. 3)

with initial and boundary conditions of

$$N'''(x,0) = 0$$
 (Eq. 4)

$$N'''(x,0) = 0$$
 (Eq. 4)  
 $N'''(-L,t) = N'''(L,t) = N'''$  (Eq. 5)

$$\frac{\partial N'''(0,t)}{\partial x} = 0 (Eq. 6)$$

where x is measured from the midpoint of the duct and 2L is the duct length. The test model represents a 0.3m x 0.3m square duct that is 6.4m long. The volume is subdivided in the x-direction with 0.3 m grid plane spacing and initialized with air. There is a tracer source at each and a control system is used to maintain a tracer concentration of 35.3 mol/m<sup>3</sup>. With this configuration, the tracer concentration should be symmetric about the center plane, and consistent with the analytic solution (DC1T) as shown in Fig. 5b. [3]

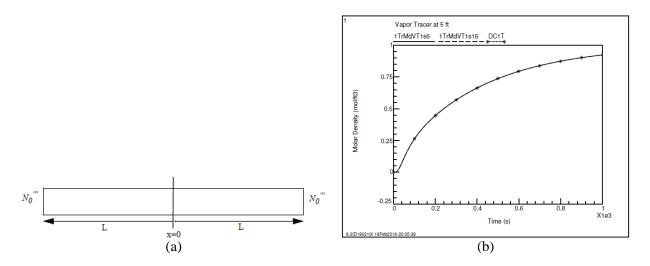


Fig. 5. Model for Tracer Diffusion Verification [3].

#### **Generalized Filters**

The generalized filter model in GOTHIC can be used to remove tracers, particulates and drops/aerosols from the flow passing through the filter, including the following filtering functions:

- Remove and retain specified fractions of selected tracers from the vapor phase flowing through the filter.
- 2. Remove and retain specified fractions of selected tracers from the liquid phase flowing through the filter.
- 3. Remove and retain specified fractions of selected liquid solid particle components from the liquid phase flowing through the filter.
- 4. Remove and retain specified size-dependent fractions of drops passing through the filter, including any liquid solid particle components in the drops.
- 5. Maintain tracer inventories, including decay effects for all tracers retained in the filter.
- 6. Maintain liquid component inventories for all liquid solid particle components retained in the filter.
- 7. Maintain a liquid inventory for all liquid from drops retained in the filter.

The filter model includes the following assumptions:

- 1. There is no pressure loss associated with the filter component itself. Any pressure losses must be accounted for in the associated Flow Path loss factors. A valve component may be included on the Flow Path to account for increased resistance as filtered materials accumulate.
- 2. Other than particulates, the liquid phase is not trapped by the filter.
- 3. The filter does not include any drainage mechanism. All filtered material is retained by the filter.

The filtration rate for tracer k in the liquid or vapor phase  $\varphi$  is

$$\dot{N}_{F_{\phi k}} = A u_{\phi} \alpha_{\phi} N_{\phi k}^{\prime \prime \prime} \epsilon_{F_k}^t \tag{Eq. 7}$$

where A is the flow path flow area,  $u_{\varphi}$  is the phase velocity,  $\alpha_{\varphi}$  is the phase volume fraction in the upstream volume,  $N_{\varphi k}^{\prime\prime\prime}$  is the upstream tracer concentration in phase  $\varphi$  and  $\epsilon_{F_k}^t$  is the specified efficiency factor for the tracer. [1]

The filter accumulation for tracer k is

$$N_{F_{\phi k}} = \int_0^t \dot{N}_{F_{\phi k}} dt - \lambda_{decay_{\phi k}} N_{F_{\phi k}} + \sum_{n \neq k} \lambda_{decay_{\phi n - k}} N_{F_{(\phi n)}}$$
 (Eq. 8)

where  $\lambda_{decay_{\phi k}}$  is the radioactive decay constant for tracer k in phase  $\varphi$ . [1]

The liquid and vapor tracer inventories are tabulated separately.

The model in Fig. 6a was constructed to verify the filter model. The model includes 5 tracers and each tracer is tracked in the vapor phase. Saturated air at  $0.28 \text{ m}^3/\text{s}$  is supplied with a nominal tracer mole density of 0.1 moles/s. The tracer specific multipliers for the source tracers are shown in the table within Fig. 6a. The Tracer Set for the filter lists only tracers T2 and T4 with a filtering efficiency of 0.8 and 0.9, respectively. The accumulation of Tracers 2 and 4 in the filter after  $1,500 \text{ seconds of operation should be } (0.28 \text{ m}^3/\text{s})(3.53 \text{ mol/m}^3)(0.1)(0.8)(1,500 \text{ s}) = 120 \text{ moles, and } (0.28 \text{ m}^3/\text{s})(10.6 \text{ mol/m}^3)(0.1)(0.9)(1,500 \text{ s}) = 405 \text{ moles.}$  These expected results are consistent with the calculated results shown in Fig. 6b.

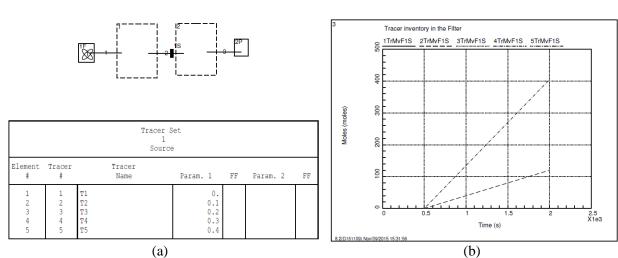


Fig. 6. Model for Tracer Filter Accumulation Verification [4].

#### **Charcoal Filters**

The charcoal filter model in GOTHIC collects and retains iodine from the vapor flow through the filter. The model considers physical adsorption of the iodine on the surface of activated charcoal, chemical adsorption of the iodine onto the activated charcoal and desorption of the physically adsorbed iodine back to the vapor flow. The model also considers diffusion of the iodine in the vapor phase inside of the filter and to the adjacent fluid cells. This allows GOTHIC to consider the release of iodine from the filter to the surrounding environment once the flow through the filter has stopped. The filter model is based primarily on the work of Wren, Qin and Moore [5], [6].

For a particular iodine isotope or compound,  $c_{m_f}$ , the concentration of the isotope in the vapor phase as it moves through the filter is governed by

$$\frac{\partial c_{m_f}}{\partial t} = D_f \nabla^2 c_{m_f} - \left( U \Delta c_{m_f} \right) - \frac{\epsilon}{\sigma_v} \left( \frac{\partial c_{p_f}}{\partial t} + \frac{\partial c_{c_f}}{\partial t} \right)$$
 (Eq. 9)

 $c_{m_f}$  is referred to as the mobile phase concentration for the isotope.  $c_{p_f}$  and  $c_{c_f}$  are the physisorbed and chemisorbed concentrations respectively.  $D_f$  is the molecular diffusivity of iodine in air. The last term is for the transfer to and from the sorbed state. Note the concentration units for  $c_{p_f}$  and  $c_{c_f}$  are mass iodine per mass charcoal. The rate of physisorption is proportional to the concentration of iodine in the mobile phase less the rate of desorption (proportional to the stationary physisorbed phase).

The mass balance for iodine concentration in the physisorbed phase is [1]

$$\frac{\partial c_{p_f}}{\partial t} = \frac{\sigma_v}{\epsilon} k_{PHYS}^A c_{m_f} - k_{PHYS}^D c_{p_f}$$
 (Eq. 10)

where  $\epsilon$  is the packing density defined as the mass of the charcoal filter divided by the macroscopic volume of the filter. The filter void fraction,  $\sigma_v$ , is defined as the macro porosity of the charcoal filter (ensemble of charcoal particles) and does not include the micro voids within the charcoal particles (micro porosity).

The physical adsorption rate constant  $k_{PHYS}^{A}$  ( $s^{-1}$ ) and the physical desorption rate constant  $k_{PHYS}^{D}$  ( $s^{-1}$ ) may have dependence on iodine concentration, conditions of the carrier vapor, and properties of the charcoal filter.

A simple GOTHIC model was constructed to test the charcoal filter model in comparison to the analytical results of Wren, Qin and Moore [6] with respect to tracer breakthrough concentration. A noding diagram for the model is shown in Fig. 7a. A boundary condition provides carrier flow of air through the system of flow paths and volumes. The volumes are very small to eliminate the storage capacity of tracers. A tracer source which represents CH<sub>3</sub>I is associated with the upstream flow boundary condition and is controlled separately from the carrier gas flow. The tracer source is shut off at 14,700 sec although the carrier gas continues to flow. As seen in Fig. 7b, GOTHIC shows good agreement with the analytical solution for charcoal filters.

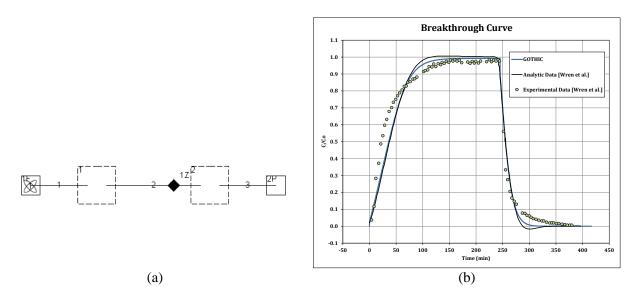


Fig. 7. Model for Charcoal Filter Tracer Breakthrough Verification [15].

### **Phebus FPT3 Benchmark**

GOTHIC's fission product migration physics models were benchmarked to the Phebus Fission Product Test 3. The Phebus FP testing program and specifically the Phebus FPT3 benchmark are briefly discussed to illustrate the applicability of GOTHIC's fission product migration models.

The Phebus Fission Product testing program consisted of 5 experiments performed by the French Institut de Radioprotection et de Surete Nucleaire (IRSN). The test facility is representative of a 1/5000 scale 900 MWe PWR, including a fuel bundle, reactor vessel, primary circuit and the containment. The objective was to investigate bundle degradation and the subsequent material release, transport and deposition in the model primary circuit and containment building for severe accident conditions in a light water reactor [8].

The FPT3 test studied the impact of a boron carbide control rod using fuel irradiated to 24.5 GWd/tU. Fuel pin gases and solid material were expelled (along with steam) into the hot leg. The material continued through a steam generator, cold leg section and then was discharged into a containment vessel. Measurements were made of various nuclides deposited on surfaces as well as conditions in the containment vessel and the sump [9].

The GOTHIC model tracks cesium, iodine, molybdenum and tellurium as well as the injected noble gases, hydrogen, nitrogen, carbon monoxide and carbon dioxide. The suspended aerosol mass in the containment is shown in Fig. 8. The data is from Figure 5.3.25 in [9]. There is a large amount of uncertainty in the experimental data, but GOTHIC captures the overall magnitude and trends exhibited in the test. These results demonstrate GOTHIC capabilities for modeling aerosol and fission product transport, agglomeration and deposition relative compared to available experimental data.

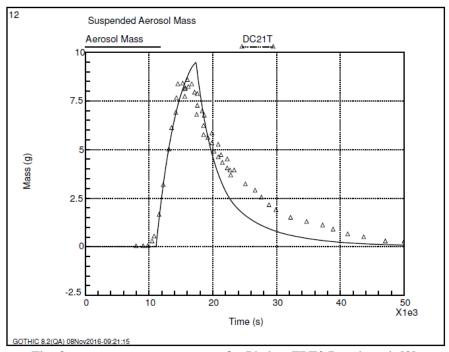


Fig. 8. Aerosol Buildup and Decay for Phebus FPT3 Benchmark [8].

#### **Hot Cell Model Results**

As evidenced, GOTHIC's tracer and filter models have been verified against multiple separate effects tests including tracer conservation, tracer diffusion, generalized filter tracer accumulation, and charcoal filter tracer breakthrough. The Phebus FPT3 benchmark demonstrated GOTHIC's performance and agreement for modeling integral effects. The hot cell demonstration model further progresses the tracer and filter models of GOTHIC to real world application for investigation of forced convection, negative pressures and isotope migration to atmosphere. Selected results from the demonstration model are provided below.

The negative pressure HVAC system establishes a vapor circulation pattern that dictates the migration of isotope migration. Fig. 9 depicts this circulation pattern using vapor flow vectors in the irradiation area on the highest z-plane (top square) and the lowest z-plane (bottom square) of the irradiation area. The vectors indicate that the circulation pattern at the bottom of the irradiation area is smaller in magnitude as it is farther away from the air entering and exiting the volume whereas the circulation at the top of the volume is highly impacted due to the HVAC inlet and exhaust occurring in this z-plane.

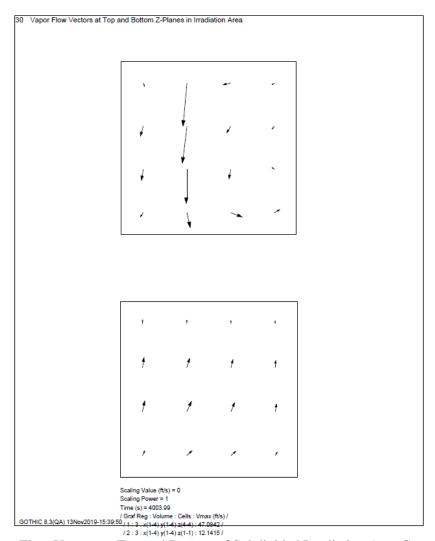


Fig. 9. Vapor Flow Vectors at Top and Bottom of Subdivided Irradiation Area Control Volume.

Fig. 10 illustrates the introduction of I-131 into the airspace and its accumulation on the outgoing filters with respect to time. The initial spike is the total I-131 activity released (effectively instantaneously) from the tracer source elements within the irradiation area, hot cell, and glovebox. The next three curves depict the accumulation and eventual saturation of available I-131 on the outgoing filters from the irradiation area, hot cell, and glovebox. The final curve is the I-131 activity which bypasses the outgoing filters from the contaminated areas, passes through the common exhaust header and ultimately accumulates on the final plant stack filter.

Fig. 11 shows the same plot fur the full duration of the transient to illustrate the retention of the accumulated I-131 on the filters. These activities would decay if the simulation was extended beyond the 8.03 day half-life of I-131 or over the remainder of the transient for a shorter-lived isotope.

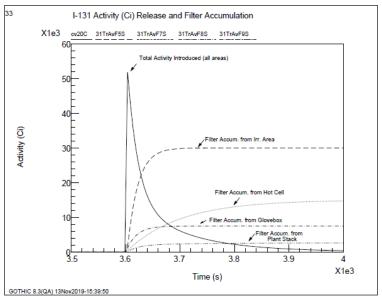


Fig. 10. Accumulation and Saturation of I-131 on HEPA Filters.

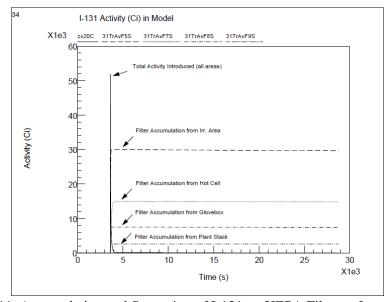


Fig. 11. Accumulation and Saturation of I-131 on HEPA Filters – Long-term.

### **CONCLUSIONS**

ADAMS ML071581053 (titled "Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications") poses guidelines for applying single phase CFD codes in nuclear reactor safety problems and GOTHIC is listed as a "tool for 3D flows" and "dispersal and deposition of radionuclides." The Quality Assurance pedigree of GOTHIC is an important aspect for applications in the nuclear industry. The fundamental tracer models (convective transport, molecular and turbulent diffusion, removal mechanisms, etc.) have been verified using analytical solutions and validated against applicable separate effects tests. Also, GOTHIC has been benchmarked to many integrated effects tests, including Phebus FP (Fission Product). GOTHIC gives good agreement for the buildup and decay of fission products in Phebus Test 3.

ZNE's hot cell model demonstrates the aptitude of GOTHIC's physics models for application to multicompartment radioactive isotope tracking through HVAC systems including various components such as isolation valves, HEPA filters, charcoal filters, and volumetric fans. Specifically, the GOTHIC model can be used to produce a variety of parameters for understanding the introduction and migration of radioactive isotopes in and through facility HVAC configurations. And tracer activities calculated in GOTHIC can be used in downstream radiation transport and shielding codes like RADTRAD-NAI©, MCNP®, and MicroShield® to determine on-site and off-site doses.

#### **ACKNOWLEDGMENTS**

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