Development of a Water Ingress Analysis Module in COPA

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1. Introduction

In a modular high temperature gas-cooled reactor (HTGR), the pressure of water/steam in the secondary system is generally much higher than the pressure of helium in the primary system, so water/steam may flow into the core due to a leak in the steam generator heat transfer pipe or damage to the steam circulation equipment [1]. Water/steam ingress into the hot reactor core poses three major safety concerns: positive reactivity insertion, chemical attack, and radioactive confinement failure. Positive reactivity insertion causes a significant temporary increase in reactor power. Due to chemical attack by moisture, oxidation and corrosion occur in the graphite material of the core and the exposed coated fuel particles. The reaction of moisture and graphite increases pressure in the primary system and creates gases such as carbon monoxide and hydrogen, creating additional safety issues. In steam cycle designs, rupture of steam generator tubes can cause pressure surges in the primary system and radioactivity deposited on the tube surfaces can be washed away and released outside the confinement building.

The study reviews the fuel behaviors during a water ingress in an HTGR and treats the development of a water ingress analysis module for the COPA code [2] that is an HTGR fuel performance analysis code.

2. Oxidation of fuel materials

2.1. Chemical reactions

During a water ingress accident, graphite gasification in an HTGR occurs through a thermal or radiolytic reactions. Considering only the thermal reaction, the overall reaction between water vapor and carbon is as follows [3]:

$$C(s) + H_2O(g) \rightarrow CO(g) + H_2(g) . \qquad (1)$$
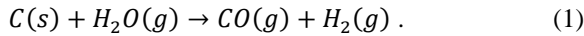
2.2. Water-vapor conservation equation

For a hollow cylinder, the water-vapor conservation equations are given by:

$$\delta \frac{\partial Y}{\partial \tau} + Pe \frac{\partial Y}{\partial r} - \frac{1}{r} \frac{\partial}{\partial r} \left(r \Phi \frac{\partial Y}{\partial r} \right) + \frac{1}{\varepsilon} \left(Pe \cdot Y - \Phi \frac{\partial Y}{\partial r} \right) \frac{d\epsilon}{dr} = Y \sum_j Da_j , \quad (2)$$

where τ ($= kt$) is the dimensionless time, k is the intrinsic reaction rate (s^{-1}), t is the time (s), $r = R/R_o$, R is the radial coordinate (cm), R_o is the outer radius (cm), Y is the pore-volume-averaged mass fraction of water vapor ((volume-averaged mass fraction of water vapor)/(mass fraction of water vapor in a coolant)), $\delta = R_o^2 k/(\phi_0 D)$, ϕ_0 is the tortuosity coefficient for a porous carbon material that is not reacted yet (dimensionless), D is the free-gas diffusion coefficient for water vapor (cm^2/s), $Pe = R_o v_D/(\phi_0 D)$ = Peclet number, v_D is the convective (Darcy) velocity for transport in graphite (cm/s), $\Phi = \phi/\phi_0$, ϕ is the tortuosity coefficient for a porous carbon material (dimensionless), ε is the void fraction ((pore volume)/(volume of pore and solid)), $Da_j = \delta_j \xi_j/Y$, $\delta_j = R_o^2 k_j/(\phi_0 D)$, $\xi_j = (V_j/\sum_i V_i) m_j (W/W_j)(\varrho_j/\epsilon) F_{b,j} F_{c,j} k_j$, V is the volume fraction (dimensionless), m is the stoichiometry coefficient ((mole of material)/(mole of carbon)) ($m = -1$ for water), W is the molecular weight (g/mol), F_b is the burnoff factor (dimensionless), F_c is the catalysis factor (dimensionless), the subscript j is the fuel material reacting with water vapor (matrix, shim particle, outer pyrocarbon, exposed kernel).

If the inner radius is facing a coolant, the boundary conditions are as follows:

$$-\phi \frac{dY}{dr}\Big|_{r=r_i} = Sh \frac{R_o}{D_h} \left(Y_\infty - Y_{r=r_i} \right) , \qquad (3)$$

$$\frac{dY}{dr}\Big|_{r=1} = 0 , \qquad (4)$$

where Y_∞ is the Y in a coolant, $r_i = R_i/R_o$, R_i is the inner radius (cm), Sh is the Sherwood number (dimensionless), D_h is the coolant hydraulic diameter (cm).

2.3. Porous carbon conservation equation

The total fractional burnoff at any location within a fuel element is given by:

$$b = 1 - \sum_j \rho_j V_j / \sum_j \rho_{j,0} V_j , \qquad (5)$$

where b is the total burnoff fraction (dimensionless), ρ is the density (g/cm^3), the subscript 0 means initial or unreacted value. The mass balance for the fuel material j is given by:

$$\frac{d\rho_j}{dt} = -F_{b,j} F_{c,j} k_j \rho_j . \qquad (6)$$

The void fraction is given by:

$$\epsilon_j = \epsilon_{j,0} - b_j(1 - \epsilon_{j,0}) = 1 - \rho_j/\rho_{th,j}, \qquad (7)$$

where ρ_{th} is the theoretical density (g/cm^3).

3. Development of a water ingress analysis module

The conservation equations for water vapor and carbon mass are coupled in a nonlinear manner, with additional nonlinearities arising from burnoff-dependent model parameters. To linearize the problem, the semi-implicit finite difference method is used to solve the water-vapor conservation equation and its boundary conditions. In the semi-implicit solution, only the linear terms of Y are evaluated at the current time step, and the nonlinear burnoff-dependent terms are evaluated and then updated at the previous time step. To increase accuracy, users can specify multiple iterations within a time step, or achieve the same results using smaller time steps. For most practical problems of interest, the burnoff does not change rapidly with time and the solution is stable and accurate over relatively large time steps.

While the water-vapor conservation equation is expressed as a product of Da and Y. In the case of numerical solutions, Y in $Da \times Y$ is evaluated at the current time step, and Y contained in Da is evaluated at the previous time step. This adds stability to the numerical solution and produces a right-hand vector containing non-zero entries only for the first node corresponding to the boundary conditions.

A FORTRAN program was developed for the above solution procedure and the completed program was inserted into the COPA code under the module name WING, as shown in Fig. 1.

4. Verification

The developed program performed some code-to-code verifications with the REACT_COMPACT [3] code on two issues: (1) comparison with experimental data for the total burnoff in a graphite test sample, (2) corrosion of the graphite web and fuel compact, and hydrolysis of exposed fuel kernels under representative water ingress conditions.

4.1. Problem 1

An out-of-pile corrosion test using water vapor in helium was performed on 2020 grade graphite. The experimental conditions are shown in Table I. The rate constant for this 2020 grade graphite has been reported to be approximately 5 times that of H-451 graphite. Therefore, the intrinsic reaction rate constant of H-451 graphite was used with $F_c = 5$. The tortuosity coefficient for diffusion in graphite can vary with burnup. Since the pressure gradient across the graphite was small enough to be ignored, the Peclet number was set to 0.

Seventy-five radial areas were applied across the graphite thickness. Only two times corresponding to the start and end of the test were used. A comparison of the calculated and measured results of burnoff at 11.92 hours is shown in Fig. 2. The COPA and REACT_COMPACT calculation results are in perfect agreement and also match well with the measurement results.

Table I: Conditions for graphite-corrosion experiment

| Parameter	Value
Type of graphite	Grade 2020
Specimen inner radius (mm)	3
Specimen outer radius (mm)	7.71
Graphite-gas interface	Inner radius
Unreacted graphite density (g/cm^3)	1.77
Graphite BET surface area (cm^2/g)	5000
Structural parameter, Ψ_0	50
Oxidation time (h)	11.92
Graphite/gas temperature (°C)	1000
System pressure (atm)	55
Gas H$_2$O concentration (ppmv)	9090
Gas H$_2$ concentration (ppmv)	455
Gas (He) flow rate (g/s)	15.04
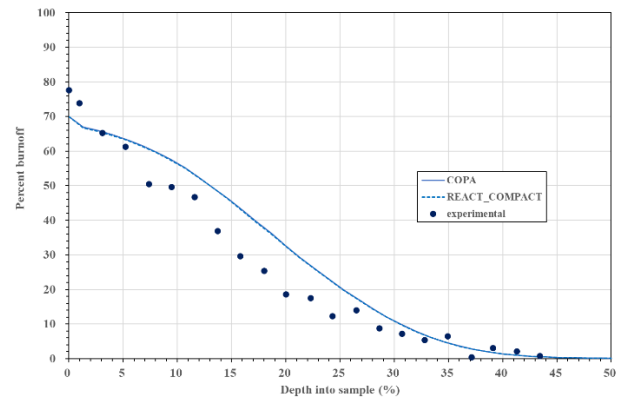
Fig. 2. Code predictions and experimental results for the burnoff profile of Problem 1.

4.2. Problem 2

This verification models a typical water ingress incident. The H$_2$O, H$_2$, and CO concentrations were all set to 1000 ppmv for 20 hours of simulation. Parameter calculations were performed in 50 °C increments for unit cell temperatures ranging from 600 °C to 1000 °C. The system pressure was maintained at 70 atm and the coolant channel flow rate was set to a low value (0.02 g/s, $Re \approx 36$) to simulate natural convection conditions.

Fig. 3 and 4 show the radial values within the unit cell of water vapor, burnoff, and exposed kernel after 20 hours when the unit cell temperature is 700 °C. The reaction rate constant of H-451 grade graphite was applied to the graphite web and graphite shim particles in the compact. The compact matrix was assumed to be 20 times more reactive than H-451 graphite. The pyrocarbon coating layer was assumed to be 0.4 times less reactive than H-451 graphite. Considering these

assumptions, the burnoff profiles of graphite shim particles, compact matrix material, and pyrocarbon coating layer shows the expected behavior. The COPA and REACT_COMPACT calculation results are in perfect agreement.
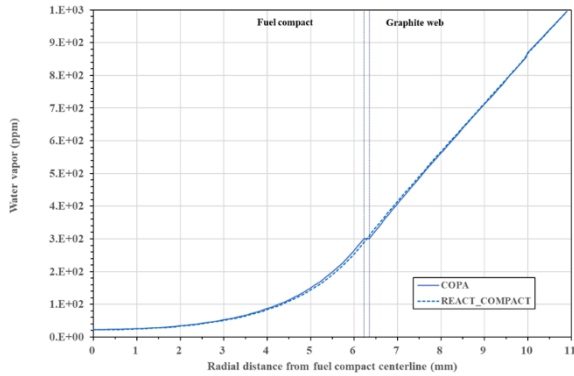

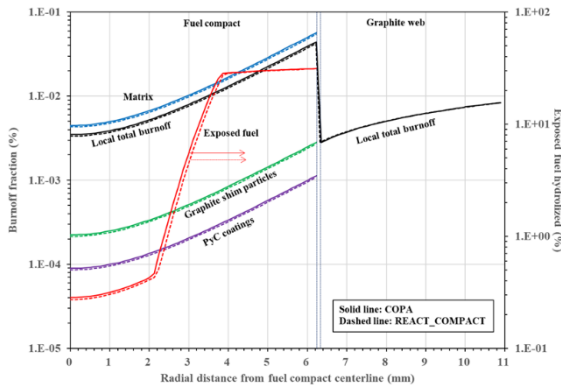Fig. 3. Radial water vapor concentration after 20 hours at a unit cell temperature of 700 °C in Problem 2.

Fig. 4. Radial burnoff fraction and hydrolyzed exposed kernel after 20 hours at a unit cell temperature of 700 °C in Problem 2.

5. Summary

In the event of a water ingress, the water-vapor conservation equation and the carbon conservation equation were established. The finite difference solution scheme for the conservation equations was obtained and programmed in FORTRAN language. The completed FORTRAN program was inserted into the COPA code as a module named COPAWING. The developed program performed some code-to-code verifications with the REACT_COMPACT code on two issues: (1) comparison with experimental data for the total burnoff in a graphite test sample, (2) corrosion of the graphite web and fuel compact, and hydrolysis of exposed fuel kernels under representative water ingress conditions. The COPA and REACT_COMPACT code calculation results were perfectly consistent. The experimental data of verification problem (1) and the calculation results of the two codes also matched well.

ACKNOWLEDGEMENTS

REFERENCES

[1] IAEA, 2008. Accident Analysis for Nuclear Power Plants with Modular High Temperature Gas Cooled Reactors. Safety Reports Series No. 54.
[2] Kim, Y. M. and Jo, C. K., 2019. COPA ver. 1.0: Theory Report. KAERI/TR-7945/2019.
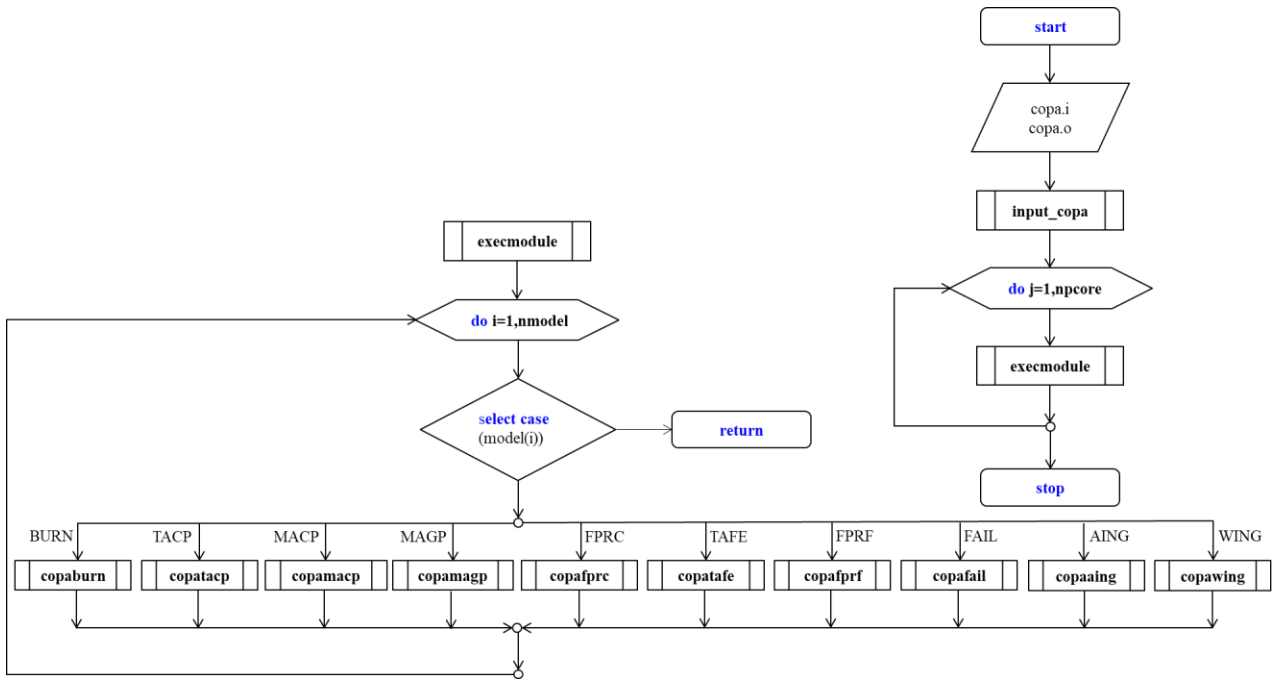[3] Richards, M., 2014. REACT_Compact Software Design Description and User's Manual. USNC-KAERI-MCP-00001, Rev. 0.

Fig. 1. Modules of COPA code.