

## One-Dimensional Model for Fission Product Plateout and Circulating Coolant Activities in a HTGR

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### 1. Introduction

Numerical prediction of fission product plateout and circulating coolant activities under normal operating conditions are crucial in the design of a high temperature gas-cooled reactor (HTGR) [1,2]. The results are used in the design of the purification system and the shielding of the components of the coolant systems for maintenance and repair. In addition, circulating coolant activities and plateout fission products significantly contribute to early source terms under loss of coolant accident scenarios [3]. Thus, a number of computer codes have been developed to evaluate the fission product plateout and circulating coolant activities in a HTGR [4]. In the past, Korea Atomic Energy Research Institute (KAERI) also developed the GAMMA-FP code [5] for the fission product plateout. However, critical limitations were found in GAMMA-FP for the simulation of a long period of time (e.g., 20-60 years) due to poor computational performance [6]. Therefore, a development of a new computer code named POSCA (Plate-Out Surface and Circulating Activities) has been in progress targeting simulations of hundreds of nuclides during whole periods of reactor life time.

This paper presents the numerical model of the POSCA code. In order to confirm the accuracy and reliability of the numerical model, a simple benchmark problem has been solved using POSCA and compared with analytical solutions.

### 2. Physical Model

#### 2.1 Governing Equations

Fig. 1 illustrates the fission product plateout across the primary coolant loop of a HTGR. Radioactive nuclides can enter the primary coolant as the result of release from wetted surfaces in the reactor core or by direct production in the coolant. Radioactive nuclides are removed by the following phenomena:

- (1) Nuclide decay
- (2) Deposition on cooler wetted surfaces (i.e., plateout)
- (3) Coolant purification
- (4) Coolant leak

In order to describe these phenomena accurately, one-dimensional model is preferred in a HTGR since the major physical parameters are not uniform across the primary loop. For example, sorption mechanism is strongly temperature dependent and a large temperature gradient exists across the primary loop of a HTGR.

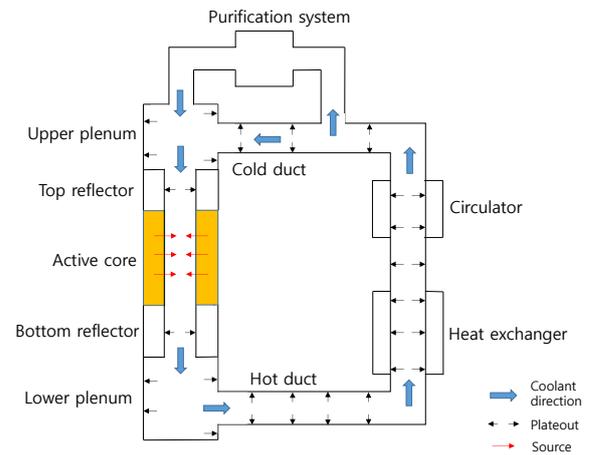


Fig. 1. Fission product plateout across the primary coolant loop of a HTGR.

Fig. 2 shows the three region model (i.e., coolant bulk, thin boundary layer, and structural surface) adopted in the POSCA code to model the fission product transport from the coolant to the wall surface. Here, the concentration of radioactive nuclide  $i$  in the coolant bulk ( $C_i$ ) is introduced under the assumption that the coolant is well mixed across the flow area. In general, a large gradient in the concentration exists between the bulk and the thin boundary layer ( $B_i$ ). It is assumed that the transport of the nuclide from the bulk to the boundary layer can be described by the mass transfer coefficient ( $h$ ). It is further assumed that the relationship between the concentration of the plateout surface ( $S_i$ ) and the boundary layer is governed by a sorption mechanism. The surface concentration is divided into two kinds, i.e., reversible ( $S_{R,i}$ ) and irreversible ( $S_{I,i}$ ) forms. Irreversible forms of the surface concentration can result from chemical reactions on or diffusion into the wetted surface material.

Based on these assumptions, the mass conservation equations throughout the coolant and surface regions can be formulated as follows:

#### Mass conservation in coolant bulk

$$\frac{\partial C_i}{\partial t} = \dot{q}_{c,i} + \sum_{j=1}^{N_t} a_{i,j}^* C_j - \frac{P_W}{A_F} h_i (C_i - B_i) - \frac{1}{A_F} \frac{\partial}{\partial x} (A_F v C_i) \quad (1)$$

Where  $\dot{q}_{c,i}$  = generation source in coolant,  $N_t$  = total number of considered nuclides,  $a_{i,j}^*$  = decay chain and

removal matrix,  $\rho_w$  = wetted perimeter,  $A_F$  = flow area,  $v$  = coolant velocity. The removal mechanism includes nuclear reaction, purification, and coolant leak.

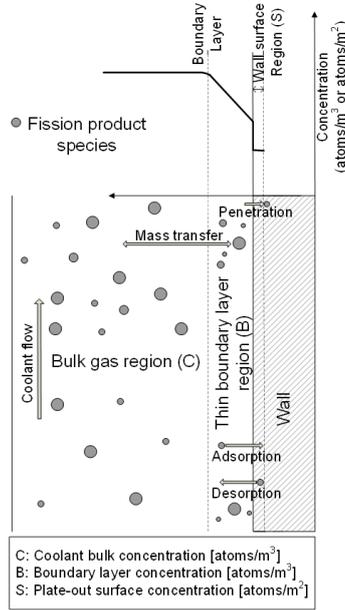


Fig. 2. Three layer model adopted in the POSCA code.

#### Mass conservation of reversible nuclide on wall surface

$$\frac{\partial S_{R,j}}{\partial t} = \dot{q}_{R,j} + \sum_{i=1}^{N_r} b_{i,j}^* S_{R,j} + h_i (C_i - B_j) \quad (2)$$

Where  $\dot{q}_{R,j}$  = reversible nuclide generation source,  $b_{i,j}^*$  = decay chain and removal matrix. The removal coefficient includes nuclear reaction and transformation into irreversible form.

#### Mass conservation of irreversible nuclide on wall surface

$$\frac{\partial S_{I,j}}{\partial t} = \dot{q}_{I,j} + \sum_{i=1}^{N_r} c_{i,j}^* S_{I,j} + \beta_i S_{R,j} \quad (3)$$

Where  $\dot{q}_{I,j}$  = irreversible nuclide generation source,  $c_{i,j}^*$  = decay chain and removal matrix,  $\beta_i$  = rate constant for transformation from reversible to irreversible form.

### 2.2 Sorption Equation

In general, the boundary layer concentration is known as a non-linear function of the surface concentration of reversible nuclide.

$$B_j = f(S_{R,j}) \quad (4)$$

For example, in the case of a Freundlich sorption mechanism, Eq. (4) becomes

$$B_j = K(x,t) S_{R,j}^{\gamma(x,t)} \quad (5)$$

For this reason, the POSCA code has to solve coupled non-linear partial differential equations, Eqs. (1)~(4).

### 3. Numerical Method

Because of the non-linearity of the governing equations and the fact that most of physical parameters change with time and space, a finite difference procedure is used to solve the equations (1)~(4). In order to speed up the calculation in the POSCA code, non-linear terms of Eq. (4) are linearized as

$$B_j \approx \phi_j^* + \sum_{j=1} \psi_{i,j}^* S_{R,j} \quad (6)$$

Where

$$\psi_{i,j}^* = \left. \frac{\partial B_j}{\partial S_{R,j}} \right|_{S_{R,j}^0}, \quad \phi_j^* = B_j(S_{R,j}^0) - \sum_{j=1} \psi_{i,j}^* (S_{R,j}^0) S_{R,j}^0$$

Using Newton-Raphson iteration procedure, the iteration can be converged efficiently and the linearization approaches to be exact.

The finite difference discretization with time and space for coupled linear differential equations and its solution method are well known and straightforward. In the POSCA code, the fully implicit discretization is used for time and the upwind scheme is used for coolant convection.

### 4. Comparison with GAMMA-FP Models

Table I compares the physical and numerical models of POSCA and GAMMA-FP.

Table I: Comparison of Physical and Numerical Models

Models	POSCA	GAMMA-FP
Governing equations	1-D	1-D
Thermo-fluid solver	no	yes
Time step limitation	no	yes
Solver for non-linear coupled equations	linearized sorption model + Newton-Raphson iteration	fractional step + Runge-Kutta solver
Sorption model	linear and non-linear correlations	non-linear correlations
No. of considered nuclides	several hundreds	several
Decay chain	yes	no
Irreversible penetration	yes	no
Neutron reaction	yes	no
Coolant leak	yes	no

The largest difference is the availability of the thermo-fluid solver. The POSCA code does not have a thermo-fluid solver and the thermo-fluid conditions are supplied by a user as boundary conditions. In addition, the POSCA code does not have any time step limitation for

converged solutions. Therefore, it is obvious that the computational speed of POSCA is much faster than GAMMA-FP. Due to the fast computation capability, the POSCA code will be able to consider hundreds of nuclides during whole periods of reactor life time. Such a capability is required for the design of the purification and shielding systems.

The efficiency of the solvers for non-linear coupled equations needs to be carefully examined. But more detailed physical models such as decay chain are going to be implemented in the POSCA code as shown in Table I.

### 5. Analytic Benchmark

In order to confirm the accuracy and reliability of the numerical model, a single loop benchmark problem has been computed using the POSCA code.

Fig. 3 shows the concept of the single loop benchmark and the input parameters are provided in Table II. Irreversible form of nuclide is not considered in the benchmark. A linear sorption equation (Eq. (7)) is used. Since the present benchmark is not dependent on space, the analytical solutions of the coupled equations of Eqs. (1) and (2) are available.

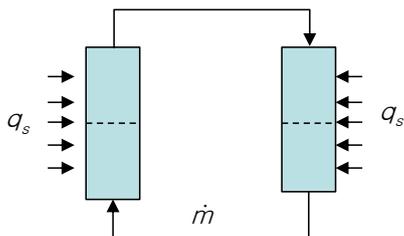


Fig. 3. Single loop benchmark.

Table II: Input parameters of single loop benchmark

Parameters	Value
Loop length (cm)	20
Pipe diameter (cm)	2
Mesh spacing (cm)	5
Initial coolant concentration	0
Initial surface concentration	0
Decay constant (1/s)	10
Helium flow rate (g/s)	42.085
Coolant/wall temperature (°C)	800/800
Coolant pressure (atm)	50
Coolant source rate	0
Surface source rate (#/cm <sup>2</sup> s)	2.2E+7
Linear sorption model	Eq. (7)
Transformation rate to irreversible form	0

$$\rho = \frac{S}{10^{20}} (10^{3.88-3730/T_w}) \quad (7)$$

Where  $p$  = vapor pressure in Pa.

Fig. 4 shows the comparison of the POSCA results with the analytic solutions. It can be seen that the POSCA results are in exact agreement with the analytic solutions.

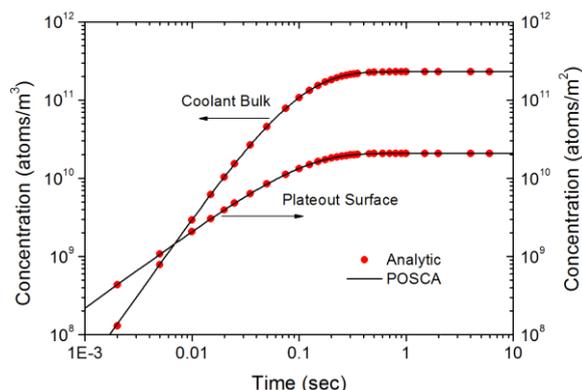


Fig. 4. Comparison of the POSCA results with analytic solutions of the single loop benchmark.

### 6. Conclusions

In this work, the numerical model of the POSCA code to predict the fission produce plateout and the circulating coolant activities was presented and it was benchmarked against the analytic solutions of a single loop problem. The comparison of the POSCA results with the analytical solutions shows that the numerical model of POSCA is accurate as well as reliable. Further development of the POSCA code is on-going toward practical applications to HTGR designs.

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