Verification of the POSCA Code Using Analytic Benchmark Examples

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1. Introduction

In order to predict fission product plateout and circulating coolant activities under normal operating conditions of a high temperature gas-cooled reactor (HTGR), development of a new computer code named POSCA (Plate-Out Surface and Circulating Activities) has been in progress [1]. The results of the POSCA code can be used for the design of the purification system and the shielding of the components as well as the early source analysis under loss of coolant accident scenarios.

This paper describes a verification study of the POSCA code using analytic benchmark examples. The existing examples which have analytic solutions [2] were adopted to verify the POSCA code.

2. Physical Models of POSCA

The major physical models of the POSCA code are:

(1) Fission product release into coolant circuit
(2) Advection by coolant flow
(3) Mass transfer between coolant bulk and boundary layer
(4) Sorption onto structural surface
(5) Nuclide transformation by decay chain or neutron absorption
(6) From reversible to irreversible transformation
(7) Coolant leak and purification

In order to describe these phenomena accurately, one-dimensional mass conservation equations across a primary loop of a HTGR were formulated as follows:

<u>Mass conservation in coolant bulk</u>

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

Where $\dot{q}_{c,i}$ = generation source in coolant, N_T = total number of nuclides, $a^*_{i,j}$ = decay chain and removal matrix, P_w = wetted perimeter, A_F = flow area, h_i = mass transfer coefficient, B_i = boundary layer concentration, v = coolant velocity.

<u>Mass conservation of reversible nuclide on wall surface</u>

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

Where $\dot{q}_{R,i}$ = reversible nuclide generation source, $b^*_{i,j}$ = decay chain and removal matrix. The mass conservation for irreversible nuclides adopted in POSCA is not considered in this paper.

In addition, sorption is modeled as:

$$B_i = f(S_{R,j}) \quad (3)$$

3. Analytic Benchmarks

Analytic solutions of Eqs. (1)~(3) can be obtained in the following limited conditions.

(1) Eqs. (1) & (2) are either time independent or space independent.
(2) Sorption equation (i.e. Eq. (3)) is simple (e.g., linear).

General Atomics (GA) theoretically derived analytical solutions of Eqs. (1)~(3) and six examples were addressed to verify their own code, PADLOC [2]. For the verification of the POSCA code, the existing analytic solutions and examples of GA were adopted. The verification of POSCA using the first example was carried out in the previous work of the authors [1]. In the present paper, the results of the verification study for the other five examples are presented.

3.1 Steady-state multi-blocks

Fig. 1 shows the POSCA model to simulate steady-state multi-blocks which consists of 7 branches.

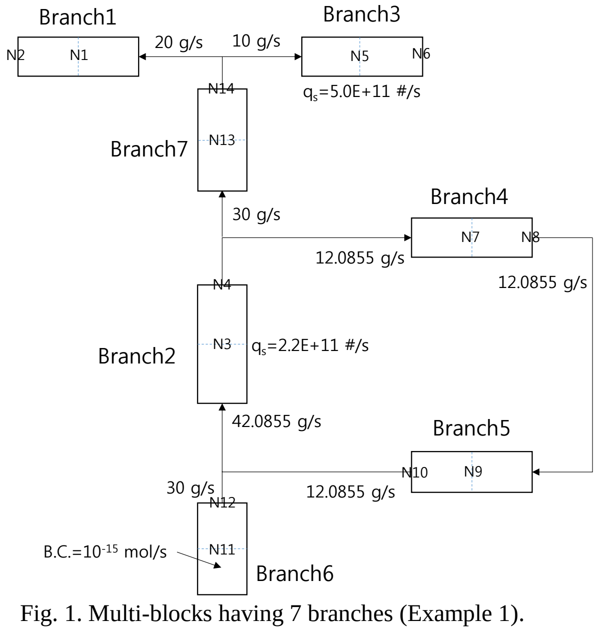

Fig. 1. Multi-blocks having 7 branches (Example 1).

Table I presents the geometry and thermo-fluid conditions of each branch. The linear sorption model is applied to Branch 1 whereas the Freundlich model is applied to the other Branches to test the applicability of each model.

A POSCA calculation shows that steady-state results are achieved within the simulation time of 50 seconds. Table II shows the percent error of the steady-state coolant (C_i) and surface concentrations (S_i) calculated by POSCA against the analytic solutions. It can be seen that the POSCA results are in exact agreement with the analytic solutions. The largest error is only 0.05%.

Table I: Geometry and thermo-fluid conditions of Example 1

	Length (cm)	Dia. (cm)	Pres. (atm)	Temp. (°C)	Sorption
Branch1	10	1	30	500	LS[a]
Branch2	10	2	50	800	F[b]
Branch3	10	3	30	500	F
Branch4	10	4	40	750	F
Branch5	10	5	30	700	F
Branch6	10	6	30	500	F
Branch7	10	7	30	750	F

LS[a] = linear with saturation, F[b] = Freundlich

Table II: Verification result of Example 1

		Error of POSCA results (%)	
	Node	Ci (#/m^3)	Si(#/m^2)
Branch1	1	2.7E-04	2.7E-04
	2	2.7E-04	2.7E-04
Branch2	3	-6.0E-03	-5.9E-05
	4	7.3E-05	9.5E-07
Branch3	5	3.4E-04	1.1E-06
	6	5.0E-02	2.7E-04
Branch4	7	5.4E-05	1.2E-05
	8	5.4E-05	1.2E-05
Branch5	9	-5.3E-05	-1.1E-05
	10	-5.3E-05	-1.1E-05
Branch6	11	-1.8E-10	-3.1E-11
	12	-1.8E-10	-3.1E-11
Branch7	13	1.6E-05	3.4E-06
	14	1.6E-05	3.4E-06

3.2 Steady-state multi-blocks with flow reversal

Example 2 is the same as Example 1 except a flow reversal in the loop (Compare Fig. 1 and Fig. 2). In addition, only linear sorption model is applied for all branches.

Table III shows the percent error of the steady-state results of POSCA against the analytic solutions. It shows that the POSCA results are in perfect agreement with the analytic solutions. It also proves that complex flow networks having flow split, merging, and reversal can be reliably modelled by POSCA.

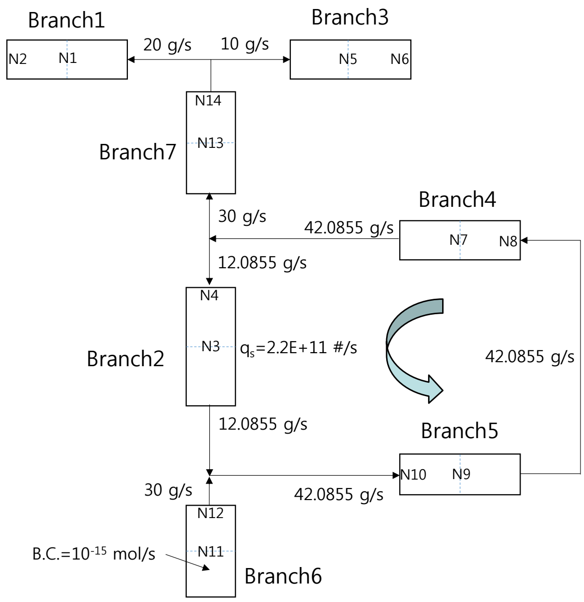

Fig. 2. Multi-blocks with flow reversal (Example 2).

Table III: Verification result of Example 2

		Error of POSCA results (%)	
	Node	Ci (#/m^3)	Si(#/m^2)
Branch1	1	2.7E-04	2.7E-04
	2	2.7E-04	2.7E-04
Branch2	3	1.6E-04	6.3E-06
	4	1.6E-04	3.4E-06
Branch3	5	4.5E-05	4.6E-05
	6	4.5E-05	4.6E-05
Branch4	7	-1.1E-04	-1.1E-04
	8	-1.1E-04	-1.1E-04
Branch5	9	3.4E-04	3.4E-04
	10	3.4E-04	3.4E-04
Branch6	11	-1.8E-10	1.1E-04
	12	7.4E-07	1.2E-04
Branch7	13	1.6E-05	1.6E-05
	14	1.6E-05	1.6E-05

3.3 Steady-state closed loop

Fig. 3 considers a single closed loop which is space-dependent. Whereas the surface source rate of Branch 1 is zero, a positive surface source rate of 2.2E+7 #/cm^2/s is applied to Branch 2. The main input parameters are provided in Table IV.

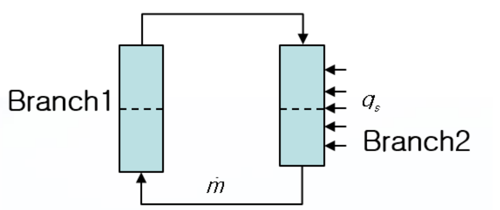

Fig. 3. Closed loop having two branches with different surface source rates (Example 3).

Table IV: Main input parameters of Example 3

Parameters	Value
Loop length (cm)	20
Pipe diameter (cm)	2
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

Figs. 4 & 5 compare the steady-state POSCA results against the analytic solutions. Very good agreements can be seen. The coolant concentration at Branch 1 is linearly decreased due to sorption whereas the coolant concentration at Branch 2 is linearly increased due to the surface source rate. The surface concentrations are not changed with location. It was found that small discrepancy in the coolant concentration is mainly due to coarse mesh size adopted. It was confirmed that the difference from the analytical solution is decreased as the mesh size is decreased.

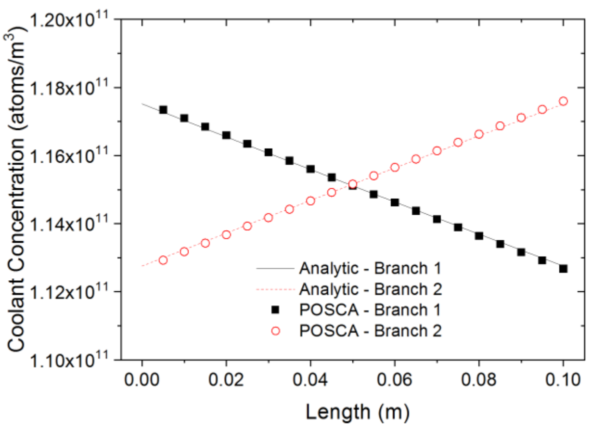

Fig. 4. Verification result for coolant concentration in Example 3.

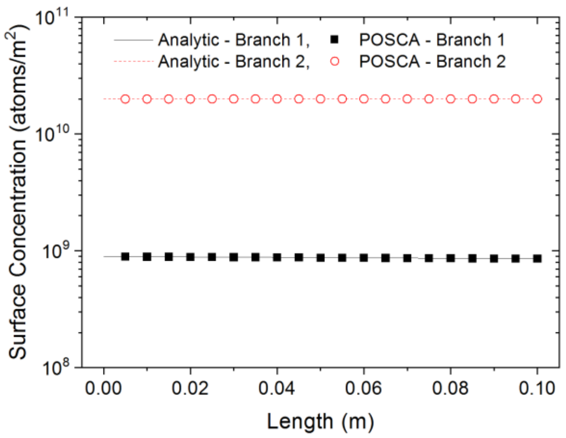

Fig. 5. Verification result for surface concentration in Example 3.

3.4 Space independent simple loop with decay coupling

Example 4 is conceptually the same as the one in Ref. [1] except a decay coupling. The system model is shown in Fig. 6 (It is the same as Fig. 3 in Ref. [1]). However, three nuclides are considered in this example. They are coupled by decay as shown in Fig. 7. In the case of decay coupling, off-diagonal terms of a_{ij}^{*} and b_{ij}^{*} appear in Eqs. (1) and (2).

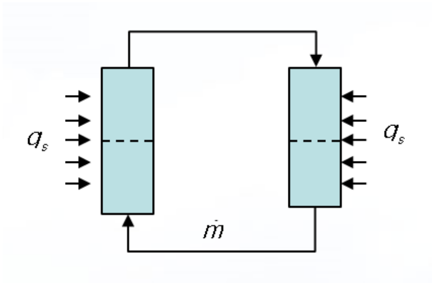

Fig. 6. Space independent simple closed loop (Example 4).

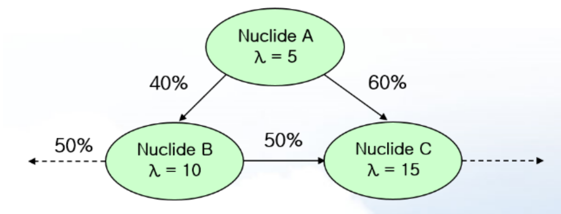

Fig. 7. Decay coupling of three nuclides considered in Examples 4 & 5.

The geometry and thermo-fluids conditions are the same as Table II of Ref. [1] if they are not specified in Table V.

Table V: Main input parameters of Example 4

Parameter	Nuclide A	Nuclide B	Nuclide C
Pipe diameter (cm)	1.6		
Coolant source rate (#/cm^{3}s)	1.0E-9	2.0E-9	3.0E-9
Surface source rate (#/cm^{2}s)	1.0E-10	2.0E-10	3.0E-10
Mass transfer coefficient (cm/s)	4.801886	4.821669	4.867107
Linear sorption coefficient (cm^{-1})	5.788849	3.441000	1.729748

Fig. 8 compares the predicted surface concentrations by POSCA against the analytic solutions. It shows perfect agreements for all the nuclides. Therefore, it is concluded that the POSCA code can reliably simulate the plateout behavior of multi-nuclides with decay coupling.

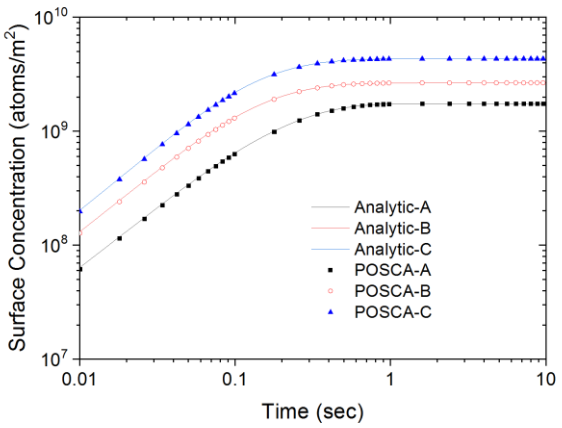

Fig. 8. Verification result for surface concentration in Example 4.

3.5 Steady-state long pipe with decay coupling

Example 5 considers a long pipe having three nuclides coupled by decay chain. The same nuclides shown in Fig. 7 are used. As shown in Fig. 9 and Table VI, the inlet coolant concentration of each nuclide is fixed as boundary condition. The modeling parameters such as mass transfer coefficients are the same as the values shown in Table V. Additional input parameters for Example 5 are provided in Table VI.

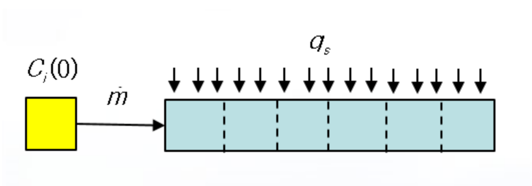

Fig. 9. Long pipe with fixed inlet coolant concentration (Example 5).

Table VI: Main input parameters of Example 5

Parameter	Nuclide A	Nuclide B	Nuclide C
Pipe diameter (cm)	1.6		
Pipe length (m)	10		
Flow velocity (m/s)	17.81808		
Inlet coolant concentration (#/m^3)	3.0E-10	2.0E-10	1.0E-10

Steady-state solutions of POSCA was achieved within the simulation time of 2 seconds. Figs. 10 & 11 show the verification results of the POSCA calculations for Example 5. Very good agreement can be seen in the figures. Small differences in the figures are mainly due to coarse mesh size. It was confirmed that they are decreased as the mesh size is decreased.

4. Conclusions

In this work, the verification study of the POSCA code was made using the existing five benchmark examples which have analytic solutions. It is believed that the tested examples can verify key physical behaviors modelled in the POSCA code. The comparisons of the POSCA results against the analytic solutions show very good agreements. Therefore, it can be concluded that the POSCA code solves its governing equations accurately and reliably. Validation study using experimental data is on-going for quality assurance of the POSCA code.

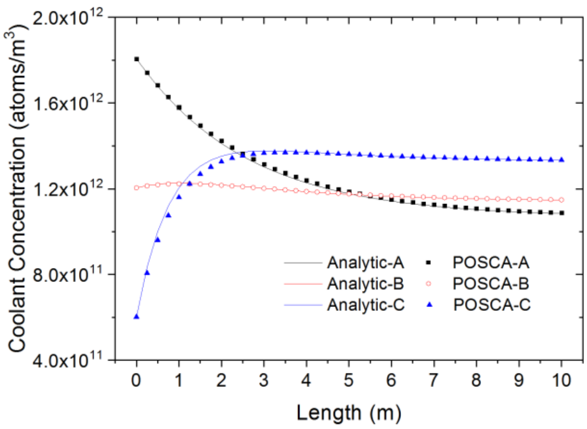

Fig. 10. Verification result for coolant concentration in Example 5.

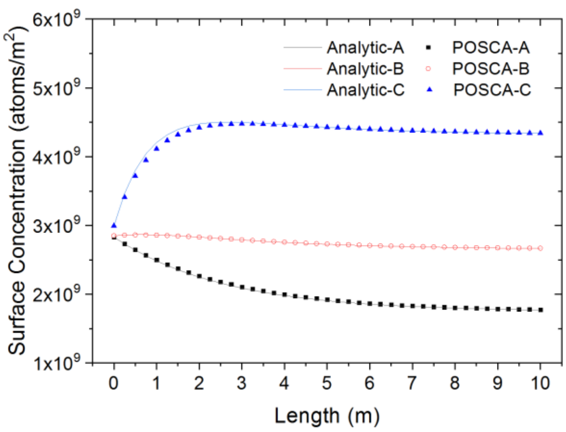

Fig. 11. Verification result for surface concentration in Example 5.

Acknowledgements

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[1] N. I. Tak, S. N. Lee, and C. K. Jo, "One-Dimensional Model for Fission Product Plateout and Circulating Coolant Activities in a HTGR," *Transactions of the Korean Nuclear Society Spring Meeting*, Jeju, Korea, May 17-18, 2018.
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