*Transactions of the Korean Nuclear Society Autumn Meeting*
*Gyeongju, Korea, October 26-27, 2023*

# Verification of Gaseous Radionuclide Transport Module in the MENTAS Code

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***Keywords :** MENTAS, verification, radionuclide, fission product

## 1. Introduction

Korea Atomic Energy Research Institute (KAERI) has been developing a new computer code named MENTAS (Mechanistic Estimation of radioNuclide Transport with Aerosol Species) for mechanistic calculations of radionuclide transport within the reactor building of a high temperature gas-cooled reactor (HTGR) [1]. Radionuclides released into the reactor building of an HTGR are transported as either gaseous or aerosol phase. They may be transported with the combination of non-radioactive aerosols such as graphite dust. The latest version of the nuclear data library for MENTAS has 216 nuclides and 127 decay chains. Nuclides with a fission yield larger than 0.1% and with a half-life longer than 1 minute are basically considered. In addition, some short-lived noble gases (such as Kr-90, Kr-91, Xe-139, and Xe-140) which have important daughters are included.

This work focuses on transport of gaseous phase of radionuclides. A two-step method is employed in the MENTAS code to speedup calculations of gaseous radionuclide behavior imposing complex decay chains with one-dimensional advection. In the first step, decay chains are solved neglecting the advection with fluid flow. Then, one-dimensional transport with fluid flow is analyzed at the second step. This two-step method well harmonizes with the two-step method employed in the aerosol analysis module in the MENTAS code.

In this paper, verification studies of the gaseous radionuclide transport module incorporated in the MENTAS code are presented. Either analytic solutions or reliable results obtained by the other tools are used for comparisons.

## 2. Modeling of Gaseous Radionuclides

Major phenomena of gaseous phase of radionuclides within the reactor building of an HTGR may be identified as decay chains, advection with bulk fluid flow, leakage across the reactor building, removal by filter, and plateout on the surfaces of the structural materials (or on the aerosol surface). A governing equation to describe the key phenomena for gaseous radionuclides can be written as:

$$\frac{\partial C_k}{\partial t} = Q_k + \sum_j \lambda_{j,k} C_j - R_{w,k} - R_{a,k} - \frac{1}{A_f}\frac{\partial}{\partial x}(A_f u C_k) \quad (1)$$

where $C_k$ = concentration of nuclide $k$ (atoms/m$^3$), $\lambda_{j,k}$ = transformation constant from nuclide $j$ to nuclide $k$ ( $\lambda_{k,k}$ = minus decay constant of nuclide $k$) (1/s), $R_{w,k}$ = plateout onto wall surface, $R_{a,k}$ = plateout onto aerosol surface, $A_f$ = flow area (m$^2$), $u$ = bulk fluid velocity (m/s). The advection term in Eq. (1) may be replaced with the leakage term (= $-\gamma C_k$, where $\gamma$ = leakage rate (1/s)).

Significant economy of calculation time can be achieved by dividing the calculation of Eq. (1) into two steps: (1) zero-dimensional behavior (i.e., decay chains and plateout) and (2) one-dimensional advection. The fundamental premise behind this approach is that during a time step of small enough duration the interdependence of the two components of a calculation can be neglected. That is, nuclide decay and plateout equation can be solved during a time step without considering the simultaneous phenomenon of transport between numerical cells. Likewise, the transport equation defining transfer of nuclides between numerical cells during a time step can be solved numerically without taking account of decay and plateout processes over that period. Such a premise is widely used in analyzing radionuclide transport phenomena in nuclear systems.

The first step to solve Eq. (1) can be expressed as:

$$\frac{dC_i}{dt} = Q_i + \sum_j \lambda_{j,i} C_j - R_{w,i} - R_{a,i} \quad (2)$$

Among various methods to solve decay chains, the MENTAS code adopts the linearized decay chain method proposed in the CINDER code [2].

The equation for the second step describes one-dimensional fluid network including leakage:

$$\frac{dC_{i,k}}{dt} = \sum_{j \in T_j} \alpha_j C_{up,k} - \sum_{j \in I_j} \alpha_j C_{i,k} \quad (3)$$

$$\alpha_j = \eta_{j,k} \frac{u_j A_j}{V_i} \text{ for convection flow}$$
$$= \gamma_j \text{ for leakge flow} \quad (4)$$

where $\eta_{j,k}$= 1- filter efficiency of nuclide $k$ and $V_i$ = fluid volume (m$^3$). After being discretized with time, Eq. (3) can be rearranged as:

$$\left[1+\Delta t\sum_{j\in I_j}\alpha_j\right]C_{i,k}^{n+1}-\Delta t\sum_{j\in T_j}\alpha_j C_{up,k}^{n+1} = C_{i,k}^{n} \tag{5}$$

Eq. (5) forms a matrix equation and can be solved with a sparse matrix solver.

## 3. Verification Results

In the present verification studies, plateout phenomena are neglected since they generally contain empirical correlations which require experimental validations.

### *3.1 Verification of Decay Chains*

Table I lists the test cases performed for verification of the decay chain solver implemented in the MENTAS code. Among the five cases shown in Table I, the results of two cases (i.e., Example 1.3 and Example 1.5) are presented in this paper for the compactness of the paper.

Table I: Test Cases Performed for Verification of Decay Chain Solver of MENTAS

| | Descriptions |
|---|---|
| Example 1.1 | One-level decay with source |
| Example 1.2 | Two-level serial decay chain |
| Example 1.3 | Four-level serial decay chain |
| Example 1.4 | Three-level network decay chain |
| Example 1.5 | Six-level network decay chain |

Example 1.3 considers a four-level serial decay chain shown in Fig. 1. As shown in Fig. 2, the results of the MENTAS code are compared with the analytic solutions. The analytic solutions are obtained using the Excel sheet provided by the reference [3]. Perfect agreements are shown in the figure.

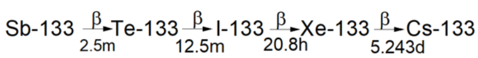


Fig. 1. Four-level serial decay chain (Example 1.3)

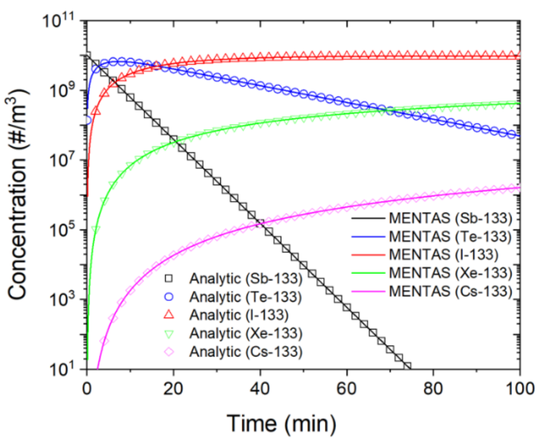


Fig. 2. Verification of decay chain solver using Example 1.3.

Example 1.5 considers a six-level network decay chain shown in Fig. 3. Branching of decay process is included and forms a complex network decay chain.

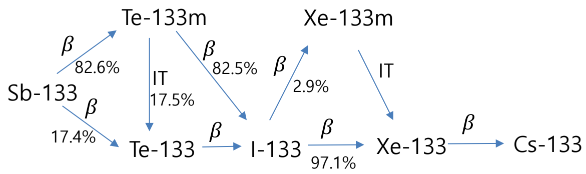


Fig. 3. Six-level network decay chain (Example 1.5).

Fig. 4 shows the verification result for Example 1.5. The results of the MENTAS code are compared with those of on-line calculator [4] developed by the Oak Ridge National Laboratory (ORNL) of U. S. Excellent agreements are shown in the figure.

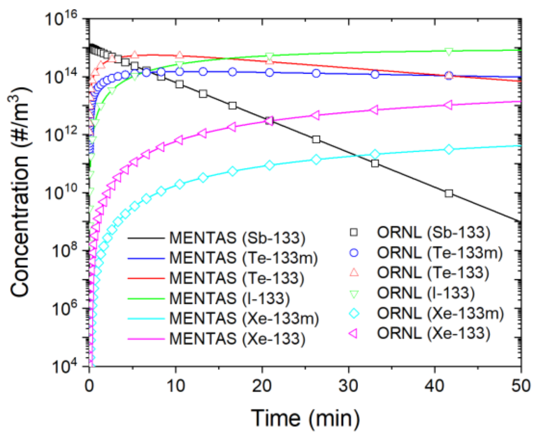


Fig. 4. Verification of decay chain solver using Example 1.5.

### *3.2 Verification including One-Dimensional Advection*

Table II lists the test cases performed for verification of gaseous nuclide transport. They cover all the key phenomena except plateout. Among the seven cases tested, the results of four cases (Example 2.2, Example 2.4, Example 2.5, and Example 2.7) are presented in this paper for the compactness of the paper.

Table II: Test Cases Performed for Verification of Gaseous Nuclide Transport Module of MENTAS

| | Descriptions |
|---|---|
| Example 2.1 | Steady-state decay |
| Example 2.2 | Steady-state decay with source |
| Example 2.3 | Transient convection |
| Example 2.4 | Transient convection with decay |
| Example 2.5 | Transient decay with sine inlet |
| Example 2.6 | Leakage without decay |
| Example 2.7 | Leakage with daughter in-growth |

Fig. 5 shows the concept of Example 2.2. A sinusoidal source is assumed with the initial condition given in Eq. (6).

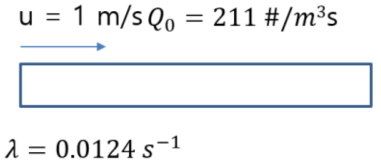


Fig. 5. Steady-state decay with source (Example 2.2)

$$C_i(x,0) = 0,\ Q_i(x) = Q_0 \sin(\pi x)\, e^{-\frac{\lambda_i}{u}x} \quad (6)$$

The analytic solution of Example 2.2 is obtained by

$$C(x) = \frac{Q_0}{\pi u} e^{-\lambda_i x/u}\left[\sin\left(\pi x - \frac{\pi}{2}\right) + 1\right] \quad (7)$$

Fig. 6 compares the MENTAS result with the analytic solution, i.e., Eq. (7). A good agreement is shown. A slight difference seems to be mainly due to the numerical error.

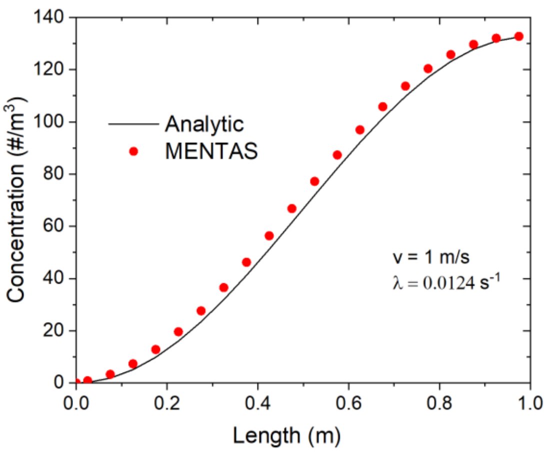


Fig. 6. Verification result of Example 2.2.

It is assumed that there is no source in the remaining examples. Example 2.4 simulates a transient convection problem with decay. The fluid velocity and the decay constant are assumed to be 1 m/s and 5 $s^{-1}$, respectively. The initial condition is:

$$C(x,0) = 10x \quad (8)$$

The analytic solution of Example 2.4 is obtained by

$$C(x,t) = 10(-ut + x)\, e^{-\lambda_i t} \quad (9)$$

Fig. 7 compares the MENTAS result with the analytic solution (= Eq. (9)). Good agreements are shown in the figure.

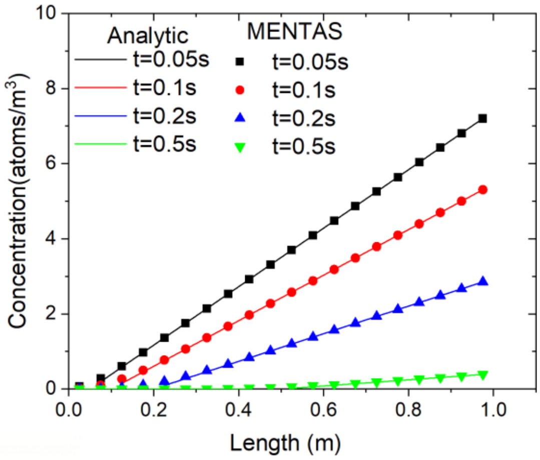


Fig. 7. Verification result of Example 2.4.

Example 2.5 considers a sinusoidal inlet with decay problem. The boundary and initial conditions are:

$$C(0,t) = 200 + 100\sin(\pi t)$$
$$C(x,0) = 200e^{-\lambda x/u} \quad (10)$$

The analytic solution of Example 2.5 is:

$$C(x,t) = \begin{cases} 200e^{-\lambda x/u}, & t < x/u \\ e^{-\lambda x/u}\left[200 + 100\sin(\pi t - \frac{\pi x}{u})\right], & t > x/u \end{cases} \quad (11)$$

The verification result of Example 2.5 is shown in Fig. 8. A good agreement is shown. The largest difference occurs around the position at $t = x/u$. This fact is reasonable since the numerical solutions of MENTAS should be smooth.

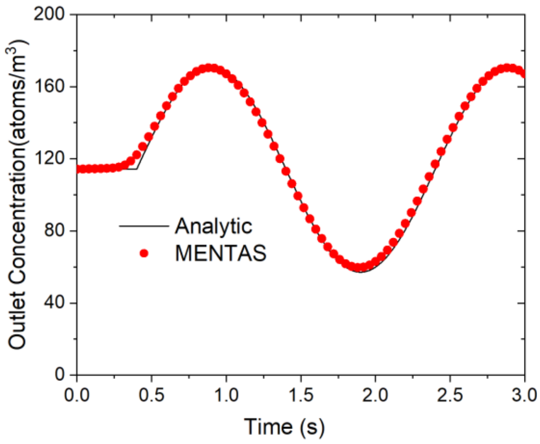


Fig. 8. Verification result of Example 2.5.

Fig. 9 shows the concept of Example 2.7. It considers I-131 leak across the containment. A growth of daughter nuclide (= Xe-131m) is also considered. The analytical solution of Example 2.7 exists but MATLAB, which is a commercial software, is used for verification to minimize a mistake.

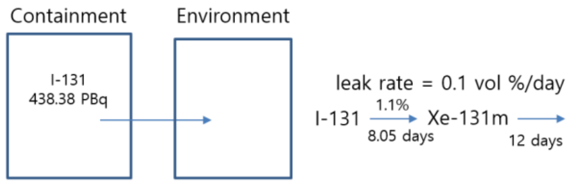


Fig. 9. Leakage with daughter in-growth (Example 2.7).

Fig. 10 compares the MENTAS result with that of MATLAB. Excellent agreement is shown in the figure.

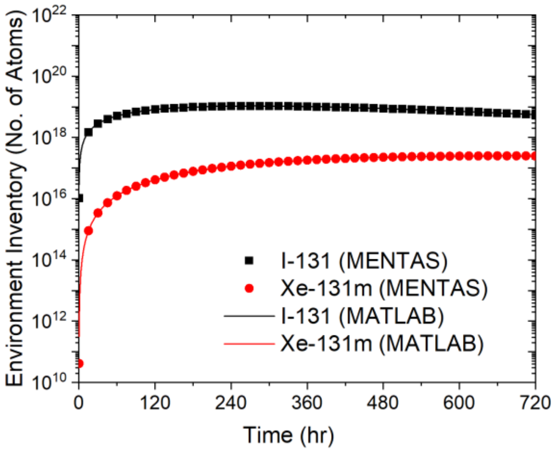


Fig. 10. Verification result of Example 2.7.

## 4. Conclusions

In this work, a series of verification studies of the gaseous radionuclide transport module in the MENTAS code were performed. Analytic solutions or reliable results obtained by the other tools are used for comparisons. The results of the present verification studies clearly show that the gaseous radionuclide transport module incorporated in the MENTAS code is highly reliable and reasonably accurate. Therefore, the MENTAS code can be a useful tool for a licensing analysis which assumes all the radionuclides released are gaseous phase. As further researches, validation studies are required including plateout phenomena. In particular, gaseous radionuclide transport attached on graphite dust is a great concern in an HTGR design.

## Acknowledgements

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2020M2D4A2067322).

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