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Development of Fission Product Behavior Analysis Code for Molten Salt Reactor under Accident Condition

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1. Introduction

The analysis of fission product behavior involves the evaluation of phenomena associated with the release, transport, and phase transformation of fission products generated and accumulated in a nuclear reactor under accident conditions. As the temperature of the reactor core increases, various fission products are released in gaseous form. These gaseous fission products are transported by a mixture of steam and non-condensable gases toward relatively cooler regions, where they may undergo condensation and be converted into aerosols.

Similar to gaseous species, fission product aerosols are transported with the carrier gas mixture; however, unlike gases, they tend to deposit on surfaces such as floors and walls through mechanisms including gravitational settling, diffusiophoresis, and thermophoresis. As a result, only a fraction of the released fission products may ultimately reach the environment through specific pathways. The analysis of fission product behavior is therefore performed to quantify the mass of fission products released to the environment.

The overall procedure for fission product behavior analysis is illustrated in Fig. 1 and can be divided into the following steps:

1. Specification of the initial fission product inventory
2. Release of high-temperature fission product gases
3. Transport of fission product gases by the carrier gas mixture
4. Conversion of fission product gases into aerosols
5. Deposition and removal of fission product aerosols
6. Release to the environment

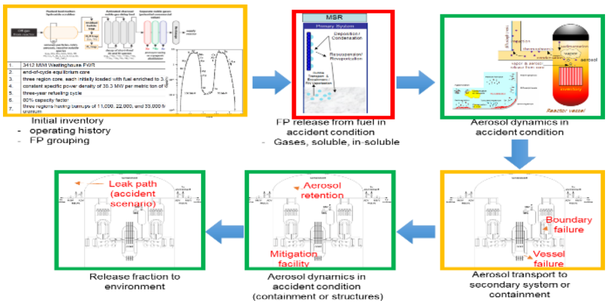

Fig. 1. Conceptual diagram of fission product behavior analysis in a molten salt reactor

For the evaluation of fission product releases to the environment resulting from molten salt leakage in a molten salt reactor (MSR), the following analyses are required:

- Determination of the inventory and physicochemical states of fission products in the molten salt
- Specification of the postulated accident scenario
- Evaluation of the spreading and cooling behavior of the leaked molten salt
- Calculation of fission product release from the molten salt
- Analysis of the transport and chemical interactions of released fission products prior to discharge to the environment

First, the inventory and physicochemical states of fission products in the molten salt prior to the initiating event are specified. Unlike pressurized water reactors, fission products generated under normal operating conditions in MSRs may exist in the fuel salt as various chemical compounds. Depending on the assumed accident scenario, a leakage pathway for the molten salt is postulated, and the subsequent spreading behavior of the leaked salt is evaluated. Based on the thickness and surface area of the spread molten salt, its cooling characteristics are assessed. As functions of the thermodynamic conditions of the molten salt and its surrounding environment, the release of fission products from the molten salt is then calculated, followed by analyses of their transport, aerosol formation, deposition, and other interactions with the environment, up to their eventual release to the atmosphere or surrounding media.

This study presents STEP-MSR (Source Term Evaluation via Pathways for MSRs) code, developed for analyzing fission product behavior in MSRs via a lumped-parameter approach. The report is based on version 1.0.1.1 of the code, and its major developments to date are summarized below:

- The code enables release calculations based on the saturation vapor pressures of compounds in molten salt.
- Saturation vapor pressure data for four compounds in the PSI-MSFR (LiF–ThF_4–UF_4) system and six compounds in the K-MSR (NaCl–KCl–UCl_3) system have been implemented in the code; release calculations are limited to these compounds.
- For the PSI-MSFR, saturation vapor pressure data reported in Ref. [1] were adopted.

- For the K-MSR, saturation vapor pressure data calculated using FactSage.
- Atmospheric conditions are assumed to consist of N_2 gas.
- The current version supports analysis for a single node only.
- The cross-sectional area of the node is assumed to be identical to that of the molten salt.
- Time-dependent values of key thermodynamic variables required for release calculations must be provided as input.
- Both steady-state and transient analyses are supported.

2. Fission Product Release Model in Molten Salt Reactors

In pressurized water reactors, fission products generated during normal operation accumulate within the solid fuel matrix, particularly at grain boundaries and fuel–cladding gaps, where they are primarily retained in gaseous form under self-generated pressure, with negligible inter-nuclide reactions. Under severe accident conditions, once cladding integrity is compromised, fission products are released in gaseous form on a nuclide-by-nuclide basis. Empirical models developed from experimental data to describe this behavior include CORSOR, CORSOR-O, and CORSOR-M. These models compute the release rates of gaseous fission products for individual nuclides as functions of fuel temperature using Arrhenius-type rate expressions. Alternatively, diffusion-based approaches, such as the CORSOR-BOOTH model, may be employed.

Unlike pressurized water reactors, there is no cladding in MSRs, allowing fission products generated under normal operating conditions to circulate freely within the liquid fuel salt. Consequently, these fission products may undergo chemical reactions and form chemical bonds with the molten salt during steady-state operation. Condensation and evaporation can be evaluated based on the concentration gradient between the liquid fuel salt interface and the overlying atmosphere.

As illustrated in Fig. 2, a molten salt leakage accident in an MSR is expected to result in the release of numerous chemical compounds from the molten salt. Information on releasable compounds can be obtained through Gibbs free energy–based evaluations of molecular bonding stability among nuclides, using thermochemical codes such as FactSage [2] and GEMS [3].

STEP-MSR code implements a fission product release model for MSR accident scenarios based on the methodologies described in Refs. [1,4]. The time-dependent evaporation rate of compound i from the molten salt is calculated using Eq. (1).

$$\frac{dm_i}{dt} = Ak_i(C_i^s - C_i^a) \tag{1}$$

$$C_i^s = \frac{P_i^s(T)M_i}{RT} \tag{2}$$

Table I. Definition of variables used in equations (1)-(2)

Symbol	Description	Unit
$\frac{dm_i}{dt}$	Evaporation rate of compound i	kg/s
A	Surface area of molten salt	m^2
k_i	Mass transfer coefficient of compound i	m/s
C_i^s	Saturation concentration of compound i at the surface	kg/m^3
C_i^a	Concentration of compound i in the atmosphere	kg/m^3
$P_i^s(T)$	Saturation vapor pressure of compound i as a function of gas temperature	Pa
M_i	Molar weight of compound i	g/mol
R	Gas constant	J/mol-K
T	Gas temperature	K

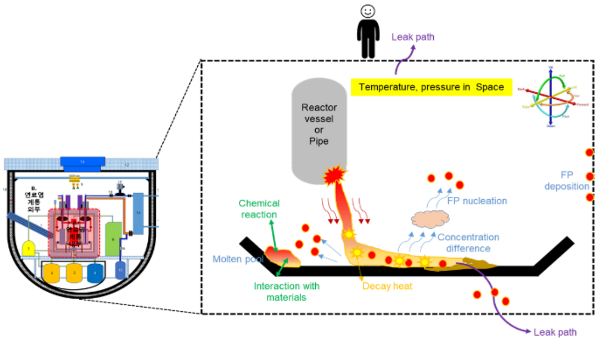

Fig. 2. Conceptual diagram of environmental fission product release due to molten salt leakage

Molten salt may consist of numerous chemical compounds, and Eq. (1) describes the calculation of the evaporation or condensation rate from the molten salt based on the difference between the saturation mole fraction of compound i in the molten salt and its corresponding mole fraction in the atmosphere. Eq. (2) provides the saturation mole fraction derived from the saturation vapor pressure using the ideal gas law. The mass transfer coefficient (k_i) is determined using the relationships given in Eqs. (3) through (10).

$$\frac{k_i}{k_{st}} = \frac{D_{i,N_2}}{D_{st,a}} \tag{3}$$

$$k_{st} = \frac{Sh\, D_{st,a}}{L_c} \tag{4}$$

$$D_{st,a} = \frac{4.7931 \times 10^{-5}\, T^{1.9}}{P_a} \tag{5}$$

$$D_{i,N_2} = \frac{0.0018583\, T^{3/2} \sqrt{M_i^{-1} + M_{N_2}^{-1}}}{P_a\, \sigma_{i,N_2}^2\, \Omega_{D_{i,N_2}}} \tag{6}$$

$$\sigma_{i,N_2} = 0.5(\sigma_i + \sigma_{N_2}) \tag{7}$$

$$\Omega_{D_{i,N_2}} = \frac{1.06036}{T^{*0.15610}} + \frac{0.19300}{exp(0.47635T^*)} + \frac{1.03587}{exp(1.52996T^*)} + \frac{1.76474}{exp(3.89411T^*)} \tag{8}$$

$$T^* = \frac{kT}{\epsilon_{i,N_2}} \tag{9}$$

$$\epsilon_{i,N_2} = \sqrt{\epsilon_i\, \epsilon_{N_2}} \tag{10}$$

Table II. Definition of variables used in equations (3)-(10)

Symbol	Description	Unit
k_{st}	Steam mass transfer coefficient	m/s
D_{i,N_2}	Diffusivity of compound *i* in N_2	m^2/s
$D_{st,a}$	Diffusivity of steam in air	m^2/s
Sh	Sherwood number	-
L_c	Characteristic length	m
P_a	Pressure	Pa
M_{N_2}	Molar weight of N_2	g/mol
σ_{i,N_2}	Lennard-Jones collision diameters	Å
$\Omega_{D_{i,N_2}}$	Collision integral for diffusion	-
T^*	Temperature coefficient	-
k	Boltzmann constant	J/K
ϵ_{i,N_2}	Lennard-Jones energy parameters	J

Although the time-dependent Lennard–Jones parameters can, in principle, be obtained through thermodynamic behavior analyses, STEP-MSR code does not explicitly simulate the thermodynamic behavior of species other than fission products; therefore, these parameters must be provided as user inputs. The thermodynamic data required for fission product release analysis in STEP-MSR code is summarized in Table III.

Table III. Thermodynamic data required for STEP-MSR code

Variable	Description	In equations	Unit
pressure	Node pressure	P_a	Pa
tempg	Node gas temperature	Used in T calculation	K
t_salt	Surface temperature of molten salt	Used in T calculation	K
D_ST	Diffusivity of steam in air	$D_{st,a}$	m^2/s
T_STAR	Temperature coefficient	T^*	-
SIGMA	Collision integral	$\Omega_{D_{i,N_2}}$	-
COL_DIAM	Collision diameter	σ_{i,N_2}	Å
MTC	Steam mass transfer coefficient	k_{st}	m/s

The variables listed in Table I may be specified either as single time-point values (at *t* = 0) for each node or as time-dependent inputs. When provided as single time-point values, STEP-MSR code performs steady-state calculations by treating these variables as constants. When specified as time-dependent values, transient calculations are carried out. The temperature (T) used in the calculations of Eqs. (5), (6), (8), and (9) is defined as the average of the molten salt surface temperature and the temperature of the atmosphere in contact with the surface.

In addition, initial conditions such as geometric information and molten salt composition are required; the corresponding input variables are listed in Table IV.

Table IV. Initial conditions for STEP-MSR code

Variable	Description	Unit
volume	Node volume	m^3
area	Node area	m^2
N2_gas_mass	Node N2 gas mass	Kg
user_defined	Number of salt component	#
salt_comp1	Salt component1 mass	Kg
⋮	⋮	⋮
salt_comp15	Salt component15 mass	Kg
Molar_weight	Molar weight of salt component	g/mol

Among the variables listed in Table II, the parameter “area” represents the surface area of the molten salt. The parameter “N2_gas_mass” is required to calculate the mole fractions of compounds in the atmosphere. For model development, the current version of STEP-MSR code assumes an atmospheric environment composed solely of N_2 and therefore accepts input only for this gas. The number of compounds to be analyzed is specified using the parameter “user_defined.” The variables “salt_comp1” through “salt_comp15” denote the masses of individual compounds in the molten salt, while “Molar_weight” represents the molecular weight of each compound. These compound-specific masses and molecular weights are used to calculate mole fractions in the molten salt and must be provided in the prescribed order.

STEP-MSR code is capable of analyzing two types of MSR. For the PSI-MSFR (LiF-ThF_4-UF_4) system, four compounds are considered as potential releasable species from the molten salt; their types and ordering are presented in Table V. For this system, no additional input regarding the initial masses of individual compounds is required.

Table V. Types of compounds considered in PSI-MSFR calculations in STEP-MSR code

No.	Compound	Release?	Molar weight (g/mol)
1	LiF	O	25.94
2	ThF_4	O	308.03
3	UF_4	O	314.02
4	CsF	O	151.9

For the K-MSR ($NaCl$-KCl-UCl_3) system, up to 15 compounds may be considered in the molten salt composition, of which release calculations are performed for six compounds. The types and sequence of the compounds in the molten salt composition are presented in Table VI.

Table VI. Types of compounds considered in K-MSR calculations in STEP-MSR code

No.	Compound	Release?	Molar weight (g/mol)
1	UCl_3	O	306.01
2	NaCl	O	58.44
3	KCl	O	74.55
4	$PuCl_3$	X	339.41
5	$ZrCl_4$	X	233.03
6	$NdCl_3$	X	246.24
7	CsCl	O	168.36
8	$CeCl_3$	X	246.74
9	$BaCl_2$	X	208.23
10	$LaCl_3$	X	263.81
11	$SrCl_2$	O	158.53
12	RbCl	X	120.92
13	UI_3	X	407.87
14	$MgCl_2$	X	95.21
15	NaI	O	149.89

Compounds within molten salt form binary, ternary, or higher-order systems to achieve chemical stability; therefore, their individual saturation vapor pressures must account for vapor pressure depression resulting from Gibbs free energy minimization, in contrast to the behavior of independent compounds. Saturation vapor pressures for individual compounds can be obtained using thermochemical codes such as FactSage and GEMS.

For evaporation calculations of molten salt compounds, saturation vapor pressure data were formulated as functions of mole fraction or molten salt surface temperature and implemented in STEP-MSR code. For the PSI-MSFR system, saturation vapor pressure data for the four compounds listed in Table III, calculated using GEMS, were input using the Clausius–Clapeyron approximation as functions of molten salt surface temperature.

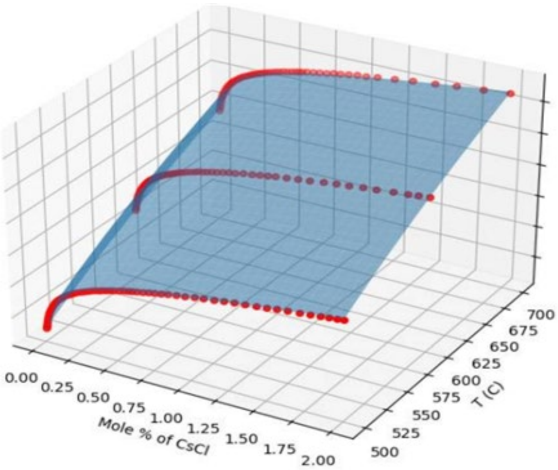

Fig. 3. Saturated vapor pressure as a function of CsCl mole fraction and molten salt surface temperature

For the K-MSR system, saturation vapor pressure data for the six compounds listed in Table IV, calculated using FactSage, were implemented as follows: for the three base salt compounds, the data were expressed as functions of molten salt surface temperature, while for the three fission product–based compounds, they were expressed as functions of both molten salt surface temperature and mole fraction as shown in Fig. 3.

3. Model Verification

To verify the validity of the developed model, molten salt release calculations for the PSI-MSFR presented in Ref. [1] were performed. Among the thermodynamic data obtained from the coupled GEMS–MELCOR calculations in Ref. [1], the pressure and temperature conditions used in the present analysis are shown in Figs. 4 and 5, and the corresponding nodes are illustrated in Fig. 6.

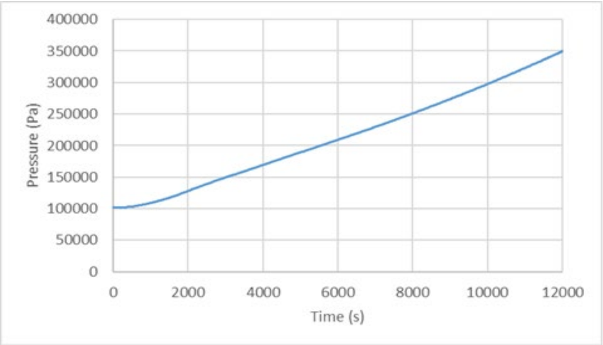

Fig. 4. PSI-MSFR calculation conditions – pressure

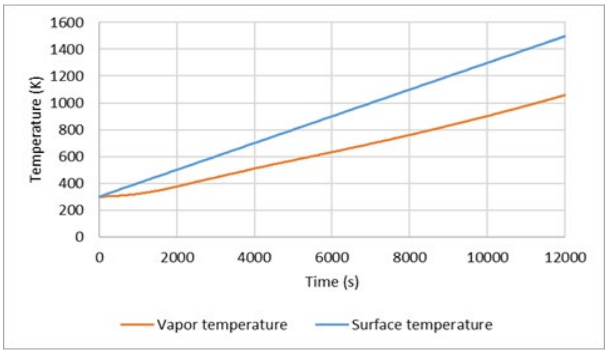

Fig. 5. PSI-MSFR calculation conditions – temperature

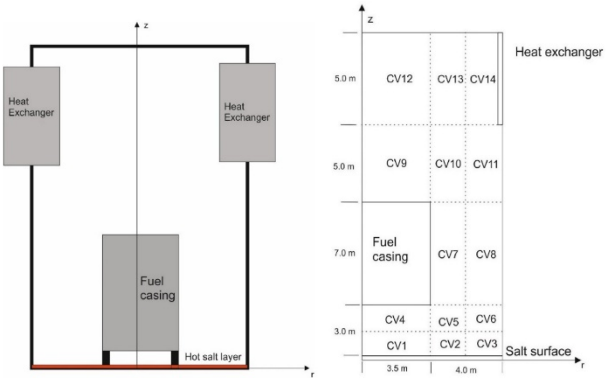

Fig. 6. PSI-MSFR nodalization for GEMS-MELCOR

In the coupled GEMS–MELCOR calculations presented in Ref. [1], not only the release of fission products but also their transport to other nodes by N_2 gas, transformation into aerosols, and subsequent deposition were considered. Consequently, the fission product gases released into the atmospheres of the three bottom nodes, where molten salt release was calculated, did not remain in those nodes but were transported to larger-volume nodes located above or converted into aerosols. As a result, the atmospheric compound concentrations in these nodes were calculated to be close to zero at all times.

In STEP-MSR code, the atmospheric compound concentration coefficient can be specified through user input. When this coefficient is set to zero, the node in which release is calculated is assumed to be a closed system, and fission products released from the molten salt continuously accumulate, leading to a gradual decrease in the release rate over time. When the coefficient is set to unity, the node is assumed to be a fully open system in which the released fission products do not remain in the atmosphere, resulting in zero atmospheric compound concentration. In this case, fission product release is calculated solely as a function of the saturation vapor pressure.

For the PSI-MSFR calculations performed using STEP-MSR code, the coefficient was set to unity in order to apply conditions similar to those used in the GEMS–MELCOR calculations, and the releases of the molten-salt-based compounds LiF, ThF_4, and UF_4 were evaluated. It was confirmed that the saturation vapor pressures of compounds in the molten salt reported in Ref. [1] differ slightly from those used in the actual GEMS–MELCOR calculations. Therefore, instead of using the saturation vapor pressures provided in Ref. [1], temperature-dependent saturation vapor pressures of the molten salt compounds were estimated in the form of the Clausius–Clapeyron equation based on the GEMS–MELCOR calculation results.

Fig. 7 presents the released mass results. The released mass represents the cumulative value of the release rate over time. Under identical conditions, slight differences were observed between the results obtained from STEP-MSR code and the coupled GEMS–MELCOR calculations. As mentioned above, the estimation of saturation vapor pressures resulted in minor differences in the predicted release rates, particularly for ThF_4. In addition, GEMS–MELCOR calculates release rates separately for three individual nodes, and the thermodynamic conditions applied to each node differ slightly. Therefore, when representative thermodynamic conditions are applied to an equivalent single node, as in STEP-MSR code, minor differences in the release rates may arise. In conclusion, the model implemented in STEP-MSR code demonstrates comparable capability to the GEMS–MELCOR framework in simulating compound release in MSRs.

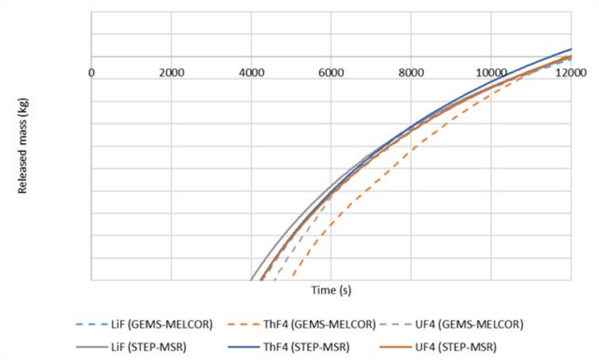

Fig. 7. PSI-MSFR calculation results – released masses of LiF, ThF_4, and UF_4

Fig. 8 compares the calculated release amounts of molten-salt-based compounds under identical thermodynamic conditions, including LiF, ThF_4, and UF_4 in the PSI-MSFR and UCl_3, NaCl, and KCl in the K-MSR. From a theoretical standpoint, chloride-based compounds are expected to exhibit higher evaporation rates than fluoride-based compounds due to their relatively weaker chemical bonding. The calculation results obtained using STEP-MSR code are consistent with this expectation.

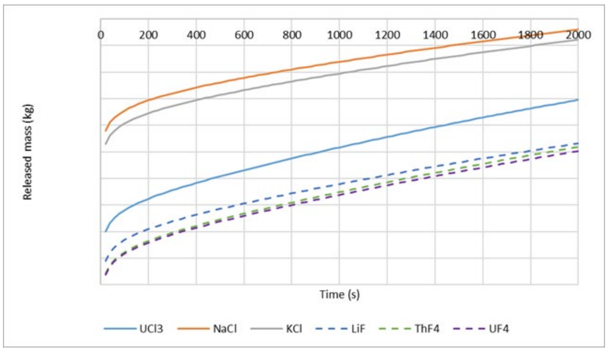

Fig. 8. Comparison of released masses of K-MSR and PSI-MSFR under same thermodynamic conditions

4. Conclusion

This study presents the modeling approach and verification results of STEP-MSR code (ver. 1.0.1.1), developed to analyze fission product release behavior during accidents in MSRs.

STEP-MSR code is based on a lumped-parameter approach and calculates evaporation amounts using the saturation vapor pressures of compounds in molten salt. Unlike in pressurized water reactors, the code reflects the characteristics of MSRs, which have no cladding, by modeling condensation and evaporation phenomena driven by concentration differences between the liquid fuel surface and the surrounding atmosphere. The code can simulate two types of MSRs, namely the PSI-MSFR (LiF–ThF_4–UF_4) and the K-MSR (NaCl–KCl–UCl_3), with saturation vapor pressure data implemented for four and six major compounds, respectively. By adjusting the gas removal rate in the atmosphere, both open-node and closed-node conditions can be simulated, and transient analyses that account for time-dependent changes in thermodynamic variables are possible.

Validation of the code for the PSI-MSFR demonstrated that STEP-MSR code can adequately simulate fission product release behavior from molten salt, as confirmed through comparison with the coupled GEMS–MELCOR calculation data provided by PSI.

The main future plans for optimal source term analysis of the K-MSR are as follows:

- Expansion of saturation vapor pressure data to include additional compounds
- Inclusion of saturation vapor pressure data estimated using other thermochemical codes, such as GEMS
- Application to PSA (Probabilistic Safety Assessment) accident scenarios
- Use of realistic values for molten salt spreading and cooling, including coupling with results from other codes
- Implementation of design-basis atmospheric conditions
- Multi-node analysis
- Simulation of transport and aerosolization of released fission product gases
- Modeling of interactions with the surrounding environment up to the point of environmental release

Acknowledgement

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