



Technical Note

Interfacing between MAAP and MACCS to perform radiological consequence analysis

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ABSTRACT

Interfacing the output of severe accident analysis with the input of radiological consequence analysis is an important and mandatory procedure at the beginning of Level 3 PSA. Such interfacing between the severe accident analysis code MELCOR and MACCS, one of the most commonly used consequence analysis codes, is relatively tractable since they share the same chemical groups, and the related interfacing software, MelMACCS, has already been developed. However, the linking between MAAP, another frequently used code for severe accident analyses, and MACCS has difficulties because MAAP employs a different chemical grouping method than MACCS historically did. More specifically, MAAP groups by chemical compound, while MACCS groups by chemical element. An appropriate interfacing method between MAAP and MACCS has therefore long been requested by users. This study suggests a way of extracting relevant information from MAAP results and providing proper source term information to MACCS by an appropriate treatment. Various parameters are covered in terms of magnitude and manner of release in this study, and special treatment is made for a bypass scenario. It is expected that the suggested approach will provide an important contribution as a guide to interface MAAP and MACCS when performing radiological consequence analyses.

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1. Introduction

In order to conduct a radiological consequence analysis, connecting the employed severe accident analysis code and the consequence analysis code is essential, as the source term information from the output of the severe accident analysis is provided as the input of the consequence analysis. In other words, interfacing the two codes plays a significant role as the end point of Level 2 PSA (probabilistic safety assessment) and the starting point of Level 3 PSA. Source term information describes postulated radionuclide releases to the environment, including both magnitude and manner of release. The magnitude of release expresses the release amount as a release mass directly or as a combination of release fraction and core inventory. The manner of release, also called the release parameters, is composed of the following:

- starting time of the release after accident initiation,
- duration of the release,
- height of the release,
- amount of energy associated with the release, and
- particle size distribution of aerosols.

MACCS (MELCOR Accident Consequence Code System) [1] is one of the most commonly used offsite consequence analysis codes for nuclear power plants. When the MELCOR code is used to perform severe accident analysis, MelMACCS software extracts and provides source term information from a MELCOR plot file to MACCS. With this developed interfacing tool, it is relatively convenient to link MELCOR and MACCS since they share the same chemical groups, i.e., each chemical group is organized with elements having similar chemical and physical properties. Other terminologies such as chemical class or radionuclide group are also used instead of chemical group. Although MACCS is very flexible in defining up to 150 chemical groups and does not provide a specific guideline for chemical grouping in the manual, grouping into 9 chemical groups

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was frequently employed, historically. From the original list of 9 chemical groups in MACCS as defined in the NUREG-1150 report [2], an update of the 9 groups was carried out as part of the SOARCA (State-of-the-Art Reactor Consequence Analyses) project [3]. Table 1 and Table 2 present the 9 chemical groups from when the NUREG-1150 report was published and those after the SOARCA project was performed, respectively.

However, when MAAP (Modular Accident Analysis Program) is used as the severe accident analysis code, the situation becomes totally different from the case using MELCOR. This is because MAAP employs 18 chemical groups called fission product (FP) groups, where each FP group is composed of chemical compounds rather than chemical elements. Table 3 lists the FP groups of MAAP. MAAP version 4 had 12 FP groups, to which 6 additional FP groups were added in MAAP version 5. It should be noted that the non-radioactive inert aerosols in FP group 1 are not considered in radiological consequence analysis.

Since MAAP is also a frequently used severe accident analysis code, it is necessary to establish a method to interface MAAP and MACCS, as illustrated in Fig. 1. This study provides an interfacing

method between MAAP and MACCS that can be used to conduct radiological consequence analyses.

2. Comparison between chemical groups of MAAP and MACCS

Tables 4–7 compare the chemical groups between each version of MAAP and the historical groupings of MACCS. The chemical elements that are not common in both cases are excluded from the MACCS list, since they do not have to be interfaced. To avoid reader confusion, the group numbers of MAAP and MACCS are expressed with a lower case “g” and an upper case “G”, respectively.

3. Interfacing method between MAAP and MACCS

In this section, an approach to interface MAAP and MACCS is introduced in detail with regard to magnitude and manner of release. First, printing out the MAAP output with the mandatory data in a proper format is the necessary starting point of the interfacing procedure. MAAP users should be careful to print out the variables of the affiliated release junction (*jj*) and donor

Table 1
Chemical groups of MACCS in NUREG-1150 [2].

Group Number	Group Name	Representative	Member Elements
1	Inert Gases	Xe	Kr, Xe
2	Iodine	I	I
3	Cesium	Cs	Rb, Cs
4	Tellurium	Te	Sb, Te
5	Strontium	Sr	Sr
6	Ruthenium	Ru	Co, Mo, Tc, Ru, Rh
7	Lanthanum	La	Y, Zr, Nb, La, Pr, Nd, Am, Cm
8	Cerium	Ce	Ce, Np, Pu
9	Barium (part of group 5 in Reactor Safety Study [4])	Ba	Ba

Table 2
Chemical groups of MACCS after the update from SOARCA [3].

Group Number	Group Name	Representative	Member Elements
1	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	Alkali Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	Halogens	I	F, Cl, Br, I, At
5	Chalcogens	Te	O, S, Se, Te, Po
6	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	Tetravalents	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	Trivalentes	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf

Table 3
Chemical groups of MAAP [5,6].

MAAP4 & MAAP5	FP Group	Member	Only MAAP5	FP Group	Member
	1	VAPOR (V): Noble gases (Xe + Kr) AEROSOL (A): All non-radioactive inert aerosols		13	Ag (activation product, not FP)
	2	V & A: CsI + RbI		14	V: I ₂ (iodine in elemental form)
	3	V & A: TeO ₂		15	V: CH ₃ I (iodine in organic form)
	4	V & A: SrO		16	V & A: Cs ₂ MoO ₄
	5	V & A: MoO ₂ + RuO ₂ ^a + TcO ₂ ^b + RhO ₂ ^b		17	V & A: RuO ₂
	6	V & A: CsOH + RbOH		18	V & A: PuO ₂ (fuel, not FP)
	7	V & A: BaO			
	8	V & A: La ₂ O ₃ + Pr ₂ O ₃ + Nd ₂ O ₃ + Sm ₂ O ₃ + Y ₂ O ₃ + ZrO ₂ ^b + NbO ₂ ^b + AmO ₂ ^b + CmO ₂ ^b			
	9	V & A: CeO ₂ + NpO ₂ + PuO ₂ ^a			
	10	V & A: Sb			
	11	V & A: Te ₂			
	12	V & A: UO ₂ (fuel, not FP)			

^a Only MAAP4.

^b Implemented since MAAP version 4.0.5.

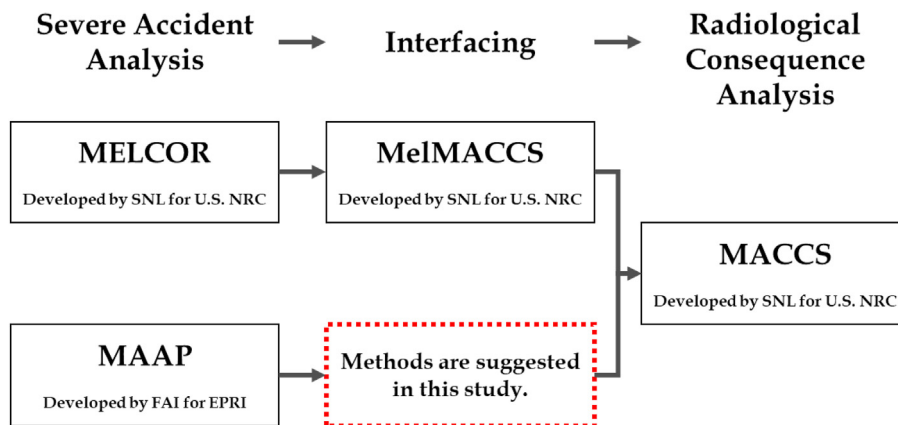


Fig. 1. Interfacing between severe accident analysis and radiological consequence analysis.

Table 4
Comparison of chemical groups between MAAP4 and MACCS-NUREG-1150.

MACCS (NUREG-1150)		G1	G2	G3	G4	G5	G6	G7	G8	G9
MAAP4		Xe, Kr O	I O	Cs, Rb O	Te, Sb O	Sr O	Ru, Rh, Mo, Tc O	La, Pr, Y, Nd, Am, Cm, Zr, Nb O	Ce, Np, Pu O	Ba O
g1	Xe + Kr									
g2	CsI + RbI		O	O						
g3	TeO ₂				O					
g4	SrO					O				
g5	MoO ₂ + RuO ₂ + TcO ₂ + RhO ₂						O			
g6	CsOH + RbOH			O						
g7	BaO									O
g8	La ₂ O ₃ + Pr ₂ O ₃ + Nd ₂ O ₃ + Sm ₂ O ₃ + Y ₂ O ₃ + ZrO ₂ + NbO ₂ + AmO ₂ + CmO ₂							O		
g9	CeO ₂ + NpO ₂ + PuO ₂								O	
g10	Sb				O					
g11	Te ₂				O					
g12	UO ₂									

Table 5
Comparison of chemical groups between MAAP5 and MACCS-NUREG-1150.

MACCS (NUREG-1150)		G1	G2	G3	G4	G5	G6	G7	G8	G9
MAAP5		Xe, Kr O	I O	Cs, Rb O	Te, Sb O	Sr O	Ru, Rh, Mo, Tc O	La, Pr, Y, Nd, Am, Cm, Zr, Nb O	Ce, Np, Pu O	Ba O
g1	Xe + Kr									
g2	CsI + RbI		O	O						
g3	TeO ₂				O					
g4	SrO					O				
g5	MoO ₂ + TcO ₂ + RhO ₂						O			
g6	CsOH + RbOH			O						
g7	BaO									O
g8	La ₂ O ₃ + Pr ₂ O ₃ + Nd ₂ O ₃ + Sm ₂ O ₃ + Y ₂ O ₃ + ZrO ₂ + NbO ₂ + AmO ₂ + CmO ₂							O		
g9	CeO ₂ + NpO ₂								O	
g10	Sb				O					
g11	Te ₂				O					
g12	UO ₂									
g13	Ag									
g14	I ₂		O							
g15	CH ₃ I		O							
g16	Cs ₂ MoO ₄			O			O			
g17	RuO ₂						O			
g18	PuO ₂								O	

Table 6
Comparison of chemical groups between MAAP4 and MACCS-SOARCA.

MACCS (SOARCA)		G1	G2	G3	G4	G5	G6	G7	G8	G9
MAAP4		Kr, Xe	Rb, Cs	Sr, Ba	I	Te	Ru, Rh	Nb, Mo, Tc	Zr, Ce, Np, Pu	Y, La, Pr, Nd, Sm, Am, Cm
g1	Xe + Kr	0								
g2	CsI + RbI		0		0					
g3	TeO ₂					0				
g4	SrO			0						
g5	MoO ₂ + RuO ₂ + TcO ₂ + RhO ₂						0	0		
g6	CsOH + RbOH		0							
g7	BaO			0						
g8	La ₂ O ₃ + Pr ₂ O ₃ + Nd ₂ O ₃ + Sm ₂ O ₃ + Y ₂ O ₃ + ZrO ₂ + NbO ₂ + AmO ₂ + CmO ₂							0	0	0
g9	CeO ₂ + NpO ₂ + PuO ₂								0	
g10	Sb									
g11	Te ₂					0				
g12	UO ₂									

Table 7
Comparison of chemical groups between MAAP5 and MACCS-SOARCA.

MACCS (SOARCA)		G1	G2	G3	G4	G5	G6	G7	G8	G9
MAAP5		Kr, Xe	Rb, Cs	Sr, Ba	I	Te	Ru, Rh	Nb, Mo, Tc	Zr, Ce, Np, Pu	Y, La, Pr, Nd, Sm, Am, Cm
g1	Xe + Kr	0								
g2	CsI + RbI		0		0					
g3	TeO ₂					0				
g4	SrO			0						
g5	MoO ₂ + TcO ₂ + RhO ₂						0	0		
g6	CsOH + RbOH		0							
g7	BaO			0						
g8	La ₂ O ₃ + Pr ₂ O ₃ + Nd ₂ O ₃ + Sm ₂ O ₃ + Y ₂ O ₃ + ZrO ₂ + NbO ₂ + AmO ₂ + CmO ₂							0	0	0
g9	CeO ₂ + NpO ₂								0	
g10	Sb									
g11	Te ₂					0				
g12	UO ₂									
g13	Ag									
g14	I ₂				0					
g15	CH ₃ I				0					
g16	Cs ₂ MoO ₄		0					0		
g17	RuO ₂						0			
g18	PuO ₂								0	

compartment (IV), because *jj* and *IV* can differ for each source term scenario, even when regarding the same reactor type. In this section, the time-dependent variables of MAAP and MACCS are written with a lower case “t”.

3.1. Amount of release

MACCS employs the release fraction (*RELFR*) of each chemical group to calculate the release amount of each radionuclide by multiplying the core inventory (*CORINV*) of each radionuclide. Thus, the fundamental concept to calculate the release fraction is to divide the release amount by the initial amount of a radionuclide. Radionuclides in the same chemical group have the same release fraction because they are grouped together by assuming they have similar chemical properties and transport characteristics. Accordingly, MACCS assigns dry deposition velocities and release fractions by chemical groups [1].

As aforementioned, it has been regarded as relatively difficult to interface the amount of release between MAAP and MACCS since MAAP employs chemical compounds to classify the fission product groups rather than chemical elements. Despite this, even if many users are unaware of this function, the MAAP code is also able to print out element information. Therefore, the approach to interfacing the release amount can vary widely depending on whether

this printing function of element information is known to code users or not. In this section, not only an advanced method using element information but also the old method using compound information is introduced with a historical overview.

3.1.1. Without chemical element information

When the element information is unknown, the interfacing method is based on decomposing the chemical compounds of MAAP to elements and then assigning them into the chemical groups of MACCS. The calculating method between MAAP4 and MACCS-NUREG-1150 in Table 4 is introduced as an example for its simplicity to explain. Among all 9 chemical groups of MACCS, only G3 and G4 correspond to multiple groups of MAAP; accordingly, the MACCS groups excluding G3 and G4 can be directly linked with MAAP groups without treatment. For instance, the release fraction of g5 of MAAP can be directly adopted by G6 of MACCS. To obtain the release fractions for G3 and G4 of MACCS, a procedure for decomposing the chemical compounds of MAAP and then recomposing them is needed.

To calculate the release fraction of G3 of MACCS, an assumption is made that Cs represents the relevant calculations excluding Rb. The release mass of Cs can be easily extracted from the release masses of CsI and CsOH using the molecular weights:

$$MFPREL_t(CsI) \cdot \frac{W(Cs)}{W(CsI)} + MFPREL_t(CsOH) \cdot \frac{W(Cs)}{W(CsOH)}, \quad (1)$$

where $MFPREL$ is the release mass of the FP group (kg) until time t in MAAP and W is the molecular weight (g).

The initial mass of Cs can be calculated by dividing the release masses by the release fractions printed as $FREL$ in MAAP:

$$\frac{MFPREL_t(CsI)}{FREL_t(CsI)} \cdot \frac{W(Cs)}{W(CsI)} + \frac{MFPREL_t(CsOH)}{FREL_t(CsOH)} \cdot \frac{W(Cs)}{W(CsOH)}. \quad (2)$$

Hence, the release fraction of the Cs group, which is expressed as $RELFR(Cs)$ in MACCS, can be obtained from dividing Eq. (1) by Eq. (2):

$$RELFR_t(Cs) = \frac{FREL_t(CsI) \cdot FREL_t(CsOH) [MFPREL_t(CsI) \cdot W(CsOH) + MFPREL_t(CsOH) \cdot W(CsI)]}{FREL_t(CsOH) \cdot W(CsOH) \cdot MFPREL_t(CsI) + FREL_t(CsI) \cdot W(CsI) \cdot MFPREL_t(CsOH)}. \quad (3)$$

If the initial masses of CsI and CsOH are provided as $MFPO$ (kg) in MAAP, $MFPREL/FREL$ in Eq. (2) can be changed into $MFPO$. Then, Eq. (3) can be simplified to:

$$RELFR_t(Cs) = \frac{MFPREL_t(CsI) \cdot W(Cs) \cdot W(CsOH) + MFPREL_t(CsOH) \cdot W(Cs) \cdot W(CsI)}{MFPO(CsI) \cdot W(CsI) \cdot W(CsOH) + MFPO(CsOH) \cdot W(CsOH) \cdot W(CsI)}. \quad (4)$$

Along the same lines, the release fraction of the Te group (G4 in Table 4) can be estimated as:

$$RELFR_t(Te) = \frac{MFPREL_t(TeO_2) \cdot W(Te) + MFPREL_t(Sb) \cdot W(TeO_2) + MFPREL_t(Te_2) \cdot W(TeO_2)}{MFPO(TeO_2) \cdot W(Te) + MFPO(Sb) \cdot W(TeO_2) + MFPO(Te_2) \cdot W(TeO_2)}. \quad (5)$$

This approach, which has been frequently employed in the past [7], can be used when the element information is not provided by MAAP. By the above procedure, all the release fractions from G1 to G9 of MACCS can be acquired and used to perform consequence analyses. However, this approach cannot be easily applied to the recent chemical grouping methods of MAAP and MACCS. Difficulties have arisen by the fact that the chemical groups of MAAP and MACCS complexly overlap, as can be seen in both the columns and rows of Table 6 and Table 7. For example, when g16 of MAAP in Table 7 is regarded, Cs and Mo can be decomposed into G2 and G7 of MACCS and not face further problems. On the other hand, g8 for instance is composed of multiple compounds, and it is not easy to determine how the portions should be assigned to G7, G8, and G9 of MACCS. If the release fraction of G7 is the target for estimation, the assigned portion from g5 and g8 plus the extracted mass from g16 are all recomposed, a method for which it is not easy to guarantee the accuracy of the estimated release fraction.

Accordingly, it is strongly suggested not to use this approach especially for the recent chemical groupings of MAAP5 and MACCS-SOARCA, since it involves high uncertainty in the procedures of decomposing the chemical compounds and assigning the resulting chemical elements. Therefore, applying the direct linking method between element to element introduced in the following section is highly advisable.

3.1.2. With chemical element information

The MAAP code has the capability to print out the information of 25 major chemical elements such as initial mass, release mass, and element mole fraction in 18 fission product groups. The release

mass of the 25 chemical elements can be directly printed and also calculated using other variables of MAAP:

$$MRELEL_t(II) = W(II) \cdot FAFPO(IE) \cdot FREL_t(IG) \cdot MTFPO(IG), \quad (6)$$

where.

- t : Calculation time in MAAP (s),
- II : Number of the element (1–25),
- IE : Number of the element for mole fraction (1–31),
- IG : Number of FP group (1–18),
- W : Molecular weight of element II (g/mole),
- $MRELEL$: Release mass of element II (kg),
- $FAFPO$: Element mole fraction in FP group,
- $FREL$: Release fraction of FP group IG , and
- $MTFPO$: Initial number of FP atoms in group IG (mole (kg/g)).

It should be noted that W multiplied by $MTFPO$ is in units of kg rather than g because $MTFPO$ indicates the initial number of the FP calculated by mass in units of kg. The molecular weight can also be calculated from the initial mass of the element ($MFPIN(II)$) divided by the initial number of FP atoms by the element ($NFPIN(II)$), which shows the same value as W . $FAFPO$ is listed in Table 8, where the mass number in the table represents the molecular weight of each element. For example, by employing Eq. (6), the release mass of Xe-131 until time t is calculated as:

$$MRELEL_t(1) = 131 \cdot FAFPO(1) \cdot FREL_t(1) \cdot MTFPO(1). \quad (7)$$

As another example, the release mass of I-131 should include the I-131 in the g2, g14, and g15 FP groups:

$$MRELEL_t(3) = 131 \cdot FAFPO(3) \cdot FREL_t(2) \cdot MTFPO(2) + 131 \cdot FAFPO(28) \cdot FREL_t(14) \cdot MTFPO(14) + 131 \cdot FAFPO(29) \cdot FREL_t(15) \cdot MTFPO(15). \quad (8)$$

Three different approaches are available to estimate the release fractions of the MACCS chemical groups until time t when the information of the chemical elements is provided by MAAP.

1. Calculating the total release masses per total initial masses of member radionuclides:

$$RELFR_t(MG) = \frac{\sum_{II} MRELEL_t(II)}{\sum_{II} MFPIN(II)}, \quad (9)$$

Table 8
MAAP5 element mole fractions in fission product groups.

Element	Variable Name	Element	Variable Name
Xe-131	FAFPO(1)	Ce-140	FAFPO(17)
Kr-84	FAFPO(2)	Pr-141	FAFPO(18)
I-131 in FP group 2	FAFPO(3)	Nd-144	FAFPO(19)
Rb-86 in FP group 2	FAFPO(4)	Sm-150	FAFPO(20)
Cs-133 in FP group 2	FAFPO(5)	Np-237	FAFPO(21)
Sr-88	FAFPO(6)	Pu-239	FAFPO(22)
Ba-138	FAFPO(7)	Rh-105	FAFPO(23)
Y-89	FAFPO(8)	Am-241	FAFPO(24)
La-139	FAFPO(9)	Cm-242	FAFPO(25)
Zr-91	FAFPO(10)	Cs-133 in FP group 6	FAFPO(26)
Nb-93	FAFPO(11)	Rb-86 in FP group 6	FAFPO(27)
Mo-96 in FP group 5	FAFPO(12)	I-131 in FP group 14	FAFPO(28)
Tc-99	FAFPO(13)	I-131 in FP group 15	FAFPO(29)
Ru-101	FAFPO(14)	Cs-133 in FP group 16	FAFPO(30)
Sb-127	FAFPO(15)	Mo-96 in FP group 16	FAFPO(31)
Te-128	FAFPO(16)		

2. Averaging the release fractions of the member radionuclides after calculating each release fraction:

$$RELFR_t(MG) = \frac{\sum_{II} \frac{MRELEL_t(II)}{MFPIN(II)}}{\text{The Number of } II}; \quad (10)$$

3. Choosing the representative release fraction of the representative radionuclide for the group:

$$RELFR_t(MG) = \frac{MRELEL_t(II_{represent})}{MFPIN(II_{represent})}, \quad (11)$$

where.

- *t*: Calculation time in MAAP (s),
- *MG*: Chemical group of MACCS,
- *II*: Number of the element in MAAP (1–25),
- *RELFR*: Release fraction of MACCS chemical group *MG*,
- *MRELEL*: Release mass of element *II* (kg), and
- *MFPIN*: Initial mass of element *II* (kg).

The elements of MAAP (*II*) are combined into the relevant chemical groups of MACCS (*MG*). When regarding the Ce chemical group in the MACCS-SOARCA grouping as an example, Eq. (9) to Eq. (11) can be expressed as Eq. (12) to Eq. (14):

$$RELFR_t(Ce) = \frac{MRELEL_t(10) + MRELEL_t(17) + MRELEL_t(21) + MRELEL_t(22)}{MFPIN(10) + MFPIN(17) + MFPIN(21) + MFPIN(22)} \quad (12)$$

$$RELFR_t(Ce) = \frac{\frac{MRELEL_t(10)}{MFPIN(10)} + \frac{MRELEL_t(17)}{MFPIN(17)} + \frac{MRELEL_t(21)}{MFPIN(21)} + \frac{MRELEL_t(22)}{MFPIN(22)}}{4} \quad (13)$$

$$RELFR_t(Ce) = \frac{MRELEL_t(17)}{MFPIN(17)}. \quad (14)$$

The appropriate choice among Eq. (9) to Eq. (11) is up to users, but using Eq. (10) looks to carry less conviction since it is just an averaging. In addition, it should be noted that creating a chemical group for each of the 25 elements can eliminate the approximation error inherent in Eq. (9) to Eq. (11), a method that might be suitable for users who do not need to run a large number of accident scenarios or who have ample resources for an extended MACCS running time to process the increased number of groups. This study basically covers an interfacing method relevant to the 9 historically categorized chemical groups of MACCS in NUREG-1150 and the SOARCA project, with a grouping method that reduces the number of chemical groups but that can introduce approximation error, as discussed above. Users may choose the appropriate solution by their situation.

The above release fractions mean cumulative release fractions until time *t*. MACCS simulates atmospheric dispersion and ground deposition by plume segments, and each plume segment has its

own timing and magnitude. Therefore, the release fraction of each plume segment (*RELFR* in MACCS) can be expressed by using the above expression of cumulative release fraction:

$$RELFR(MG, MP) = RELFR_{PDELAY+PLUDUR}(MG) - RELFR_{PDELAY}(MG), \quad (15)$$

where.

- *MG*: Chemical group of MACCS,
- *MP*: Number of plume segment of chemical group *MG* in MACCS (1–*NUMREL*),
- *NUMREL*: Number of plume segments that are released,
- *PDELAY*: Release time of each plume segment (s),
- *PLUDUR*: Duration of each plume segment (s), and
- *RELFR*: Release fraction of MACCS chemical group *MG*.

MRELEL is a cumulative value but it can decrease in some cases in which the FP flowing through a junction (*WFPJ*) becomes negative. This represents when mass flows from the environment to the containment, a phenomenon that occurs when the pressure in the containment becomes lower than the air pressure of the outside environment, for example, when the containment spray system operates. However, as the absolute amount of this negative flow is expected to be negligible, and MACCS does not allow a negative release fraction, a treatment to convert negative release into zero release is suggested. Moreover, cutting off the plumes with negligible release amounts, including zero release plumes, can help to shorten the running time of a MACCS analysis by reducing the number of plume segments.

The duration of the plume segment is recommended to be set the same as the time interval of the meteorological data to reflect and capture changes in meteorological conditions dynamically. Table 9 shows the three standard levels in performing radiological consequence analysis with regard to multiple plumes. This standard supports the importance of the plume timing setting.

There exists a concept of a maximum risk plume segment (*MAXRIS*) in MACCS analysis [1]. The selection of the risk-dominant plume is usually utilized to perform a conservative analysis, especially for the emergency phase. The risk-dominant plume is aligned with the first hour of the weather sequence or precipitation time. Therefore, it is recommended to select the plume segment that has a relatively large release amount of a major radionuclide. Selection of the risk-dominant plume does not influence the consequence result when all of the 8760 weather trials are encompassed in the analysis.

3.1.3. Multiple release paths and diverse chemical forms

In order to develop MACCS input accounting for multiple release paths and different chemical forms such as aerosol and gas separately, the flow of FPs through release junctions *WFPJ(IG, IS, JF)* should be employed instead of the release mass of the element *MRELEL(II)*, because all release paths and chemical forms are already integrated in *MRELEL*. In that case, the below terms supersede the *MRELEL* in Eq. (9–11):

Table 9
ASME/ANS standard for multiple plumes [8].

Capability Category I	Capability Category II	Capability Category III
DEVELOP a single plume for each release category.	DEVELOP multiple plumes for each release category (e.g., to reflect significant changes in the source term as a function of time, to capture meteorological changes).	DEVELOP multiple plumes for each release category at the same resolution as the underlying meteorological data (e.g., to reflect significant changes in the source term as a function of time, to capture meteorological changes).

$$MRELEL_t(II) \rightarrow W(II)K \cdot \frac{WFPJ_t(IG, IS, JJ)}{MFPO(IG)} \cdot FAFPO(IE) \cdot MTFPO(IG), \tag{16}$$

where.

- *t*: Calculation time in MAAP (s),
- *II*: Number of the element (1–25),
- *IG*: Number of the FP group (1–18),
- *IS*: Chemical form (1: Vapor, 2: Aerosol),
- *JJ*: Release junction number,
- *IE*: Number of the element for mole fraction (1–31),
- *W*: Molecular weight of element *II* (g/mole),
- *WFPJ*: Fission product flow through junction *JJ* (kg/s),
- *MFPO*: Initial mass of FP group *IG* (kg),
- *FAFPO*: Element mole fraction in FP group, and
- *MTFPO*: Initial number of FP atoms in group *IG* (mole (kg/g)).

Equation (16) is similar to Eq. (6) which uses *FREL* instead of *WFPJ* and *MFPO* after integrating the chemical forms and release junctions. By using the above expression, the release fraction of a plume with diverse chemical forms and multiple release paths can be calculated by:

$$RELFR(JJ, MG, IS, MP) = \frac{\int_{PDELAY}^{PDELAY+PLUDUR} \left\{ \sum_{II} \left[W(II) \cdot \frac{WFPJ_t(IG, IS, JJ)}{MFPO(IG)} \cdot FAFPO(IE) \cdot MTFPO(IG) \right] \right\} dt}{\sum_{II} MFPIN(II)}, \tag{17}$$

where *IE* and *IG* are connected to *II* in the equation and *II* is combined into the corresponding MACCS chemical group *MG*. It is important to note that integration is used in Eq. (17) in contrast to Eq. (15), since *WFPJ* is not a cumulative value.

3.2. Particle size distribution

MAAP5 defines 30 particle size bins, which cannot be modified arbitrarily by users. MAAP5 prints out the sizes of the bins by radius, and the bin sizes themselves change by time, although with no fluctuation. Minimum and maximum particle diameters (*d*) are about 0.05 μm and 500 μm, respectively, and the particle diameter of a size bin expands by multiplying $(d_{max}/d_{min})^{(1/30)}$ to the previous bin. The particle sizes of the bins in MAAP are presented in Table 10, while noting that care should be taken as these values are

Table 10
Particle size diameter (μm) of each particle size bin in MAAP.

Bin No.	Minimum size of bin	Maximum size of bin	Bin No.	Minimum size of bin	Maximum size of bin
1	5.00E-02	6.80E-02	16	5.00E+00	6.80E+00
2	6.80E-02	9.24E-02	17	6.80E+00	9.24E+00
3	9.24E-02	1.26E-01	18	9.24E+00	1.26E+01
4	1.26E-01	1.71E-01	19	1.26E+01	1.71E+01
5	1.71E-01	2.32E-01	20	1.71E+01	2.32E+01
6	2.32E-01	3.15E-01	21	2.32E+01	3.15E+01
7	3.15E-01	4.29E-01	22	3.15E+01	4.29E+01
8	4.29E-01	5.83E-01	23	4.29E+01	5.83E+01
9	5.83E-01	7.92E-01	24	5.83E+01	7.92E+01
10	7.92E-01	1.08E+00	25	7.92E+01	1.08E+02
11	1.08E+00	1.46E+00	26	1.08E+02	1.46E+02
12	1.46E+00	1.99E+00	27	1.46E+02	1.99E+02
13	1.99E+00	2.71E+00	28	1.99E+02	2.71E+02
14	2.71E+00	3.68E+00	29	2.71E+02	3.68E+02
15	3.68E+00	5.00E+00	30	3.68E+02	5.00E+02

rough estimates and there exist temporal changes of the size of each bin in the MAAP code.

By using the ADJUST subroutine of the code [6], MAAP lumps all the mass of the aerosol size distribution greater than 2 μm in radius into one size bin. Therefore, the particle size bins 16 to 30 of MAAP are rarely used. As can be checked in Table 10, particles with sizes above 2 μm in radius appear from bin number 15, and all particles having a size above 2 μm are assigned into bin 15. Since ADJUST is a subroutine that operates on particles in the containment building, particles in the reactor coolant pump or steam generator can have a distribution in particle size bins 1 to 30. Therefore, bin numbers 16 to 30 would likely be used in a SGTR (steam generator tube rupture) scenario. When particle size bins 16 to 30 are not used in a MAAP analysis, they can be combined into the last particle size bin of MACCS or be disregarded. Bins with zero fractions do not influence the radiological consequences but possibly increase the running time of a MACCS analysis.

Particle size distribution is not a time-dependent value in MACCS analyses, and thus a particle size distribution is not assigned to each plume segment. Rather, one representative distribution for each chemical group is an input of MACCS. Conversely, the particle size distribution of MAAP changes temporally but is calculated for all radionuclides together, irrespective of chemical group. Therefore, a reasonable way to interface the particle size bins of MAAP and MACCS would be to infer the cumulative particle size distribution after weighting the release mass of each chemical group of MAAP. Eq. (18) can be adopted for the weighting:

$$PSDIST(MG, MB) \text{ by mass} = \int \left\{ \sum_{II, SB, IS, JJ} \left[FMXRB_t(SB, IV) \cdot W(II) \cdot \frac{WFPJ_t(IG, IS, JJ)}{MFPO(IG)} \cdot FAFPO(IE) \cdot MTFPO(IG) \right] \right\} dt, \tag{18}$$

where *FMXRB* is the fraction of aerosols in each particle size array *SB* in compartment *IV* of MAAP. During the integration, *IE* and *IG* are associated with *II* in the equation, and *II* is combined into the affiliated MACCS chemical group *MG*. In addition, the size bin *SB* of MAAP is linked with the affiliated size bin *MB* of MACCS. Due to the flexibility to set MACCS particle size bin *MB*, users can set an adequate number of *MB* and assign *SB* into the affiliated *MB*. The integration is suggested to be done over the entire period of release since the current version of MACCS does not consider the particle size distribution for each plume segment [1].

The above equation is a particle size distribution expressed by mass rather than fraction. A particle size distribution as a MACCS

input in fraction format can be calculated by:

$$PSDIST(MG, MB) = \frac{PSDIST(MG, MB) \text{ by mass}}{\sum_{MB} PSDIST(MG, MB) \text{ by mass}} \quad (19)$$

The particle size distribution influences the dry deposition velocity of each chemical group in MACCS. Regarding the size of the particles, dry deposition velocity is calculated by two ways based on gravitational settling or expert elicitation [9]. The major difference between the two methods is that gravitational settling accounts for only aerosol size while expert elicitation incorporates not only aerosol size but also wind speed and surface roughness.

Dry deposition velocity by gravitational settling is calculated by using the following equation [10]:

$$v_d = \frac{d_g^2 g (\rho_p - \rho_a) C_C}{18 \mu_a \chi} \quad (20)$$

where.

- v_d : Dry deposition velocity (m/s),
- d_g : Geometric diameter of the particle (m),
- ρ_p : Density of the particle (kg/m^3),
- ρ_a : Density of air (kg/m^3),
- $g = 9.8$: Acceleration of gravity (m/s^2),
- C_C : Cunningham slip correction factor,
- $\mu_a = 1.8 \times 10^{-5}$: Viscosity of air at 25 °C ($\text{N}\cdot\text{s/m}^2$), and
- $\chi = 1$: Dynamic shape factor.

The Cunningham factor expresses slipping effects of fine particles:

$$C_C = 1 + \frac{\lambda_a}{d_g} \left(2.514 + 0.8e^{-0.55 \frac{d_g}{\lambda_a}} \right) \quad (21)$$

where λ_a is 0.069×10^{-6} m which is the mean free path of air at 25 °C.

The calculation method via expert elicitation was updated when the SOARCA Sequoyah analysis [11] was carried out. Specifically, the square term of surface roughness from the MelMACCS document was removed by the update. The correlation coefficients used in the Sequoyah analysis are tabulated in Table 11. The equation reads:

$$\ln(v_d) = a + b \cdot \ln(d_p) + c \cdot \ln(d_p)^2 + d \cdot \ln(d_p)^3 + e \cdot z_0 + f \cdot V \quad (22)$$

where.

- d_p : Aerodynamic diameter of particle (0.05–20 μm),
- z_0 : Surface roughness length (0.01–0.2 m),
- V : Wind speed (0.5–10 m/s), and
- a, b, c, d, e, f : correlation coefficients.

Referring to the MELCOR reference manual [13], logarithmic mass mean diameter \bar{D} can be calculated by the following equation:

Table 11
Correlation coefficients of expert elicitation employed in NUREG/CR-7245 [12].

Correlation coefficient	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	<i>f</i>
Value used in NUREG/CR-7245	-2.964	0.992	0.19	-0.072	1.061	0.169

$$\ln(\bar{D}) = \frac{\int_0^\infty \ln(D) f_m(D) dD}{\int_0^\infty f_m(D) dD} \quad (23)$$

where $f_m(D)dD$ is the mass in the distribution between diameter D and $D + dD$. Therefore, $f_m(D)$ is proportional to D^3 . When we know maximum diameter D_{max} and minimum diameter D_{min} of particle size bin MB , \bar{D} can be estimated by:

$$\begin{aligned} \bar{D} &= \exp \left[\frac{\int_{D_{min}}^{D_{max}} \ln(D) D^3 dD}{\int_{D_{min}}^{D_{max}} D^3 dD} \right] \\ &= \exp \left\{ \frac{D_{max}^4 [\ln(D_{max}) - 0.25] - D_{min}^4 [\ln(D_{min}) - 0.25]}{D_{max}^4 - D_{min}^4} \right\}. \end{aligned} \quad (24)$$

\bar{D} can be calculated for each particle size bin MB and used as the representative diameter in Eq. (22).

The maximum particle size considered in expert elicitation is 10 μm in diameter [14] but the MelMACCS algorithm by default allows for the correlation to be up to 20 μm , an extension by a factor of 2. The SOARCA Sequoyah analysis calculated dry deposition velocity using the gravitational settling concept when the particle size was greater than 20 μm . Otherwise, the expert elicitation approach was applied. Note that gravitational settling uses geometric diameter d_g (m), whereas expert elicitation adopts aerodynamic diameter d_p (μm). Both diameters can be converted by the following equation:

$$d_p = 10^6 \cdot d_g \sqrt{\frac{\rho_p}{1000}} \quad (25)$$

Gaseous forms of iodine such as elemental iodine (I_2) and organic iodide (CH_3I) can also be considered and incorporated in radiological consequence analysis. Dry deposition velocity is a key characteristic to distinguish the aerosol form of iodine (CsI), elemental iodine, and organic iodide. Different dry deposition velocities can be utilized to perform consequence analyses incorporating various forms of iodine; a detailed method is introduced in Kim [15].

3.3. Height of release and plume rise

Height of release is an important factor that influences radiological consequences as the starting position of atmospheric dispersion. Plumes rise by buoyancy flux or momentum flux in the environment, and the height of release (h) along with plume rise (Δh) is usually called the effective plume height:

$$h_{eff} = h + \Delta h. \quad (26)$$

MACCS simulates plume rise only by buoyancy flux, and users can choose between two options to determine plume buoyancy [1]. The first option is to calculate plume buoyancy by sensible heat release rate (\dot{Q}) of a plume using Eq. (27):

$$F = 8.79 \times 10^{-6} \dot{Q}. \quad (27)$$

The other option estimates plume buoyancy with the mass flow rate (\dot{m}) and density (ρ) of a plume by the following formula:

$$F = \left(1 - \frac{\rho}{\rho_a}\right) \frac{g\dot{m}}{\pi\rho}, \quad (28)$$

where ρ_a is the density of the surrounding air at ambient conditions (1.178 kg/m³) and g is gravitational acceleration (9.8 m/s²).

The rest of this section introduces how to obtain and interface the information of height (h), sensible heat release rate (\dot{Q}), mass flow rate (\dot{m}), and density (ρ) of a plume from MAAP results to MACCS input.

3.3.1. Height of release

The release height of a plume from ground level (*PLHITE* in MACCS) is calculated as follows:

$$PLHITE(MP) = ZFRB(IV) + ZJUNC(JJ) + \frac{XHJUNC(JJ)}{2}, \quad (29)$$

where.

- *MP*: Number of plume segments of chemical group *MG* in MACCS (1–*NUMREL*),
- *IV*: Donor compartment index of release junction,
- *JJ*: Release junction number,
- *PLHITE*: Release height of each plume segment above ground level (m),
- *ZFRB*: Floor elevation of compartment *IV* relative to ground level (m),
- *ZJUNC*: Bottom of junction height with respect to donor compartment floor (m), and
- *XHJUNC*: Height of junction *JJ* (m).

3.3.2. Heat of release

The sensible heat release rate of a plume (*PLHEAT* in MACCS) is the sensible heat content of the plume divided by its release duration (*PLUDUR* in MACCS). *PLHEAT* can be calculated by:

$$PLHEAT(MP) = \frac{\int_{PDELAY}^{PDELAY+PLUDUR} [HGRB_t(IV) \times WRB_t(JJ)] dt}{PLUDUR}, \quad (30)$$

where.

- *t*: Calculation time in MAAP (s),
- *MP*: Number of plume segments of chemical group *MG* in MACCS (1–*NUMREL*),
- *IV*: Donor compartment index of release junction,
- *JJ*: Release junction number,
- *PLHEAT*: Release rate of sensible heat in each plume segment ($W = J/s$),
- *PDELAY*: Start time of each plume segment from the time of accident initiation (s),
- *PLUDUR*: Duration of each plume segment (s),
- *HGRB*: Enthalpy in compartment *IV* (J/kg), and
- *WRB*: Mass flow rate through junction *JJ* (kg/s).

3.3.3. Mass flow rate and density of release

The mass flow rate of a plume segment (*PLMFLA* in MACCS) is derived using the following equation:

$$PLMFLA(MP) = \frac{\int_{PDELAY}^{PDELAY+PLUDUR} WRB_t(JJ) dt}{PLUDUR}. \quad (31)$$

Equation (32) estimates the mass density of a plume segment (*PLMDEN* in MACCS):

$$PLMDEN(MP) = \frac{\int_{PDELAY}^{PDELAY+PLUDUR} WRB_t(JJ) dt}{\int_{PDELAY}^{PDELAY+PLUDUR} \left[VGRB_t(IV) \times WRB_t(JJ) \times \frac{PEXO_t(IV)}{PEXO_t(E)} \right] dt}, \quad (32)$$

where *VGRB* is the specific volume in compartment *IV* (m³/kg), *PEXO* is the pressure in the compartment (Pa), and *E* means environment compartment.

It is not suggested to account for the counter-current mass flow rate (*WRBCC*) though junction *JJ* with *WRB*, since counter-current mass flow from the environment is expected to be zero or negligible. In case that counter-current mass flow is not negligible but important, $WRB_t(JJ) + WRBCC_t(JJ)$ can be used instead of $WRB_t(JJ)$ in Eq. (30), Eq. (31), and Eq. (32).

3.4. Special treatments for bypass scenarios

3.4.1. SGTR (Steam generator tube rupture) case

When the SGTR scenario is considered, care should be taken to exchange the MAAP output variables into appropriate ones for SGTR, since in this scenario radionuclides are released into the environment through the secondary side of the ruptured steam generator and then through the main steam safety valve (MSSV). The MAAP output variables that should be changed are as below:

$$FMXRB(SB, IV) \rightarrow FMXSG(SB, SG) = \frac{PLT(SB, SG)}{\sum_{SB} PLT(SB, SG)}$$

$$WFPJ(IG, IS, JJ) \rightarrow WFPSGOUT(IG, SG) \\ = WFVSGT(SG) \times \sum_{IS} MFPSG(IG, IS, SG)$$

$$WRB(JJ) \rightarrow WSGT(SG)$$

$$HGRB(IV) \rightarrow HG2SG(SG)$$

$$VGRB(IV) \rightarrow VG2SG(SG)$$

$$PEXO(IV) \rightarrow PSGGEN(SG)$$

where.

- *SB*: Number of the particle size bin in MAAP5 (1–30),
- *SG*: Donor steam generator loop index,
- *IG*: Number of FP group (1–18),
- *IS*: Chemical form (1: Vapor, 2: Aerosol),
- *FMXSG*: Fraction of aerosol in each particle size array of the steam generator,
- *PLT*: Aerosol mass concentration in each particle size array of the steam generator (kg/m³),
- *WFPSGOUT*: Flow rate of FP from the steam generator (kg/s),
- *WFVSGT*: Volumetric release fraction rate from the steam generator (/s),
- *MFPSG*: Mass of FP in the steam generator (kg),
- *WSGT*: Combined flow rate out of the steam generator through relief valves, safety valves, and main steam line including main steam line break (kg/s),
- *HG2SG*: Enthalpy in the steam generator (J/kg),
- *VG2SG*: Specific volume in the steam generator (m³/kg), and
- *PSGGEN*: Pressure in the steam generator (Pa).

It should be noticed that $FMXSG(SB, SG)$ is a defined parameter for user convenience and does not exist in MAAP originally. $PLT(SB, SG)$ can be directly printed and used instead of defining $FMXSG(SB, SG)$. It is also important to notice that $PLT(SB, SG)$, which handles the particle size distribution of the secondary side of the steam generator, is generated using the MAAP5 API (application programming interface). Therefore, applying the DLL (dynamic-link library) file made via MAAP5 API is necessary to obtain $PLT(SB, SG)$.

Similarly, $WFPSGOUT$ is also not an original parameter of MAAP but a defined parameter. $WFVSGT$ and $MFPSG$ can be directly used to calculate the FP flow rate from the steam generator instead of using $WFPSGOUT$.

The release height in the SGTR scenario can be defined by the height of the centerline of the main steam line break above ground level:

$$PLHITE(MP) = ZFRB(IV) + ZNMSLB, \quad (33)$$

where.

- MP : Number of plume segments of chemical group MG in MACCS (1– $NUMREL$),
- IV : Donor compartment index,
- $ZFRB$: Floor elevation of compartment IV relative to ground level (m), and
- $ZNMSLB$: Height of the centerline of the main steam line break above the floor of the receiving compartment (m).

Care should be taken to link the donor compartment, as it is related with the main steam line.

3.4.2. ISLOCA (interfacing system loss of coolant accident) case

ISLOCA is another type of bypass scenario similar to SGTR; however, special treatment for this case is not needed because the bare pool concept rather than a complicated concept can be employed to simulate decontamination and release of radionuclides in the ISLOCA scenario, like other non-bypass scenarios.

4. Conclusions

This study attempted to provide a solution to interface between MAAP and MACCS in order to respond to code users' requests. The extraction and conversion methods of this study are based on the magnitude and manner of release. In light of the historical overview, interfacing methods of the release magnitude were introduced assuming both awareness and absence of information related to chemical elements in the MAAP output. The manner of release comprising particle size distribution, height of release, and plume rise was covered, and a special treatment for a bypass scenario was also considered. It is expected that the suggested methods in this study will play an important role as a reference to link MAAP and MACCS.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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