MAAP 3.0B/PWR REVIEW

Part 4: Fission Product Release and Transport

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ABSTRACT

This report presents the forth part of a preliminary review of the MAAP 3.0B/PWR code. The review covers in-vessel and ex-vessel fission product release, aerosol dynamics, and fission product scrubbing by water pools, ice condensers and sprays. Detailed comments are made on basic assumptions, analytical modeling, selection of empirical correlations and model parameters. Comparisons between the MAAP code and the NRC developed MELCOR code are made.

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1. INTRODUCTION

This report summarizes a preliminary review of the MAAP 3.0B/PWR code.[1] The work was performed under Task 4 of the MAAP Code Evaluation Program. Task 4 of the program deals with MAAP code models for fission product release and transport in the primary system and containment building. The review includes phenomena such as in-vessel release due to cladding failure and fuel melting, ex-vessel release due to corium/concrete interaction, aerosol agglomeration, deposition and settling. An assessment of the models in MAAP for engineering safety features (i.e., pool scrubbing, sprays and ice condensers) is also presented. Comparisons between the MAAP code and the NRC developed MELCOR[2] code are made.

2. FISSION PRODUCTS TREATMENT IN PWR SYSTEM

2.1 Fission Product Species

In the MAAP and MELCOR codes, fission products refer to both radioactive and non-radioactive nuclides generated by fuel fissioning and other non-radioactive material released from structures (control rods) or corium/concrete interaction. The initial masses of 27 specific fission products (22 from fuel and 5 from structures), in the form of chemical elements, are provided by the MAAP input file as shown in Table 2.1. The 22 elements from the fuel are lumped to 12 groups when released from the fuel rods. The 12 groups, most are chemical compounds as shown in Table 2.2, are treated separately as aerosols or vapors in the MAAP code. The 5 elements from structures in Table 2.1 are lumped together into group 1 in the MAAP code (aerosol of Table 2.2). Any concrete aerosol generated by the corium/concrete interaction is also included in group 1 (aerosol of Table 2.2). The aerosol group (from structure materials) is not considered in the primary system and is only tracked in the containment.

In MELCOR, fission products are treated by the Radionuclide Package (RN). In this package, chemical elements of similar properties are grouped into 15 classes as shown in Table 2-3. Comparison with Table 2.2 shows that MELCOR treats the fission products as elements, not compounds as treated in MAAP. The different chemical forms used in the two codes will make a direct comparison of the source terms in the MAAP/MELCOR comparison exercise more complicated, because conversion of the species will have to be made. For example, CsI in class 2 and CsOH in class 6 of the MAAP species must be converted and combined in order to compare with Cs in class 2 of the MELCOR species. Although MELCOR permits the combination of two classes to form a new class upon release, such as Cs + I to CsI, all default properties have to be redefined for the new material class through user-specified input file.

MELCOR uses the VANESA model to compute the radionuclide release from the reactor cavity. Since VANESA models 25 species, mapping is employed between the 25 species defined in VANESA and the 15 material classes used in the RN package. Mapping is also performed between non-radioactive materials in the COR package (core), i.e., steel and steel oxide, etc., and the material classes in the RN package. If the default class structure is used, the default mapping applies. However, if the default class structure is revised, mapping must be modified through the input records. No mapping is needed in MAAP.

In MAAP, the total core inventory of the 27 elements given in Table 2.1 is user-specified in the input file. The initial distribution of the masses is not specified. In MELCOR, the initial distribution of the masses of core fission products can be specified in the input file to reflect the radial and axial power profiles in the core. In addition, MELCOR allows fission products to reside in the fuel-cladding gap.

2.2 Fission Product Transport

Fission products transport is closely coupled with the thermal-hydraulics. In any region of the primary system or containment, the rate of change of fission product depends on the volumetric flows and temperature of gases and structures in that region. On the other hand, the energy balance required in the thermal-hydraulic calculation needs information on the fission product decay heating. Therefore, the fission product behavior predicted by either MAAP or MELCOR strongly depend on the thermal-hydraulic behavior predicted by the codes.

In MAAP, fission product behavior is analyzed separately for the primary system, steam generators, pressurizer, quench tank and for the containment upper, lower, annulus and cavity compartments. Aerosol analysis is also performed for the auxiliary building. In each region aerosols and fission product vapors are transported along with the steam, hydrogen and other gases. If a water pool is presented in the region, as in the case of containment, pool scrubbing is estimated and the deposited aerosols are transported with water.

However, pool scrubbing is not modeled for the annulus and ice condenser regions of the containment. Pool scrubbing is also not modeled for the primary system. MAAP permits fission products mixed in the corium to be transported with corium during core relocation, discharge from the reactor vessel, and entrainment in the containment. The quantity of fission products transported with corium is determined by the fractional volume of corium involved in these processes.

In MELCOR, aerosols and fission product vapors are transported between control volumes through flow paths in a similar manner as the MAAP model. However, fission product transport in any flow path can be disabled by a user-input record to simulate the potential blockage of aerosols in the flow path. The removal of aerosols and vapors by filters in any flow path can also be modeled in MELCOR. No filter is modeled in MAAP.

2.3 Fission Product Decay Heating

MAAP tracks the energy associated with fission product decay. Each fission product species is assumed to decay at a rate proportional to that given by the ANSI decay curve. As the fuel node heats up and releases fission products, the associated decay heat energy moves out of the core into other parts of the primary system. In MAAP, each node in the primary system may have multiple heat sinks which can be heated up by the deposited fission products. Fission product masses which are deposited on each of the heat sinks are tracked separately. Decay energy associated with the suspended fission products is assumed not to heat up the atmosphere in that node. The energy is converted to one of the heat sinks which has the largest surface area. The selection of the largest heat sink is to reduce the temperature rise due to fission product decay heating. Revaporization of volatile fission products is determined by the heat sink temperature.

In the containment, MAAP allows the decay energy of the suspended fission products to be added to the atmosphere energy in that compartment. This will serve to increase the containment temperature. The decay energy of deposited fission products is added to the

single heat sink in the compartment. (In each compartment, MAAP only models one heat sink to receive the decay energy.) The surface area of the single heat sink in each containment compartment is user-specified. Note that no settling area is provided for the reactor cavity compartment.

In MELCOR, the decay energy of each fission product species can be proportional to the ANSI decay curve or be described in a tabular form provided in the input file. In each control volume, different treatments are applied to the decay energy provided by fission products in the atmosphere, in the water pool and deposited on the surface structure:

(1) Decay energy provided by fission products in the atmosphere is divided among the atmosphere of that volume, surfaces in that volume, and the atmosphere and surfaces of other volumes. The split of the decay energy is determined by user input.

(2) Decay energy provided by fission products in a water pool is completely absorbed by the pool.

(3) Decay energy associated with fission products deposited on a structure is allocated to the structure, the atmosphere of the volume, other surfaces in the volume, and the atmosphere and surfaces of other volumes. The split can be user-specified.

The above treatment in the MELCOR code is an attempt to consider energy transfer by radiation among the atmosphere and structures of the volume and other volumes.

A comparison between the two codes on the way fission products are treated is summarized in Table 2.4. It is seen that the MELCOR treatment is more flexible and many user-specified parameters are provided for performing sensitivity studies.

Table 2-1

Initial Core Fission Products in MAAP

From Fuel

1.	Xe	12.	Mo
2.	Kr	13.	Tc
3.	I	14.	Ru
4.	Rb	15.	Sb
5.	Cs	16.	Te
6.	Sr	17.	Ce
7.	Ba	18.	Pr
8.	Y	19.	Nd
9.	La	20.	Sm
10.	Zr	21.	Np
11.	Nb	22.	Pu

From Structural Materials

1.	Cd
2.	In
3.	Ag
4.	Su
5.	Mn

Table 2.2

Fission Product Species in MAAP

1. Noble Gases and Radioactivity Inert Aerosols
2. CsI + RbI
3. TeO_2
4. SrO
5. MoO_2
6. CsOH + RbOH
7. BaO
8. $La_2O_3 + Pr_2O_3 + Nd_2O_3 + Sm_2O_3 + 1/2\ O_3$
9. CeO_2
10. Sb
11. Te_2
12. $UO_2 + NpO_2 + PuO_2$

Table 2.3

Material Classes in MELCOR

Class 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. Alkaline 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, Pb, Re, Os, Ir, Pt, Au, Ni
7. Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8. Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9. Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10. Uranium	U	U
11. More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12. Less Volatile Main Group	Sn	Ga, Ge, In, Sn, Ag
13. Boron	B	B, Si, P
14. Water	H_2O	H_2O
15 Concrete	---	---

Table 2.4

Comparison of Fission Products Treatment

	MAAP	MELCOR
Initial Fission Products Masses	· Total core inventory of 25 elements are provided · No radial and axial distribution of masses are specified	· Initial masses are provided in COR and RN package · Radial and axial distribution of masses can be specified
Fission Products Species	· 12 classes (Most are chemical compounds, except noble gases and Sb) · Aerosols from structural materials are not considered in the primary system	· 15 elements (default) · A total of 20 elements can be user-specified · Chemical compound can be user-specified · Mapping is required
Fission Products Transport	· F.P. in each region is transported along with the flow · Pool scrubbing is modeled in all containment compartments, except ice-condenser and annulus region · No pool scrubbing in primary system · No filter in any flow path	· F.P. in each control volume is transported along with the flow · Pool scrubbing is allowed in every flow path and control volume as user-specified · Filter is allowed in any flow path as user-specified

	MAAP	MELCOR
Fission Product Decay Heating		
F.P. Suspended in Atmosphere	· Allowed to heatup the atmosphere in containment · Not allowed to heatup the atmosphere in primary system (Heat is transferred to the largest heat sink)	· Allowed to heat up atmosphere and structures of the current volume and other volumes · Split energy is user-specified
F.P. Deposited on Structures	· Heat-up of the single structure in containment · Heat up of multiple structures in primary system	· Allowed to heat up the structure, atmosphere and other structures of the current volume, and atmosphere and structures of other volume · Split of energy is user-specified
F.P. Deposited in Water Pool	· Complete absorption by water pool	· Complete absorption by water pool

3. IN-VESSEL RELEASE

In the MAAP code, the fission product release from the fuel rod starts at the time of clad failure. There are two criteria for clad failure: a user-specified failure temperature or when the computed burst stress of the clad is greater than the hoop stress. The failure temperature is provided by model parameter No. 46, which has a default value of 2100K. The recommended range of the failure temperature is 1200 to 2100K. Note that the default failure temperature is about 400K below the core melting temperature (2500K recommended in MAAP). The stress analysis depends on the fuel rod heat up rate and is therefore accident sequence dependent. At present, it is not known which criterion will result in early cladding failure for a given accident sequence. Since the release time, relative to the reactor vessel failure time and containment failure time, is important for the overall fission product deposition in the primary system and release to the containment, some comparative analysis should be performed to guide the selection of the two criteria for in-vessel release.

The releases of the volatile materials (noble gases, Cs, I and Te) are estimated in MAAP by either the steam oxidation model or the empirical correlations recommended in the NUREG-0772 report[3]. The steam oxidation model assumes that the release of volatile fission products follow the kinetics of fuel oxidation when UO_2 is heated in steam. The model shows that the fractional release of all volatile fission products is a function of time and temperature. The correlations recommended in NUREG-0772 provide the fractional release rate coefficient (fraction/minute) as a function of temperature only. The correlations contain empirical constants which are derived from experimental data for temperatures greater than 1000C. The two models have been compared with identical boundary conditions (core flows, temperatures, etc.) and the predicted release rates for Cs and I from the two models are reported to agree reasonably well[4].

A separate treatment is used for the release of tellurium, because tellurium can be chemically bonded to the cladding when Zr is less than 70-90% oxidized. Therefore, MAAP

provides an option to allow the tellurium to remain in the core region. The option is provided by the user-specified model parameter No. 51, FTEREL. With this parameter at zero, Te will remain in the core region, supply decay heat during the core heat up, and will be transported with Zr and molten fuel during core relocation into the containment. In the containment, Te is released from the melt as Zr is oxidized due to core/concrete interactions. When the model parameter is one, Te will be released according to either the steam oxidation model or the empirical correlations.

For non-volatile fission products, MAAP uses Kelly's correlations of the fractional release rate coefficient, which contain empirical constants for different fission product elements, similar to the correlations recommended in the NUREG-0772 report. The release of the non-volatile fission products is also limited by the transport of fluid flow computed by the MAAP code, i.e., the ability of the flow to carry the materials to the upper plenum. This implies that the concentration of any element in the atmosphere can not be greater than the saturated concentration based on chemical equilibrium. The flow blockage model, which has a strong effect on clad oxidation, can also affect the fission product release. A user-specified negative value of the model parameter No. 50, FPRAT, will turn on the blockage model which reduces the release of nonvolatile fission products. Thus, the flow reduction due to blockage will limit the release of non-volatile fission products.

Although the control rod and structural materials are not considered when calculating the core thermal-hydraulics, MAAP does consider the release of In, Cd, Ag, Su and Mn at the time the melting point of steel is reached in any node. The release of these materials is controlled by the saturation densities at the nodal temperature. However, the transport of these materials in the primary system is not accounted for. They are tracked only in the containment.

In MELCOR, the initial fission products masses are allocated to the fuel or the fuel-cladding gap. In the gap region, the fraction, not the mass, of the initial inventory is specified. The default values of the fraction of gap inventory used in MELCOR are

obtained from the CORSOR model. For example, the amount of gap inventory is taken to be 5% of the initial mass of Cs, 1.7% of I, 3% of the noble gases and 0.01% of Te. It should be noted that these values depend on the degree of irradiation of the fuel rod. Values provided by CORSOR are for highly irradiated rods and are not applicable to fresh rods.

MELCOR models the in-vessel release by two stages: gap release and fuel release. Fission products in the fuel-cladding gap are released at cladding failure defined by either a user-specified failure temperature or the loss of intact cladding geometry. The default value of the failure temperature is 1170K, which is much lower than the default failure temperature (2100K) used in MAAP for fission product release. The loss of an intact cladding is determined by the fuel melt model in the COR package.[2-5] When any fuel node reaches the above release criterion, the entire gap inventory in the fuel rods of that radial ring is released instantly to the surrounding control volume. The subsequent release from fuel as it heats up is calculated on a node by node basis. The fission products from the fuel are released to the gap inventory when the cladding is intact and are released to the surrounding control volume when cladding has failed.

Fission product release rates from the fuel are computed according to the empirical correlations provided by the CORSOR or CORSOR-M model depending on user's selection. These empirical correlations are the same as those reported in NUREG-0772, which were also used in the MAAP code. The CORSOR and CORSOR-M models consider the release rate of each material class as a function of temperature only. The surface-to-volume ratio of the material is not included. An option has been added in MELCOR to consider this ratio. A user-specified component surface-to-volume ratio is compared to a base value, derived from the CORSOR experimental data (422.5 1/m). The CORSOR or CORSOR-M computed release rate is increased or decreased by the ratio of the user-specified value to the base value. The release rate calculated for each class by the CORSOR or CORSOR-M model applies to all core components (i.e., fuel, cladding, control rod and particulate debris.)

The treatment of Te in MELCOR is slightly different than in the MAAP code. In MELCOR, the CORSOR or CORSOR-M computed Te release is used when the amount of cladding oxidation is greater than a cut-off value (default = 0.70). When the amount of cladding oxidation is less than the cut-off value, the release rate is multiplied by a multiplier (default = 0.025). Recall that in MAAP the Te release rate is determined by either the correlations without considering the oxidation effect or the release is completely prevented (i.e., no release at all).

MELCOR also considers the effect of the vapor pressure of each material class. No concentration of any element can be greater than the saturation concentration in the surrounding control volume. If the release mass is greater than the saturation value for the fission product vapor, the excess vapor mass is converted to aerosol mass. MAAP also uses the saturation concentration to limit the release of fission products. However, it is not known how MAAP treats the excess vapor mass, i.e., whether MAAP converts the excess vapor mass into aerosol mass or simply stops the release calculation.

Hobbins, et al.,[6] have pointed out that melt progression in the reactor core has important effects on fission products release as described below:

a. Burst release due to fuel microcracking during core reflooding can increase the fission products release.

b. Fuel liquification (i.e., dissolution of fuel pellet with molten zircaloy) destroys the crystal structure of the UO_2 pellet so that the release of fission products is much faster than the process of diffusion in a solid.

The above effects are not considered in MAAP or in MELCOR.

A comparison of the treatments in MAAP and MELCOR for the in-vessel release phase are summarized in Table 3.1.

Table 3.1

Comparisons of In-Vessel Release

	MAAP	MELCOR
Release Criteria		
1. User-specified Failure Temperature	Default = 2100K	Default = 1170K
2. Failure of Intact Cladding	Burst stress analysis	Clad melting analysis
Release Mode	Fuel Release	Gap release and fuel release
Volatile materials release	1. Steam oxidation model 2. Empirical correlations (NUREG-0772)	CORSOR or CORSOR-M model

Treatment of Te	User-specified option: 1. No release 2. Release but no consideration of the Zr-oxidation effect	User-specified cut-off parameter: 1. Above 70% Zr oxidation: CORSOR or CORSOR-M model 2. Less 70% Zr oxidation reduced by a user-specified multiplier (0.025)
Non-volatile Material Release	Kelly's correlation	CORSOR or CORSOR-M model

4. EX-VESSEL RELEASE

Fission product release during corium/concrete interaction is computed by the METOXA subroutine of the MAAP code. METOXA models vaporization of compounds from the molten corium pool. The compounds include those present in liquid form as corium constituents and those formed by chemical reactions between liquid corium constituents and the concrete decomposition products. A total of 23 reactions and element balances are modeled as the "basis set" in METOXA. Compounds not included in the basis set are considered in a set of auxiliary relations. The chemical reactions involve 30 x 6 condensed species and gases.

The vaporization model in METOXA assumes chemical equilibrium for all chemical reactions between the liquid corium constituents and the concrete off-gas. All gases are assumed to follow the ideal gas law. Non-ideality of the liquid compound is expressed by the activity coefficients, which are temperature and composition dependent. Four activity coefficients, expressed as user-specified model parameters, are provided by MAAP for sensitivity studies for the compounds SiO_2, SrO, BaO and K_2O or Na_2O. The recommended minimum and maximum values for these coefficients cover a large range of uncertainty.

METOXA also assumes equal oxygen potential throughout the debris pool. This assumption implies that gas agitation will create enough interfacial contact between any phases to promote oxygen diffusion to equilibrium. There is no stratification or phase separation on oxygen potential.

The ex-vessel release is sensitive to the corium temperature and all other factors that influence the corium temperature, such as corium/water and corium/concrete interactions. Thus, the ex-vessel fission products release is closely related to the analysis performed by the DECOMP subroutine. In DECOMP, a single corium temperature is computed based on the uniform mixing model.

In MELCOR, the VANESA model has been implemented and coupled to CORCON during every time step to estimate the release of fission products from the corium/concrete interaction. Two aerosol generation processes are addressed in VANESA. In addition to the vaporization release considered in MAAP, VANESA also includes the mechanical aerosol generation process.

A total of 27 species are considered in VANESA. Each species within the melt represents an element or group of elements presumed to have similar physical and chemical properties. Since CORCON assumes a multiple layer of the corium pool, each melt species is assigned to either the metallic or oxidic layer, depending upon the species' chemical characteristics. Furthermore, the oxygen potential of the oxidic layer is assumed to be the same as that calculated for the metallic layer. This assumption is equivalent to the assumption that oxygen transport between the oxidic and metallic phases is sufficiently rapid to compensate for various processes that would otherwise increase the oxygen potential of the oxidic layer.

In the VANESA vaporization model, chemical equilibrium between the gas phase and the condensed phase is assumed separately for the oxidic and metallic layers. The non-ideal effects are represented by the activity coefficient for the condensed phase and fugacity coefficient for the gas phase. However, the present version of VANESA used in MELCOR made the following approximations: (1) nearly all constituents of the metallic and oxidic phase of the core melt were assumed to be ideal, (2) Na_2O and K_2O were taken to be nonideal and have an activity coefficient of 10^{-8}, (3) all gases and vapors are ideal. The above approximations are also implemented in MAAP. (The recommended best estimate of Na_2O and K_2O activity coefficient is also 10^{-8}.)

The vaporization model considered in both MAAP and MELCOR provides the upper bound estimate of materials which are released from the core debris interacting with concrete. The kinetic factors which might prevent the vaporization process from reaching the equilibrium limit is also considered in VANESA. Since vaporization processes involve the transfer of

a volatile constituent to the free surface of the vapor phase, VANESA considers the following rate processes:

(1) The volatile constituents of the condensed phase must migrate to the free surface;

(2) Once the constituent reaches the free surface, it must transfer into a vapor; and

(3) Vapor at a surface must be conducted away from the surface lest the gas phase becomes locally saturated and net vaporization ceases.

Each of the above steps is a kinetic process that requires time. Because the steps are serially related any one of them can become rate-limiting. The kinetic processes are not modeled in MAAP. The inclusion of the kinetic model as well as the chemical equilibrium model is an important difference between the MELCOR and MAAP code.

Another important aspect of the VANESA model is the inclusion of mechanical aerosol generation, which refers to the dispersal of small droplets of melt into the containment atmosphere by gas bubbles rising through the melt. The process can occur in two ways: bursting of bubbles at a melt surface and melt entrainment. When gas generation rate is low, gases pass through the melt as discrete bubbles. At the surface of the molten debris, the bubble burst and throw the melt material upward in droplets of small dimension. As the rate of gas generation rises, entrainment of melt droplet at the melt surface can occur. Within the context of the VANESA model, only the uppermost portion of the core debris in the oxide layer participates in the mechanical aerosol production process. The particle size distribution, generation rate and aerosol composition are considered in the VANESA model.

The mechanical aerosol generation is important during the time periods when 1) gas generation rates are high during the early transient stage of corium/concrete interaction, 2) the corium temperature is low such that the aerosol generation due to vaporization becomes

insignificant at the late stage of a transient. At low corium temperatures, gas generation from the decomposition of concrete can still be high and the bubble bursting and/or entrainment can still be significant. The mechanical aerosol generation model is omitted in the MAAP code.

The comparisons of MAAP and MELCOR ex-vessel release are summarized in Table 4.1.

Table 4.1

Comparisons of Ex-Vessel Release

	MAAP	MELCOR
Chemical Reactions Considered	23	-
Elements and Compounds Involved	30 x 6	27
Vaporization Release		
Chemical Equilibrium	Yes	Yes
Gas Phase	Ideal gas	Ideal gas
Condensed Phases	Non-ideality by activity coefficient	Non-ideality by activity coefficient
Temperature-Dependent	Singe corium temperature	Separate temperatures for oxidic and metallic layers
Oxygen Potential	Uniform	Uniform for all layers
Kinetic Rates	Omitted	Rate limitation considered
Mechanical Aerosol Generation	Omitted	Burst release and melt entrainment are modeled

5. AEROSOL DYNAMICS

In MAAP, the aerosol and vapor removal rates from the gas phase to surfaces or the revaporization rates of deposited materials are computed in subroutine FPTRAN. In this subroutine, the aerosol decay or removal constant is expressed by the instantaneous aerosol concentration of any species. Brownian and gravitational motions are modeled for aerosol agglomeration using the principle of similitude. The principle states that the determination of the size distribution function can be made universal by introducing suitable scale factors, i.e., using dimensionless parameters to express the aerosol density and the aerosol decay or removal constant. The principle of similitude used in MAAP is valid only for two limiting cases when only one of the deposition process is operative. The two limiting cases are the aging of an initially specified aerosol and a steady-state aerosol generated by a constant continuous source. These two cases can indicate how the shape of size distributions vary with time or with the aerosol source strength, i.e., aerosol concentration decay or buildup. For aerosol conditions that involve both the steady-state and decay (aging) regimes of aerosol behavior or more than one particle removal processes, MAAP uses an interpolation method between the two limiting cases and the "combining law" to represent the combining effect of the two major removal processes.

Similarity treatment is also applied for particle deposition on surfaces covered by turbulent boundary layer (turbulent deposition), for deposition by inertial impaction and for particle removal by leaking. Empirical correlations of the removal rate constant as a function of aerosol mass density were developed for these mechanisms. It is noted that these dimensionless correlations involve many empirical constants. MAAP allows three of the empirical constants to be used as model parameters for sensitivity study. The parameters are:

	Best Estimate	Recommended Range	
		Minimum	Maximum
Collision Efficiency	0.33	0.33	1
Particle Collision Shape Factor	2.5	1	10
Aerosol Settling Shape Factor	1.0	1	15

The effect of such a large variation of these parameters should be demonstrated.

Water soluble aerosols are also modeled in MAAP to consider the condensational growth of hygroscopic nuclei in subsaturated or saturated steam environments. The model assumes:

(1) Particle size is uniform and the aerosol behavior is monodisperse;

(2) Particle growth by condensation is more rapid than the growth by coagulation and particle removal by gravity that the equilibrium size is attained by each particle;

(3) The initial seed particle radius is empirically determined as 0.3 microns (model parameter No. 49);

(4) The criterion for choosing between the dry aerosol model and water soluble aerosol model is based on the relative values of the predicted removal constant. The larger removal constant is taken to be the deposition of water soluble aerosols.

The aerosol dynamics performed in subroutine FPTRAN is based on an aerosol size distribution determined by the local quantities in each control volume. However, if a group of control volumes are interconnected and the inter-mixing flows are large enough to result in effectively the same size distribution, the aerosol dynamics will be computed by the

averaged quantities over the group members. The criterion of group formation is based on the product of the aerosol residence time and the removal rate. If the smaller product of all the control volumes in the group is less than 1, MAAP/PWR will take the following steps:

(1) All containment compartments are considered to be a group;

(2) All primary system nodes other than the reactor dome are considered to be a group, if recirculating flow paths in the primary system are not blocked by the presence of a water level.

MELCOR does not consider the formation of groups and does not use any averaged quantities to compute aerosol dynamics. All aerosol calculations are based on local quantities in a control volume.

MELCOR uses the MEAROS model to compute the aerosol behavior in the atmosphere of each control volume. MEAROS is a multisectional, multicomponent aerosol model, which evaluates the dynamic size distribution of each component. Different aerosol species, referred as components, are specified such that the model can track the behavior of each species individually. A number of size classes, referred to as sections, are specified to represent the particle size distribution for the suspended aerosols. Each component can have an independent source size distribution and source rate. In MELCOR, up to 5 sections and 15 components can be specified. However, limited by the computational time, specification of only one component is recommended in the present version of the MELCOR code to achieve the best calculational time. Condensation and water can be one of the aerosol components; it is referred to as fog and its mass is calculated in the Control Volume Hydrodynamics (CVH) package. The input parameters specifying the aerosol size boundaries are the lower bound and upper bound aerosol diameters. The default values are 10^{-6} and 5×10^{-5} m, respectively. The initial mass of the aerosol water is put into the smallest aerosol section.

MELCOR treats three agglomeration processes: Brownian, gravitational and turbulent agglomeration. The code allows many user-specified input parameters to control these processes for sensitivity studies. The input parameters include the material density (default 1000 kg/m^3), aerosol dynamic shape factor (default 1.0), agglomeration shape factor (default 1.0), turbulence dissipation rate (default $0.001 m^2/s^3$), particle slip coefficient (default 1.37) and particle sticking coefficient (default 1.0).

In MELCOR, aerosol deposition and settling are treated as separate processes. Aerosols can directly deposit onto a surface (ceiling, wall or floor) through deposition processes. Settling refers to large aerosols (formed by agglomeration) which fall onto horizontal surfaces in the control volume by gravity. There are four deposition processes: Brownian, gravitational, thermophoresis and diffusiophoresis. Thermophoresis is the migration of aerosol particles to surfaces due to a temperature gradient in the gas boundary layer. Diffusiophoresis is the migration of aerosol particles to surfaces in the flux of coolant vapor condensing on the surfaces.

In addition to structural surfaces, a water pool in any control volume is considered to be available for deposition and settling. Aerosols can also settle between control volumes through open flow paths, called "flowthroughs". The input parameters controlling the aerosol deposition processes are the thermal accommodation coefficient (default 1.0), particle slip coefficient (default 1.37), diffusion boundary layer thickness (default 10^{-5} m) and the ratio of the thermal conductivity of the gas to that for the particle (default 0.05).

Instead of the principle of similitude used in MAAP, aerosol dynamics in MELCOR is described by a set of ordinary differential equations. To integrate these equations forward in time, the kernel for agglomeration and the rate constants for aerosol deposition need to be known on the basis of size class used. When defined on the basis of size classes, the agglomeration kernel and the rate constants are referred to collectively as aerosol coefficients. The MELCOR/MEAROS model computes these aerosol coefficients. The pressure and temperature of the atmosphere are embedded in these coefficients and are

fixed for a single set of coefficients. Since the calculation of these coefficients is time consuming, MELCOR only computes 4 sets of coefficients at points given by combinations of two temperatures and two pressures. Changing thermal-hydraulic conditions during the transient are accommodated by interpolating between these sets of coefficients. Thus, the two temperatures and two pressures should be chosen to bound the temperatures and pressures expected during the transient. This procedure imposes some constraints as summarized below:

(1) The aerosol material density is assumed to be the same for all components.

(2) The particle shape is constant.

(3) The degree of turbulent agglomeration is constant.

(4) Deposition rate is independent of particle composition. (The ratio of the thermal conductivity of air to that of the aerosol material is fixed.)

The MEAROS model for particle growth or decay due to water condensation or evaporation on the aerosols is not used in MELCOR. MELCOR uses the fog mass (aerosol water) calculations of the Control Volume Hydrodynamics (CVH) package to determine the amount of water present in the atmosphere. The model accounts both for the diffusivity of water vapor in air and for the conduction of heat associated with condensation or evaporation.

The comparisons of MAAP and MELCOR aerosol dynamics are summarized in Table 5.1.

Table 5.

Comparisons of Aerosol Dynamics

	MAAP	MELCOR
Treatment Method	Numerical solution Aerosol decay or removal constant is related to aerosol concentration by the principle of similitude	MAEROS analytical model for the determination of aerosol coefficient
Aerosol Agglomeration Processes	Brownian and gravitational	Brownian, gravitational and turbulent
Aerosol Deposition		
Structures	Singe structure in containment Multiple structures in primary systems Structure orientation not specified	Multiple structures in each control volume Structure orientation specified
Processes	Gravitational, inertial impact, turbulent, leakage and thermophoresis	Brownian, gravitational, thermophoresis and diffusiophoresis
Aerosol Settling	On horizontal surfaces only	On horizontal surface only
Water Aerosol	Condensation and evaporation considered	Treated as fog in CVH package

6. ENGINEERING SAFETY FEATURE MODELS

6.1 Pool Scrubbing

Pool scrubbing refers to the removal of aerosols by several physical processes which are involved in transporting gas-borne particles to the liquid interface (bubble surface) when steam/gas mixtures are bubbled through a water pool. The processes modeled in MAAP include gravitation, inertial impaction, Brownian diffusion, and thermophoresis. The term used to quantify the reduction is the decontamination factor (DF). In MAAP, pool scrubbing is considered for the upper, lower and cavity compartments, and for the auxiliary building. In these regions, a water pool above the molten corium will remove a fraction of aerosols entrained by gases released from the corium/concrete interaction. A tube rupture in the steam generator and a pipe break in the primary system can also result in pool scrubbing of fission products and are modeled in MAAP. Pool scrubbing in the annulus compartment and ice-condenser region are not modeled in MAAP.

The pool scrubbing model used in MAAP consists of the computation of DFs for the incoming aerosols and for condensable gases that form aerosols upon entering the pool. The total DF for the incoming aerosols is computed by empirical correlations which depend on the following parameters:

(1) Gas injection mode: Two modes are modeled in MAAP for the PWR systems. A sparger is assumed for containment compartments involving corium/concrete interaction. A side vent is assumed for steam generator tube rupture and the auxiliary building for conservative consideration. (The DF associated with side vent injection is lowest.)

(2) Aerosol particle radius: MAAP/PWR sets the particle size as 0.01 microns for the sparger injection mode by assuming that the particles are formed by homogeneous nucleation. For the side vent injection mode, the aerosol particle mass distribution

is computed by the subroutines AMDIST and ADJUST, which cover 10 particle sizes ranging 0.01 to 1 microns.

(3) System pressure: The range of system pressure covered by the model for the calculation of DF is 1 to 5 atm.

(4) Pool subcooling: The degree of pool subcooling covered by the model is up to 30K.

(5) Pool height: The maximum pool height covered by the model is 6 m for sparger injection and 1.8 m for side vent injection.

(6) Gas composition: The incoming gas composition is assumed to be hydrogen and steam for the sparger injection mode and a mixture of steam, air and hydrogen for side vent injection.

In view of the above parameters, it appears that the range of system pressure, pool subcooling and pool height are adequate under most of the severe accident conditions. However, the assumed gas composition for the case of sparger injection (i.e., corium/concrete interaction) ignores the large quantity of CO_2 and CO released from the concrete decomposition. Since physical properties of CO_2 and CO are quite different than that of H_2, ignoring these gases would cause an uncertainty on the DF calculation.

For fission product vapors that have condensed to form aerosols upon entering a cold pool, the decontamination factors are computed by analytical models in the VAPRDF subroutine. The analytical models consider the effects of vapor condensation, inertial impaction and thermophoresis. In the inertial impaction model, MAAP assumes that a higher-velocity gas jet containing fine aerosol particles enters a pool of water. The entrainment of water at the gas-liquid interface forces water droplets into the submerged jet. The aerosol particles within the gas stream are collected by the water drops at a rate proportional to the relative

velocity between the drops and the particles. The main features of the analytical model include the following:

(1) The behavior of the two-phase axisymmetric turbulent free jet is not affected by the incoming aerosol particles.

(2) After the initial expansion zone, a turbulent entrainment zone is defined based on a minimum gas velocity required for the liquid atomization process. The entrainment region length is determined by the mass and momentum equations involving correlations for the entrainment velocity, minimum gas velocity and an entrainment coefficient.

(3) The average droplet size in the entrainment zone is computed using the volume-to-surface area approach and Weber number criterion. (The critical Weber number is taken as 6.)

(4) The aerosol particles are assumed to move with the jet velocity and the droplet velocity is estimated by a force balance. The particle collection efficiency is proportional to the relative velocity between the particles and droplets.

The above features are reasonable for the analytical model. The uncertainty of the computed DF depends on the assumptions and approximations related to the entrainment length, entrainment velocity, entrainment coefficient, droplet size and velocity, etc.

For the thermophoretic process, MAAP determines the decontamination factor by using the mass balance law and a thermophoretical deposition velocity related to the temperature gradient at the gas/liquid interface. Using the assumption that the particle concentration is proportional to the gas temperature, the DF is simplified as the ratio of initial gas temperature to the final gas temperature. It is noted that the assumption of the proportionality between the gas temperature and particle concentration was derived from

an analysis involving the thermphoretic transport of small particles through a free convection boundary layer adjacent to a vertical surface.[7] The analysis is valid under two conditions: 1) natural convection boundary layer flow along a vertical surface, and 2) the product of thermophoretic transport coefficient and Prandtl number is unity. The first condition may not apply for the present pool scrubbing situation. The validity of the second condition has to be proved.

In MELCOR, the treatment of pool scrubbing is different than in MAAP. MELCOR only considers the removal of incoming aerosols in the pool; the thermophoretic process is not considered. In contrast to the empirical correlations used in MAAP, MELCOR uses analytical models to compute the aerosol particle deposition velocity. In the model, the pool is divided into an entrance region and a bubble rise region. In the entrance region, it is assumed that the gas would attain thermal equilibrium with the pool water and condensation would occur. Thus, ar inlet scrubbing factor can be estimated on the basis of the fraction of the gas that condenses. It is assumed that the particles are swept along with the condensing steam. The DF is simply expressed as the ratio of mole fraction of noncondensables at the pool temperature and entrance pressure to the mole fraction of noncondensables before entering the pool.

In the bubble rise region, aerosol particle capture by gravitational settling, inertial impaction and Brownian diffusion are determined based on the mass and momentum conservation laws for spherical particles. Once bubbles begin to rise, evaporation will begin because the bubble pressure decreases with decreasing depth. Thus, water evaporation, which decrease aerosol removal, at the gas-liquid interface is also considered in MELCOR. The net DF in the bubble rise region is the sum of aerosol removal rates by these mechanisms. The total decontamination factor for pool scrubbing is the product of the values for the entrance and bubble rise regions. The following are the restrictions of the MELCOR pool scrubbing model:

(1) The submerged depth of the flow path must be greater than the "zero efficiency bubble rise height" in order to compute the pool scrubbing. The default value of the user-specified height is 0.01m.

(2) Two bubble rise velocities must be user-specified. One is the bubble rise velocity with respect to the liquid. This velocity determines the driving force for inertial deposition in the bubble and its default value is 0.2 m/s. The other velocity is the rise velocity of the bubble swarm used to determine the position of the bubble with respect to time and the resulting evaporation from the pool to the bubble. The default value of this velocity is 1.16 m/s.

(3) Spherical bubbles are normally assumed. However, a user can specify an elliptical shape for the rising bubbles. Elliptical correction factors are computed to modify the spherical bubble velocities. For spherical bubbles, the bubble diameter must be specified and the default value is 0.005m. For elliptical bubbles, the major to minor axis is user-specified and the default value is 1.5.

The comparison of MAAP and MELCOR pool scrubbing are summarized in Table 6.1.

Table 6.1

Comparisons of Pool Scrubbing

	MAAP	MELCOR
Incoming Aerosol Particles	Empirical correlation. Parameters controlling DF are: 1. Gas injection mode 2. System pressure 3. Pool subcooling 4. Gas composition 5. Pool height	Analytical model. Pool has two regions. 1. Entrance region (vapor condensation effect) 2. Bubble rise region User-specified parameters required: bubble diameter, rise velocity, minimum pool height

Aerosol Formed by Condensable Gases		
Jet Entrainment	Analytical model involves entrainment region length, entrainment velocity, droplet size and velocity, etc.	Not modeled
Thermophoretical	Analytical model developed for natural convection boundary layer flow along a vertical surface	Not modeled

6.2 Containment Sprays

Containment sprays when available are an effective mechanism for fission product removal. An analytical model using the first order rate equation is used in MAAP. The model shows that the rate of change of aerosol particle concentration due to containment sprays is governed by the water droplet size, water droplet concentration, relative velocity of the particles and water droplets, and the collection coefficient parameter. It is not clear how MAAP treats the collection coefficient parameter which should depend on the particle size distribution and species class. Absent from the MAAP model is the spray absorption of elemental iodine. There is no user-specified parameters to control the MAAP spray model.

MELCOR also uses the first order rate equation to estimate the change of fission products mass in terms of a rate constant. The rate constant depends on the material class and droplet size, and is treated differently for vapors and aerosol particles. Aerosol removal by inertial impaction and interception, with diffusiophoresis effects are considered. Vapor removal by absorption using a stagnant film model to compute the absorption coefficient is included. The vapor removal model is important for the absorption of elemental iodine. The MELCOR code allows a user-specified partition coefficient to limit the iodine absorption. The partition coefficient is defined as the ratio of the iodine concentration in the liquid droplets to the iodine concentration in the gas under equilibrium conditions. Using the partition coefficient a user can simulate chemical solutions contained in the spray water for the control of iodine. For example the partition coefficient can vary from 100,000 for the boric acid solution to 2,500 for the sodium thiosulfate solution.

Comparisons of the MAAP and MELCOR spray models are summarized in Table 6.2.

Table 6.2

Comparisons of Containment Spray Model

	MAAP	MELCOR
Aerosol Removal	First order rate equation	First order rate equation
Vapor absorption	Not modeled	Stagnant film model with partition coefficient for iodine vapor control

6.3 Ice Condenser

Fission product removal in an ice condenser is important when early containment failure occurs and significant fission products inventory is lost from the primary system prior to the depletion of ice. In MAAP, aerosol removal by steam condensation and gravitational settling are modeled for the ice condenser and upper plenum compartments. The empirical models used to estimate the aerosol decay rate are the same as that used for other containment compartments as described in Section 4 of this report. Since conditions under which these empirical correlations were developed are different than that in the ice condenser region, the models may not be appropriate for the ice condenser. For example, in addition to the deposition on solid surface, there is retention by absorption in flowing liquid water film formed by the melting of ice and the condensation of steam. Diffusiophoretic deposition, which occurs as the result of steam condensation, and thermophoretic deposition, which is related to the large temperature difference between the entering and leaving gases, could be more important in the ice condenser region than in other containment regions.

MELCOR does not have an ice condenser model and therefore, no comparison can be made.

6.4 Filters

Filter systems are used as atmosphere cleanup systems in many ESF systems, such as the containment air recirculating system and the auxiliary building filter system. The filter systems are intended to trap iodine and aerosols from the air before it is released to the environment.

MAAP has no model for the filter system. MELCOR has a simplified model to represent the removal of aerosol particles or fission product vapor in any flow path. The model requires the following user-specified parameters:

(1) Flow path in which a filter is modeled,
(2) Type of filter, i.e., aerosol or vapor but not both,
(3) Global DF,
(4) Total mass loading.

7. SUMMARY

Comparisons of the treatment of fission products by the MAAP and MELCOR codes are given in the summary tables presented at the end of each section of this report. These tables reveal large differences between the two codes. However, many differences between individual process may not make any significant impact on the overall fission product behavior. The fission product behavior is strongly coupled with the thermal-hydraulic behavior predicted by the code. The release, transport and removal of fission products are affected by the code predictions on fuel heatup, cladding failure, fuel melt, gas and structure temperatures, inter-compartment flow, natural circulation, and the corium/water and corium/concrete interactions. Thus the fission product treatment should be reviewed on the basis of a complete examination of the MAAP and MELCOR codes. The MAAP/MELCOR comparison exercise, which will present an integrated fission product/thermal-hydraulic analysis, can be used as the basis of evaluation.

Finally, the following are BNL concerns based on this preliminary review:

(1) In the primary system, the decay energy associated with the suspended fission products is not used to heat up the atmosphere but is converted to the heat sink with the largest surface area. This treatment would affect the heat sink temperature and the revaporization of volatile fission products.

(2) The present treatment of Te release in the reactor vessel by the two limiting models could affect the environmental release of Te in the event of an early containment failure. For IPE work, guidelines should be provided for the selection of Te release model. Impact of the two release models on environmental release should be established.

(3) The omission of the mechanical aerosol generation in the ex-vessel release model will introduce uncertainties when gas generation rates are high during the early

transient stage of corium/concrete interaction and when the vaporization process becomes insignificant at the late stage of a transient. Assessment of the uncertainties should be provided.

(4) Guidelines should be provided for the selection of the two cladding failure criteria (failure temperature or burst stress) for the initiation of in-vessel release.

(5) Absorption of iodine should be added to the containment spray model.

(6) The empirical correlations used in the pool scrubbing model do not include the CO_2 and CO gases for the sparger injection mode (i.e. corium/concrete interaction). Since the properties of CO_2 and CO are quite different than that of H_2, the omission of CO_2 and CO would affect the empirically determined DF.

8. REFERENCES

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