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**ASSESSMENT OF CONTAIN AND MELCOR FOR
PERFORMING LOCA AND LOVA ANALYSES
IN ITER**

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ABSTRACT

This report describes the results of an assessment of the CONTAIN and MELCOR computer codes for ITER LOCA and LOVA applications. As part of the assessment, the results of running a test problem that describes an ITER LOCA are presented. It is concluded that the MELCOR code should be the preferred code for ITER severe accident thermal hydraulic analyses. This code will require the least modification to be appropriate for calculating thermal hydraulic behavior in ITER relevant conditions that include vacuum, cryogenics, ITER temperatures, and the presence of a liquid metal test module. The assessment of the aerosol transport models in these codes concludes that several modifications would have to be made to CONTAIN and/or MELCOR to make them applicable to the aerosol transport part of severe accident analysis in ITER.

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Assessment of CONTAIN and MELCOR for Performing LOCA and LOVA Analyses in ITER

1. INTRODUCTION

The International Thermonuclear Engineering Reactor (ITER) will generate or contain radioactivity material in the form of activation products and tritium. ITER will have a variety of energy sources that can mobilize these materials in several different forms during loss-of-vacuum-accidents (LOVAs) or loss-of-cooling-accidents (LOCAs). These energy sources include: fusion neutron and particle heat, structure decay heat, plasma stored thermal and magnetic energy, coolant pressurization, chemical reactions, and hydrogen production and possible combustion. The mobilized forms radioactive material can take are: 1) dust resulting from plasma-facing-component (PFC) erosion during normal operation which can contain tritium or activation products, 2) aerosols resulting from structure surface oxidation, 3) aerosols resulting from PFC erosion during plasma disruptions, 4) isotopic exchange of tritium from PFCs with spilt coolants, and 5) cooling system corrosion products. The extent to which these materials can be confined, and thereby the amount of radioactive material released to the environment, will depend on the degree to which the integrity of several ITER confinement barriers can be maintained during LOVAs and LOCAs.

Two computer codes, MELCOR¹ and CONTAIN,^{2,3,4} have been developed for light water fission reactor (LWR) hypothetical accident analyses. In this report, we assess^a these computer codes for application to ITER LOVA and LOCA analyses. We use the results of this assessment to arrive at recommendations regarding the use of these codes to develop input for the ITER site independent "Early Safety and Environmental Characterization Study" (ESECS) and "Preliminary Hazard Analysis Report" (PHAR) documents. Because these codes were written for studying fission reactor containments, it is important to assess both the aerosol transport and thermal hydraulic models in these codes with respect to fusion confinement issues.

Our assessment is documented in four sections. The model requirements are defined in Section 2. In the third and fourth sections, the current modeling capabilities in CONTAIN and MELCOR are critically reviewed. The fifth section presents the results of an ITER LOCA test case. In Section 6, the conclusions and recommendations section, proposed modifications and their priorities are presented.

This assessment is closely related to another part of ITER Confinement Task (NID-9c), the development of experiment requirements for a moderate scale aerosol transport facility. It is intended that items identified as weak in the CONTAIN or MELCOR code or phenomena whose importance is unknown be improved by experiments proposed for the transport facility.

^a This review of MELCOR and CONTAIN is based on the documentation in the MELCOR 1.8.0¹ and CONTAIN user's manuals^{2,3} and on calculations performed with these codes. A detailed examination of the source code listing would have required far more resources than were available.

2. CONFINEMENT COMPUTER CODE MODEL REQUIREMENTS

An important prerequisite to assessing any computer code for possible use as a fusion reactor confinement analysis tool is a definition of the issues the code will be expected to address. This section will discuss the development of code requirements and priorities in three steps. First, we review what is known about fusion reactor confinements, second we define the important confinement issues, and third we define code requirements and priorities that will support resolution of the confinement issues.

2.1 ITER Confinements

Confinement structures must address two types of issues, radioactive or other mass-transport hazards and energy-related or pressure/vacuum hazards. The mass-transport hazards are caused by the presence of tritium and induced activities as well as the toxic chemical properties of candidate structural materials like beryllium. Energy-related hazards come from the energy contained in the fusion machine plasmas, the stored energy of the magnetic fields present, and the pressures that can be produced by confined cryogenic fluids and high temperature system coolants, e.g. water.

The radioactivity confinement is a key safety barrier for fusion machines. As machines develop, confinement designs will change but it is important to be aware of the safety implications of the various designs as they are developed so that safety aspects can be optimized. For example, it is desirable to make the confinement as passive as possible to improve reliability.⁵ Practical limits of 0.1 volume percent/day for an unpressurized confinement and 1 volume percent/day for a pressurized confinement have been recommended in Reference 5.

The ITER EDA design includes as major components^{6,7} the Primary Vacuum Vessel (VV), and the vacuum-tight outer Cryostat Vessel (CV). Inerted rooms, the building itself, and additional structures like passive filters or vents may also play a role in either radioactivity confinement or pressure/vacuum confinement as the EDA design and safety strategy evolve.

The main function of the vacuum vessel is to provide the primary vacuum boundary for the containment of the plasma. The vessel contains a vacuum volume that is D-shaped in cross section, has azimuthal symmetry about a vertical axis approximately 8 m from the center of the cross section, and is about 5 meters high in the center of the D-shaped cross section. It also contains the blanket which lines the interface between the vacuum and the vacuum vessel surface. The vacuum vessel is an austenitic steel or INCONEL structure divided toroidally (circumferentially) into 32 sectors, 16 parallel and 16 wedge. The parallel sectors are located inside toroidal magnetic field coils and the wedge sections each provide three large access ports. There is a lower port for vacuum pumping and plasma impurity removal; a horizontal port for different functions like plasma heating, fueling, diagnostics, etc.; and vertical ports for the removal, replacement, and cooling of blanket segments. The most critical surfaces within the vacuum vessel are the plasma-facing surfaces of the blanket and shielding. Plasma-facing surfaces must be able to withstand radiation effects and heat loads from the plasma yet not be the source of unacceptable concentrations of high-Z impurities in the plasma. These

requirements are met in ITER with one of two options⁸:

1. beryllium-clad copper plasma facing components (PFCs) and water-cooled copper or stainless steel vacuum vessel and blanket structures
2. beryllium plasma facing components, lithium/vanadium blankets, and sodium-potassium or sodium cooled vacuum vessel structures.

The main function of the cryostat system is to minimize the heat transfer from surrounding structures to the magnet coils. The vessel and an associated refrigerated radiation shield surrounds the vacuum vessel and magnetic field coils. The cryostat vessel⁹ is a double wall system^b with both walls near room temperature. The interior is lined with thermal radiation shrouds at about 80 K or with passive, multi-layer radiation shields. The cryostat vessel (CV) also serves as a partial second tritium release barrier.

Table IV.2-1 of Reference 6 provides expected operating conditions for the confinements. The internal pressure of the vacuum vessel is specified as 4×10^{-5} Pa during normal operation and up to 0.2 MPa absolute in case of accident. The external pressures for this vessel are 10^{-3} Pa to 0.1 MPa normal and 0.2 MPa absolute in case of an accidental release of all helium cryogen to the interior of the cryostat (but coolant at 2 MPa is also present⁹).

It may be necessary to add HEPA filters or gravel scrubbers relief valves associated with vacuum pumping lines to control the release of HTO in the event of an over-pressure of the vacuum vessel. Even these would not remove elemental tritium (HT) so biological conversion of HT to HTO has been proposed as one approach if removal of HT is required. Another approach that has been proposed is the development of a catalyst to encourage the oxidation. Since the dose impact of HT is considerably smaller than the dose impact of HTO, confinement features that address removal of HTO should have higher priority in model development than models of mechanisms or proposed containment features that offer a passive way of confining or removing elemental tritium.

In addition to the role of the vacuum vessel and the cryostat vessel, the building housing the reactor will contribute to the confinement of aerosol particles. For best estimate modeling of confinement, the contribution of the building should be considered.

2.2 Important Confinement Issues

There are two major groups of issues relevant to fusion confinement behavior, radioactivity confinement and pressure confinement. These groups and their application to ITER designs are discussed in the following two subsections.

^b To allow vacuum testing during its construction, control heat transfer by convection, and avoid condensation of atmospheric vapors on the cryostat surface.

2.2.1 Radioactivity Confinement

The radioactivity confinement issues related to aerosol behavior that are most important for an analysis tool to address are (in decreasing priority) (1) the transport/retention of activated isotopes associated with tokamak dust and that produced by oxidation driven volatilization of structural material, (2) the retention of tritium present as part of water vapor, (3) the retention of tritium adsorbed on or dissolved in aerosol particles composed of structural material, and (4) the ability of the confinement to retain tritium that is present as an elemental vapor.

The tritium issues are present in any fusion machine because of the use of hydrogen isotopes in the process. The retention of tritium has been divided into three separate issues because the mechanisms for transport of the pure oxidized form, the tritium adsorbed in or absorbed on mobile oxide particles, and the elemental form differ widely. The tritium issues have lower priority than the activated isotope issues because there is more extensive experience with the behavior of tritium than there is with the behavior of the activated isotopes.

The behavior of activated isotopes involves both the mobilization of the isotopes from a surface and the ability to transport the mobilized material. Figure 1 is a schematic illustration of the four mobilization mechanisms and the most significant transport/deposition mechanisms in a tokamak environment. The four potential mechanisms for mobilization of activated or toxic aerosol particles are volatilization due to reaction with air, resuspension and chemical reaction of dust deposited during normal operation, corrosion of surfaces by steam, and vaporization by plasma disruption. The transport/deposition phenomena believed to be the most important are¹⁰ the nucleation of aerosol particles from the vapor, agglomeration of aerosol particles, vapor condensation onto particles, particle deposition due to gravity, and particle deposition because of impaction due to the centripetal acceleration required to force particles to follow non-linear fluid flow.

Differences in the mobilization mechanisms are a major cause of the difference between fusion reactor confinement analysis and fission reactor source term analysis. In fission reactor accidents, the fission products and the energy available to mobilize them are concentrated in the fuel. In fusion, the activation product sources are more numerous and the potential energy sources to mobilize the material are more numerous and diffuse.

Both the mobilization and transport of the activated isotopes are strongly dependent on the reactor materials used since both the activation and the physical/chemical properties of the species with the activated isotopes are materials-dependent. A design with 316 SS/copper/beryllium components leads to concerns about the mobilization of activated stainless steel components like cobalt or manganese compounds and about the mobilization of beryllium or its oxides. A design with a lithium/vanadium blanket and beryllium plasma facing components leads to concerns about the possible mobilization and transport of oxides from lithium fires and isotopes produced by transmutation of vanadium (e.g. scandium, sodium).

In spite of the differences just discussed, many aspects of fusion activation product mobilization and transport are generally similar to the behavior of fission products in reactor containments. For instance, such basic mechanisms of aerosol transport as agglomeration and

Figure 1. Key aerosol mobilization and transport phenomena in tokamaks.

particle deposition as well as evaporation and condensation of vapors onto aerosol particles are not a function of the mobilization mechanisms or the materials that form aerosol particles. This observation suggests it may be reasonable to adapt the CONTAIN or MELCOR computer code for use in the analysis of fusion reactor confinements. The differences that will affect the analysis of confinement structures by CONTAIN or MELCOR include the potential for generation of much more tritium in fusion machines, the presence of cryogenic fluids in

fusion machines, the use of different materials in fusion and fission reactors, and the difference of the confinement/containment structures in the two kinds of machines. Many of these differences will require the incorporation of fusion-specific materials properties and transport data.

2.2.2 Pressure Confinement

A number of over-pressure threats to confinement have been defined in past fusion safety assessments.⁷ These include:

1. Over-pressure from first wall, blanket, or divertor coolant leakage.
2. Cryogen spill.
3. H₂ generation, pressurization, and combustion following H₂O reactions with plasma facing materials (e.g. graphite, beryllium, stainless steel, copper).
4. Air ingress leading to exothermic reactions and heating.
5. External events, (e.g. earthquakes, winds, fires, etc.)

Any of these events, or combinations thereof, could result in a breach of a confinement barrier, and thereby a possible release of radioactive material to the environment. Most of these over-pressure threats are specific to fusion, and will not be directly addressed by the CONTAIN or MELCOR codes. The heat transfer correlations and fluid properties of these codes will have to be extended to account for conditions that could range from cryogen to liquid metal temperatures, as well as properties added for cryogens and liquid metals. In addition, the chemical kinetics of oxidation of fusion specific PFC materials, and the consumption and generation of gases by these reactions will have to be added to these codes.

2.3 Aerosol Model Requirements

Any fission reactor containment computer code must be modified to produce an adequate simulation of activation product confinement in a fusion machine. However, it is neither feasible nor necessary to model all known aerosol phenomena. The practical approach is to use engineering judgement to establish preliminary priorities, install any missing models judged to be important, remove models that are inappropriate or irrelevant, and assess the code against the most relevant experiments that can be carried out. This section defines the aerosol model requirements. Priorities will be discussed in conjunction with Table 6 of Section 6. The aerosol phenomena that have been identified as important to predicting activation product mobilization and transport in the previous subsection (Figure 1) are:

1. The injection of volatilized material from heated and possibly oxidizing surfaces.
2. The resuspension, characterization, and potential chemical reaction of activity produced and deposited as particles during normal operation (i.e. tokamak dust).

3. The transport of non-volatile activated isotopes. The probable existence of activated isotopes in aerosol particles means that the ability to model the transport and deposition of aerosol particles will be required. This requires, in turn, the capability to model the agglomeration of aerosol particles because agglomeration to larger sizes can have a significant effect on the deposition of particles. It will require the ability to model the evaporation and condensation of any vapors present at more than saturation concentrations because the condensation of vapors onto particles often has a significant effect on particulate transport/deposition. If electrostatic precipitators and filters are proposed to remove these particles^c, the capability to model aerosol particle removal by these devices will be required. If very cool temperatures are expected, the condensation and freezing of water or other vapors at temperatures as low as 4 K will also require special models that consider the effects of the large temperature gradients and low temperature of cryogenics.
4. The transport of steam/water containing tritium. This capability must include consideration of the possible nucleation of water drops, evaporation and condensation of water vapor on heat structures and/or onto aerosol particles produced from structural materials. If any of the particle materials are hygroscopic^c, the effect of the activity of aerosol seed material on the equilibrium vapor pressure of water vapor must be considered. On the other hand, any models that assume the hygroscopic properties of fission products like CsI apply to all aerosols must be modified.
5. The spallation, breakup and subsequent entrainment of particles of oxide produced by reaction of air or water vapor with walls.
6. The transport of hydrogen isotopes as adsorbed surface layers or dissolved (absorbed) impurities in aerosol particles. Adsorption in and absorption on heat structures should also be considered but the requirement has lower priority than the adsorption in and absorption on aerosol particles because of the typically greater surface area of aerosol particles.
7. Isotopic exchange between elemental hydrogen gas and water vapor or condensed water.
8. The transport of any volatile activated isotopes.
9. Chemical reactions of hydrogen and tritium with oxidizing agents. This must include the effect of intentionally introduced agents like an apparatus installed to burn hydrogen, a catalyst, or biological conversion of HT to HTO.

^c Hygroscopic materials are those that absorb and retain water vapor, thus reducing the equilibrium vapor pressure of water over solutions of hygroscopic materials. CsOH, NaOH, and LiCl are examples of hygroscopic salts.

Table 1 is a summary of the aerosol behavior requirements identified above and some additional modeling needs which affect aerosol behavior but are primarily requirements for fluid behavior modeling. Like Table 2, the corresponding list of thermal hydraulic models required, Table 1 does not address whether or how well any particular code models the item listed. These questions are dealt with in Table 6 of the conclusions and recommendations section. The remainder of this section discusses the reasons the models listed are important to the analysis of fusion reactor confinements.

The first item in the table is the basic capability to model the mixing and transport of the gas phases. In fusion machines, this phase may contain helium, nitrogen, oxygen, hydrogen, tritium, and steam in varying proportions. While not normally thought of as aerosol modeling requirements, this capability is needed to consider the transport of gas phases and as support for aerosol behavior models. For example, changes in gas composition from steam to hydrogen can affect viscosity and thus particle settling speeds by a factor of three at a given temperature and pressure.

Volatilization due to reaction with air is one of the four ways that activated material may be introduced. The capability to analyze the extent of volatilization of chemical species and the timing of the mobilization is important because the extent of activity mobilization by this mechanism will probably influence the fusion source term in severe accidents. The ability to describe the timing of the mobilization is required to perform useful analysis of the transport of the activated material associated with the aerosol particles. The modeling capability must include the ability to model not only activated material, but inert material as well because the size and number density of all aerosol particles will strongly influence the transport of those particles that have activated material.

The third item in the table, the injection of spalled oxides from surfaces is present because laboratory-scale experiments with candidate first-wall materials (e.g. copper, vanadium, steels) have produced oxides that spall as the material cools¹¹. When the spalled material is suspended in convective currents, it is observed to produce particles that are small enough to be transported as part of an aerosol. If this potential mechanism for transport of activity is to contribute significantly to the actual transport of activity, the spalling of the surface material must occur when convection is sufficient to cause the spalled material to be suspended and to strike a wall with sufficient impact stress to cause the production of small particles. Thus the model for the injection of spalled oxide must include not only a characterization of the oxide (size distribution) but the timing of the injection.

Tokamak dust is known to form during the operation of machines containing graphites and beryllium. Some means of characterizing this dust will be required but this may be done outside of the off-normal analysis computer code (MELCOR/CONTAIN) by a code designed to model normal operation. If the model for tokamak dust generation is operated outside of the off-normal code, the results could be input to the off-normal calculation as a table of dust size and amount versus time.

The fifth item in the table, mobilization of corrosion products, is required because some scenarios will involve the release of liquids like water, lithium, or lithium-lead compounds. These coolants may contain significant amounts of activated corrosion products.

The sixth item in Table 1 is the resuspension (and characterization) of activity produced and deposited as particles (dust) during normal operation. Models for the size distribution need not be mechanistic. They may be as simple as a description of measured tokamak dust resuspension versus particle size and fluid speed. The key capability of this item will be the ability to determine the timing and size distribution of the resuspension.

It is not clear at the present time whether a single model will suffice to model the resuspension of tokamak dust and spalled oxides. If the dust resuspension model is sufficiently mechanistic, it may be used to find the resuspension of both dust and spalled oxides but if a non-mechanistic correlation is used to model the resuspension of tokamak dust, it may be necessary to use a separate model for the resuspension of spalled oxide dust. Because it is not clear that the model for the resuspension of tokamak dust will also be appropriate for the resuspension, these two models are listed separately.

Table 1. Current Aerosol Modeling Requirements for a Fusion Confinement Analysis Tool.

Code Must Model	Comment
Transport and composition of gas phase	The basic capacity to model gas phase transport is required to support most other models. Gas composition (and pressure) are required for aerosol particle behavior modeling.
Injection of volatilized material from heated and possibly oxidizing surfaces	Volatilization is one of four major potential sources of activated isotopes.
Injection of spalled oxides from surfaces	Oxide spalling has been observed with many candidate materials but current estimates indicate spalled material is likely to remain in the form of large particles that settle
Formation of tokamak dust	Tokamak dust is one of four major potential sources of activated isotopes.
Mobilization of corrosion products	Corrosion products are one of four major potential sources of activated isotopes
Resuspension of tokamak dust produced during normal operation	
Resuspension of spalled oxides	
Breakup of mechanically spalled oxides	This production has been observed in small scale experiments but analysis shows the amount of small particles produced is small
Transport of non-volatile activated isotopes, i.e. aerosol particles	Transport includes several mechanisms of particle agglomeration and deposition as well as gas-particle interactions that affect particle size or charge distribution

Table 1. Current Aerosol Modeling Requirements for a Fusion Confinement Analysis Tool (cont.).

Code Must Model	Comment
Transport of steam/water with tritium.	Important for both transport of HTO and the effect of condensing water on aerosol behavior
Adsorption and absorption of tritium (hydrogen/steam) on aerosol particles	The amount of adsorption is very dependent on the aerosol chemical species and can be added to existing models easily.
ITER-specific chemical reactions	The chemical form of Be, C, Li, ^{17}Li ^{83}Pb has the potential to affect the transport of these materials.
Isotopic exchange between elemental gas and water vapor or condensed water	
Chemical reactions of hydrogen	
a. Apparatus to burn	Not a passive device.
b. Catalyst	Models should wait for development of a catalyst.
c. Biological conversion	Models should wait for development of a specific conversion.

The model for the breakup of mechanically spalled oxides is needed because particles less than 3 to 5 μm in diameter are much less likely to settle or be deposited by inertial effects than larger particles. The size range 0.1 to 1 μm in diameter is particularly mobile because many of the mechanisms that cause deposition of particles less than 0.1 μm in diameter (e.g. diffusiophoresis and particle diffusion) are not effective in this size range either.¹² Because of the mechanistic basis of this model,¹³ it should also work for particles produced during normal tokamak operation and subsequently resuspended.

The ninth item in Table 1, transport of the less-volatile activated isotopes, i.e. aerosol particles, represents many models. For example:

1. Particle agglomeration due to diffusion, differential gravitational settling, or turbulent fluid flow will affect particle size and thus the transport. If particles are charged or possess electric or magnetic dipole moments, electric/magnetic effects may affect agglomeration. Agglomeration rates are proportional to the square of the particle number density and the dominant agglomeration mechanism is a function of particle size and charge distribution.
2. Particle deposition by gravity, diffusiophoresis, thermophoresis, diffusion to walls (Brownian motion), eddy current diffusivity in turbulent flows, impaction, and electromagnetic forces. The deposition models must consider ITER-

specific geometries and the presence of any filters or electrostatic particle removal apparatus that may be installed. The particle deposition mechanisms contribute in varying degrees depending on the aerosol particle sizes, the fluid speed, temperature gradients, and particle charge distribution.

3. The strong dependence of both particle agglomeration and deposition on both particle size and charge distribution means that aerosol transport is strongly coupled to models for evaporation or condensation of vapors off of or onto particles, the breakup of larger particles, and particle charging or discharging by ions or high electric fields in the gas.

The tenth item in Table 1, the transport of steam/water with tritium, is important because the steam/water will have molecules containing tritium. It is also important because condensing steam will alter the behavior of aerosol particles. Accidents with condensing steam will result in less aerosol transport than dry accidents.

The adsorption and absorption of tritium either as water vapor or as elemental gas on aerosol particles that are not predominately water would enhance the effects already discussed in conjunction with the transport of steam/water. For hygroscopic particles, the mass of steam condensed will be enhanced. The two possible hygroscopic aerosol materials that have been identified among current materials candidates are NaOH produced by the mobilization of sodium activation products in steam and Re_2O_7 , produced by the mobilization of rhenium activation products in air.

The twelfth entry in the table, ITER-specific chemical reactions, must be considered because several potential ITER materials, e.g. Be, V, Li, and $^{17}\text{Li}^{83}\text{Pb}$, can react with air or steam to form volatile chemical species.

The thirteenth entry in Table 1 is the isotopic exchange between elemental gas and water vapor or condensed water. This mechanism supplements evaporation/condensation, adsorption, and absorption as a means of transport of tritium from aerosol particles to vapor and conversely. Of course, isotopic exchange drives the isotopic fractions toward equal fractions in all phases, no matter what phase was the initial location of the activated isotopes.

The final entry in Table 1, chemical reactions of hydrogen, is not a well characterized requirement because the devices that may be installed to promote these reaction have not been identified.

2.4 Thermal Hydraulic Model Requirements

Performing LOCA and LOVA thermal hydraulic calculations for ITER will be a formidable challenge. The time-scale can vary from milliseconds, if the blow-down phase of a large LOCA is of interest, to days, if the long-term structural heat-up from decay heat is of interest. Structural temperatures can vary from -268.7°C (cryogenic temperatures) to 1000°C (~maximum temperature due to decay heating). Three different coolants have been proposed: water, cryogens, and liquid lithium. These coolants can pressurize confinement barriers and

react chemically with plasma-facing-component (PFC) materials (e.g. beryllium, carbon, tungsten, etc), or even react with each other (e.g. water and liquid lithium). For instance, water reacts exothermically with beryllium to produce both heat and hydrogen. Hydrogen can become an explosive gas in air given the appropriate conditions. During LOCAs and LOVAs, various modes of heat transfer can exist, including: forced and natural convection, boiling, and condensation. And finally, flows can vary from sonic to natural convection conditions.

In this section, we define the thermal hydraulic models a LOCA or LOVA analysis code would require to be applicable to ITER. In the following subsections, we discuss the thermal hydraulic phenomenon that we believe to be important in modeling hypothetical accidents in ITER. We have summarized these modeling requirements in Table 2. These requirements will form the basis for evaluating the CONTAIN and MELCOR code fluid dynamic models (note Section 4).

2.4.1 Fluid flow modeling issues

Both single and two-phase fluid flow will occur during LOCAs in ITER. This flow can become sonic in the case of water and cryogens, because these coolants are pressurized and can be expelled into evacuated volumes. As a consequence, choked flow models will be required for these coolants. These coolants will also flash due to either contacting superheated structures, or from stored internal energy, and could over-pressurize ITER confinement barriers (i.e. water at 200 °C has a saturation pressure of 1.5 MPa). Consequently, the flow of both the liquid and gaseous phase of these coolants must be accounted for, including any inter-phase momentum transfer. In addition, the possibility exists for encountering non-equilibrium thermodynamic flow conditions, for example during a low temperature water spill, requiring the adopted accident analysis code to have an inter-phase mass transfer capability.

The confinement barriers of ITER have multiple penetrations which are at a variety of different elevations. These penetrations represent possible fluid flow paths during accident conditions, along which either forced flow from coolant over-pressurization or natural convective flow during long-term decay heat-up could occur. These flow paths may contain valves, rupture disks, and frictional pressure losses. The adopted accident analysis code must be able to account for multiple parallel flow paths of this type.

The presence of non-condensable gases, such as air and hydrogen, must be correctly treated, including condensation and combustion effects on fluid pressure and flow. Finally, a number of engineered safety features (ESF's) could exist for ITER, such as containment sprays, filters, scrubbing pools, pressure suppression pools, and condensers, which will also require modeling capabilities.

2.4.2 Heat transfer modeling issues

The modes of heat transfer that are anticipated to exist between the structural components and coolants of ITER during hypothetical accident conditions include: single and two-phase heat transfer for both internal (inside of pipes) and external flow (over outer surfaces of structures). This heat transfer could be either natural or forced convection, boiling (pool or film boiling), condensation (plus freezing), and thermal radiation. All of these modes are likely to occur with either water or cryogen, because there are structures in ITER that are

Table 2. Modeling requirements for hypothetical accident analysis codes applicable to ITER.

Thermal hydraulic phenomenon	Code must model
Fluid flow	<ul style="list-style-type: none"> Single and two-phase fluid flow Flow conditions <ul style="list-style-type: none"> Natural convection, Sub-sonic Sonic Sonic choking models Friction/form losses, valves, etc. Engineering Safety Features <ul style="list-style-type: none"> Scrubbing pools, filters, etc. Inter-phase momentum transfer Non-equilibrium inter-phase mass transfer Multiple parallel flow-paths between confinement barriers volumes Non-condensable gas effects including hydrogen combustion Natural convective transport between confinement barrier volumes
Heat Transfer	<ul style="list-style-type: none"> Single phase heat transfer (gas or liquid) <ul style="list-style-type: none"> Forced convection for both internal and external flow Natural convection for both internal and external flow Two phase heat transfer <ul style="list-style-type: none"> Pool, film, and convective nucleate boiling Condensation (freezing) Radiant heat transfer <ul style="list-style-type: none"> Structure to gas or liquid, including the effect of aerosol particles Structure to structure Effects of non-condensable gases Multiple heat structures within a volume <ul style="list-style-type: none"> Conduction and internal heating
Chemical reactions	<ul style="list-style-type: none"> Kinetics of chemical reactions <ul style="list-style-type: none"> Water - beryllium, carbon Lithium - water, air, concrete Hydrogen - air Heating/cooling of structures from chemical reactions

either super-heated or sub-cooled with respect to saturation conditions for these coolants. Since both phases of these coolants are expected to be present during portions of the accident, the hypothetical accident code must treat heat transfer between both phases of the coolant and the various structures of ITER.

In addition to heat transfer between coolants and structures, the ability to model radiative heat transfer between structures would be a requirement, since this becomes the predominant mode for transferring the blanket/shield decay heat to the vacuum vessel or magnet cooling system during long-term LOCA analyses. The adopted code must have the flexibility of modeling any number of structures within a given confinement barrier volume (i.e. to allow modeling of the divertor and blanket components inside the vacuum vessel), and allowing internal conduction and heating (e.g. decay heat) in these structures. We have summarized these modeling requirements in Table 2.

2.4.3 Chemical reaction modeling issues

Chemical reactions that occur between some of the proposed coolants and PFC materials, between proposed coolants, or between proposed coolants and confinement volume atmospheres must be modeled. In the case of water, exothermic reactions with beryllium and endothermic reactions with carbon will occur, producing hydrogen gas. The heating/cooling produced by these reactions must be appropriately applied to PFC structures. Since hydrogen gas poses an explosive hazard under appropriate conditions, models that account for the chemical kinetics of hydrogen burning should also be available. Lithium is very chemically reactive with water, air, and to some extent concrete. These reactions are exothermic, and can result in lithium fires, hydrogen production and potential explosion, aerosol generation, and structural over-heating. If liquid lithium remains a coolant option for ITER or is used in a test module, then the chemical kinetics of lithium would have to be modeled.

3. AEROSOL MODELS IN CONTAIN & MELCOR

The CONTAIN and MELCOR aerosol behavior models have been critically reviewed for relevance to fusion reactor confinements. The CONTAIN review is based on a current CONTAIN 1.1 reference manual² and earlier or alternate descriptions of the models referenced in the current manual.^{3,4} The MELCOR review is based on a description of MELCOR 1.8.0.¹ Since both CONTAIN and MELCOR aerosol dynamics models are based closely on the MAEROS models¹⁴, they differ only in some of the simplifications made to improve running time. Table 3 is a comparison of the aerosol models in CONTAIN and MELCOR. The models are basically the same. The major difference is that fact that CONTAIN allows more than one aerosol component while MELCOR allows only one. Models for aerosol nucleation are also different but neither is adequate for analysis of fusion reactors. Details of the reviews are in Appendix A and potential modifications to adapt CONTAIN and/or MELCOR to model ITER confinements are given in Appendix B. The following limitations of CONTAIN and/or MELCOR for ITER confinements were identified:

1. Emphasis is placed on steam/water as the condensing species in both CONTAIN and MELCOR. The MAEROS equation for diffusion of water vapor to and from aerosol particles has been replaced by an expression from cloud physics that considers both mass transfer and heat transfer. Inspection of the equation shows it is particularly relevant for species like water that can be present at high concentrations and near saturation. If accidents involving cryogenics are to be analyzed, the consideration of heat and mass transfer to aerosol particles probably will have to be extended to cryogenic fluids (nitrogen and oxygen, perhaps helium and hydrogen) because it is not clear that assuming water properties for cryogen vapors and liquids is necessarily conservative (e.g. the very low heat capacity and low boiling temperature of liquid helium causes liquid helium to vaporize much faster than water and makes helium much less effective than water at causing aerosol deposition due to condensation on small particles).
2. There is no model for aerosol resuspension in MELCOR^{1 p. 3-55} and none is described for CONTAIN. Since a major source of possible activated material is the resuspension of dust from normal operation, this omission must be corrected to make ITER analysis creditable.
3. The fission product release (more appropriately termed mobilization in the context of fusion reactors) models provided as an option in MELCOR (CORSOR and CORSOR-M) are not appropriate for ITER. They should be inerted and replaced by ITER-relevant models or user input.
4. The use of fission product classes (Noble gases, Alkali Metals, Alkaline Earths, etc.) in MELCOR may be an unnecessary approximation in ITER. A few specific ITER-relevant species will probably be sufficient to describe the aerosols. Of course, the materials properties of these species (e.g. copper, beryllium, components of stainless steel, etc.) will have to be provided.

5. The condensation of vapors is assumed to begin on existing particles.^{2 p. 4-11, 4-13 and 1 p. 3-53} For a fission reactor containment where the condensing species has a low surface tension like water and there is a background of suspended dust, this is reasonable. The assumption may be unsatisfactory for a LOVA when gas or liquid is transported into the vacuum vessel, especially if the vapor that may condense has a high surface tension like many metals and the low gas pressure of the vacuum vessel has caused all of the dust to settle.
6. Gas pressures and temperatures can be much lower in fusion accidents than in LWR accidents. All of the gas properties representations relevant to aerosol transport, e.g. viscosity, density, thermal conductivity, must be extended to the lower pressures and temperatures present in some hypothetical fusion accidents. Also in hypothetical ITER accidents, evaporation of material frozen on cold surfaces or reaction of water vapor with hot surfaces to produce hydrogen, carbon monoxide, or carbon dioxide is likely to cause significant changes in bulk gas properties during hypothetical fusion reactor accidents. This may make the MELCOR/CONTAIN practice of assuming the gas phase composition to be constant for aerosol dynamics calculations^{2 p. 4-6 and 1 p. 3-52} a poor approximation.
7. The equation used to limit evaporation rates of water in CONTAIN assumes the dissolved material in the water drop is hygroscopic^{2 p. 4-7}. This is not the case for many candidate ITER materials.
8. The MAEROS model for particle growth from water condensation onto pre-existing aerosol seed particles has not been employed. The MELCOR description says the change in aerosol size distribution is handled by the same equations as in the MAEROS condensation/evaporation model^{1 p. 3-53} but no description of these equations has been found. The CONTAIN approach is to solve rate equations for each particle size class^{2 p. 4-8}, an approach which usually causes severe Courant limits and probably is the motivation behind limiting the number of species that are allowed to affect aerosol size distributions. One consequence of incorrect models for the effect of evaporating or condensing vapors on particle size is often a failure to model the conservation of particle number density when more than one species of vapor is evaporating or condensing and no other effect is significant. Because errors in particle number density produce errors in the particle surface area and thus the particle size distribution, such errors usually lead to large errors in deposition and transport results.
9. Condensates and deposited liquids on walls are apparently assumed to be liquid in MELCOR.^{1 p. 3-32} Surface layers thicker than 0.0005 m (or an alternate user input thicknesses) are assumed to run off the wall and into the pool. In ITER, the condensates and deposited aerosol particles may be solid and remain on the wall to form thick deposits. Some sort of test to discriminate between deposits that stick on walls and those that can run down walls is necessary.
10. In MELCOR, fogs (aerosols) with more than 0.1 kg/m³ mass density are assumed to deposit immediately. In ITER, variations in condensed phase density (metals are heavy) or the fluffy nature of some solid aerosol particles,

or low viscosities in the gas phase may cause an order-of-magnitude variation in typical maximum mass densities from those of water drops. If proper aerosol agglomeration and deposition models are in place, this redundant and specialized limit is not necessary.

11. The expression for particle deposition by diffusiophoresis in CONTAIN^{2 p. 4-16} has been specialized to include only water vapor and water particles.
12. The priorities used to develop the aerosol particle dynamics models in CONTAIN and MELCOR may not be correct for ITER. There may be some unnecessarily detailed models and some more important models that are missing. For example, there is no model for the deposition of particles due to the motion of the fluids in curved paths in CONTAIN or MELCOR. Since the centripetal acceleration is likely to be on the order of the acceleration of gravity for some phases of some accidents in ITER^d, the centripetal inertial deposition model is as important as the settling models and should be added for a consistent analysis. Consistent analysis will also require generalization of the model for agglomeration due to different settling speeds to include agglomeration due to different radial speeds in curved paths and consideration of the effects of possible electric charge and electric/magnetic dipole moments on aerosol particle behavior.
13. The models for decay heat in CONTAIN and MELCOR are for LWR structure partitioning and fission products. A defensible analysis of ITER will require an ITER-relevant model or revised user input values appropriate to ITER.
14. The MELCOR model for aerosol nucleation is specialized to the case of water vapor forming a fog in a typical containment environment. The low pressures, high temperatures, and dry environment of many fusion accident scenarios require a more general model for aerosol nucleation.

^d Even for a radius of 8 m, a fluid speed of 2.5 m/s requires a centripetal acceleration of $v^2/r = 0.8 \text{ m/s}^2$ or about 0.1 times the acceleration of gravity to turn aerosol particles with the fluid. Smaller radii near structural components will require accelerations on the order of the acceleration of gravity to keep particles in the fluid. The slip of particles relative to the fluid is equivalent to effect of a gravity force field for the purposes of calculating agglomeration and particle deposition in a frame of reference moving with the fluid.

Table 3. Comparison of Aerosol Models in CONTAIN and MELCOR.

Phenomena	MELCOR	CONTAIN
Transport and composition of gas phase	Four sets of aerosol coefficients are interpolated over time. The default properties are those of air ¹ pp. 3-52,4-8.	The gas is assumed to be air. Four sets of aerosol coefficients are interpolated for some coefficients. Some coefficients are constant ⁴ pp. 2-42 & 2-43.
Injection of volatilized material	Current model consists of input initial fission product location tables and release from LWR fuel ¹ pp. 3-48,3-49.	Current model consists of input fission product source tables ⁴ p. 2-101.
Injection of spalled oxidized from surfaces	Current model for initial distribution of aerosol particles ¹ p. 3-53 could be used if the user knows when the oxide spalls.	Current model for user input of a log normal initial aerosol particle distribution ⁴ p. 2-39 might be used if the problem were started when the oxide spalls.
Formation of Tokamak dust	No model	No model
Mobilization of corrosion products	Current model for initial distribution of aerosol particles ¹ p. 3-53 could be used if the user knows when the corrosion products are mobilized.	Current model for user input of a log normal initial aerosol particle distribution ⁴ p. 2-39 might be used if the problem were started when the corrosion products are mobilized.
Resuspension models	no model ¹ p. 3-55	no model
Breakup of mechanically spalled oxides or tokamak dust	no model	no model
Transport of non-volatile activated isotopes. Size distribution	User-specified discrete size ranges (sections) with geometric progression. Aerosols that grow beyond the largest section are lost. ¹ p. 3-52	User-specified discrete size ranges (sections) with geometric progression. Aerosols that grow beyond the largest section or shrink below the smallest section are placed in a special upper bin or lower bin and assumed to deposit. ⁴ p. 2-40

Table 3. Comparison of Aerosol Models in CONTAIN and MELCOR (cont).

Phenomena	MELCOR	CONTAIN
Transport of non-volatile activated isotopes. Coagulation or agglomeration mechanisms.	Brownian motion, gravity, turbulence effects considered. Electromagnetic effects not considered. ^{1 p. 3-52}	Brownian motion, gravity, turbulence effects considered. Electromagnetic effects not considered. ^{4 p. 2-44}
Transport of non-volatile activated isotopes. Deposition mechanisms.	Brownian motion, gravity, thermophoresis, diffusiophoresis considered. Electromagnetic effects and turbulent deposition not considered. ^{1 p. 3-52}	Brownian motion, gravity, thermophoresis, diffusiophoresis considered. Electromagnetic effects and turbulent deposition not considered. ^{4 p. 2-44} The driving force for particle diffusion (i.e. Brownian motion) is represented in a constant particle diffusion boundary layer thickness. ^{4 p. 2-45}
Transport of non-volatile activated isotopes. Vapor condensation onto and evaporation from aerosol particles.	Particle size change due to condensation/evaporation is not modeled. Mass of liquid water in the atmosphere is distributed over aerosol sizes "for consistency in the overall calculation scheme". ^{1 p. 3-52} Mass addition rate for each particle size range (section) is calculated considering mass and heat transfer. ^{1 p. 3-53}	Particle size change due to condensation or evaporation is not discussed and probably not modeled. Mass addition rate for each particle size range (section) is calculated considering mass and heat transfer. ^{4 p. 2-47}
Aerosol composition	One aerosol component (i.e. one particle composition for each size range or section) is modeled. The composition is mapped back and forth into fission product classes. ^{1 p. 3-53}	More than one aerosol component (i.e. one particle composition for each size range or section) is modeled. ^{4 p. 2-38}

Table 3. Comparison of Aerosol Models in CONTAIN and MELCOR (cont).

Phenomena	MELCOR	CONTAIN
Aerosol nucleation	A fog is presumed to form when the thermal hydraulic code module calculates that liquid water should be present ^{1 p. 3-53} .	Seed nuclei are assumed to be present by the code. They are generated as needed. ^{4 p. 2-48}
Transport of steam/water with tritium	Steam/water transport is modeled.	Steam/water transport is modeled.
Adsorption and absorption of tritium (hydrogen/steam) on aerosol particles.	not modeled	Evaporation from particles is assumed to be inhibited when the mass of water and solid are comparable. ^{4 p. 2-47}
ITER-specific chemical reactions	not modeled	not modeled
Isotope exchange	not modeled	not modeled

4. THERMAL HYDRAULIC MODELS IN CONTAIN & MELCOR

The CONTAIN and MELCOR codes both model fluid behavior by solving conservation equations in terms of control volumes and flow paths. While there are some similarities between the thermal hydraulic models of CONTAIN and MELCOR, the number of conservation equations that are solved, the solution procedure adopted to solve these equations, and the number of flow paths allowed are quite different. The following two subsections describe the thermal hydraulic modeling approach adopted for the CONTAIN and MELCOR codes, assess the merits of each modeling approach, propose the code most applicable for ITER hypothetical accident thermal hydraulic analyses, and suggest required code modifications needed to make the proposed code more ITER relevant. We summarize our thermal hydraulic evaluation of the CONTAIN and MELCOR codes in Table 4.

4.1 Thermal Hydraulic Modeling Approach

The MELCOR code solves six conservation equations to determine fluid flow. These equations are: conservation of mass, momentum, and energy for both phases of a coolant. MELCOR also allows the user to specify any number of flow paths between any combination of control volumes, and either or both phases to flow along these flow paths. The CONTAIN code solves three conservation equations to determine fluid flow. These equations are: total conservation of mass and energy equations (e.g. both phases combined), and conservation of momentum for the vapor phase. CONTAIN allows the user to specify only a single flow path between control volumes, along which only vapor flow is calculated. As a consequence, CONTAIN's fluid dynamic model has limited flexibility, assumes thermodynamic equilibrium, and requires the liquid phase to vaporize in order to leave a given control volume. Our

experience with low temperature water spill predictions in the ITER CDA indicated that a thermodynamic equilibrium approach is too conservative regarding predicted confinement volume pressurization. CONTAIN does not track the liquid level within a control volume with respect to the user specified flow path elevation. If this flow path lies below the surface of a pool during a transient, CONTAIN still assumes that only vapor flows along this flow path. CONTAIN will adjust the free-volume within a given control volume to account for the existence of a pool, but what CONTAIN does if the vapor volume becomes less than or equal to zero is not stated by the authors of CONTAIN.

MELCOR and CONTAIN employ very different solutions schemes to solve their respective fluid conservation equations. MELCOR forms a linearized equation set that is only a function of fluid velocity. This equation set is formed by finite differencing the momentum conservation equations, linearizing the equation-of-state for water, and substituting for fluid densities and energies from finite differenced mass and energy conservation equations. This equation set is then solved by standard matrix inversion techniques to give new time velocities. This procedure is repeated to converge any nonlinear velocity terms, for example frictional momentum loss terms. Once the velocities are converged, new time densities and energies are calculated and the pressures based on these quantities and the equation of state for water are compared with pressures obtained from the linearized equations-of-state. If these two pressures do not agree with a user specified tolerance, the process is repeated until convergence is achieved. This solution scheme is similar to that used in RELAP5,¹⁵ but RELAP5 does not converge nonlinear terms, or re-linearize the equation-of-state. The MELCOR approach should allow for large time-steps to be taken during natural convective flow problems. The CONTAIN code also uses a two-tier convergence scheme, but based on the Secant Method.¹⁶ The inner-iteration is a point iteration to converge control volume temperature. The outer-iteration is global iteration to converge control volume pressure and flows, given the resulting temperatures of the inner-iteration. The MELCOR solution scheme is more in line with state-of-the-art fluid dynamics codes.

The authors of the MELCOR and CONTAIN codes decided to neglect the momentum fluxing term (i.e. $v \partial v / \partial x$) of the momentum conservation equations. They argue that this term is either too difficult to formulate or is unimportant for the low velocity flow conditions that hypothetical accidents produce. However, both CONTAIN and MELCOR check for sonic conditions along a given flow path, which seems like a contradiction. CONTAIN uses an ideal compressible gas formulation to check for sonic (choked) flow conditions. MELCOR uses the same relationship for the vapor phase, and the Henry-Fauske model for subcooled water, and the Moody model for saturated two-phase water as developed for the RETRAN code.¹⁷ Both codes allow frictional or form momentum loss terms for flow paths. MELCOR allows the user to specify dimensions along a flow given path, allowing a more accurate treatment of changing flow path geometry.

Both MELCOR and CONTAIN allow the user to specify any number of heat structures within a given control volume. These heat structures allow for user specified internal heating and material properties. Boundary conditions at the surfaces of these heat structures are either user specified, or calculated from heat transfer packages of these codes. The MELCOR code treats the following heat transfer modes between these structures and control volume atmospheres: single-phase convection (forced or natural, internal or external flow), pool boiling, thermal radiation, and condensation. The CONTAIN code treats: single-phase vapor

natural convection (external flow), pool boiling, thermal radiation, and condensation. To obtain two-phase pool boiling in CONTAIN, the lower cell control volume model must be invoked. The CONTAIN lower cell model only allows one heat structure to communicate thermally with the pool. MELCOR uses the Rohsenow correlation for pool boiling, the Zuber correlation for critical heat flux, and the Bromely correlation for film boiling.¹⁸ CONTAIN uses the boiling correlations from the CORCON-MOD2 code,¹⁹ which relies on the Zuber-Rohsenow correlation for critical heat flux, and scales on the basis of wall super-heat to obtain nucleate through film boiling heat transfer rates. It is unclear from CONTAIN literature if thermal radiation between the heat structures of the upper cell (i.e. walls) and the pool of the lower cell model is considered. The CONTAIN code does model radiative heat transfer between heat structures within a given control volume. This option is not yet available in MELCOR. MELCOR and CONTAIN use similar correlations for condensation heat transfer.

Both MELCOR and CONTAIN address a number of engineering features, and engineering safety features (ESF) that affect fluid flow in confinement volumes. These include: pressure suppression/scrubbing pools, ice condensers, containment sprays, fan coolers, heat exchangers, valves, and pumps. MELCOR and CONTAIN use the SPARC²⁰ model for aerosol scrubbing from atmospheres bubbling through water. The CONTAIN code containment spray model is very elaborate, while that of MELCOR is much more simplistic. CONTAIN has detailed mechanistic models for addressing the fluid flow/heat transfer affects of ice condensers, suppression pools, fan coolers, and heat exchangers. It is not clear from CONTAIN literature that these models have been validated, and are therefore more accurate than the approach allowed by MELCOR. In MELCOR, the standard fluid flow, heat transfer, and heat conduction models of MELCOR allow the user to model these safety features directly. Both codes treat valves and pumps in a similar fashion: very simplistically.

The fluids that have been proposed as coolants for ITER include: water, cryogenics (liquid helium and nitrogen), and liquid lithium. Both MELCOR and CONTAIN have thermodynamic properties for water. Neither of the versions of these codes available in the US have thermodynamic properties for cryogenics or liquid lithium. According to H. Loeffler^c a version of CONTAIN exists at GRS^f that can model liquid nitrogen. However, neither the results from this version of CONTAIN, or the code itself have been made available to the ITER community. There is a liquid sodium version of CONTAIN²¹ available in the US that could be modified to include the chemistry of liquid lithium. Both MELCOR and CONTAIN model non-condensable gases, but MELCOR has thermophysical properties for a larger number of gases. Although in the ITER environment, where structures temperatures can be as low as 4 K, it is hard to imagine these gases remaining non-condensable. Neither code treats the freezing of water, either in the atmosphere or on super-cooled structures.

MELCOR and CONTAIN have models that calculate the rate at which hydrogen and carbon monoxide gases are produced by water oxidation of metals. In particular, MELCOR treats zircaloy, steel, and B₄C oxidation by using standard Arrhenius rate relationships. This

^cITER JCT Second Technical Meeting on Safety, Environment, and Licensing, San Diego, CA., November 3-12, 1993.

^fGesellschaft fuer Reaktorsicherheit, Koeln, Germany.

oxidation occurs only within what MELCOR calls "core" control volumes. The authors of CONTAIN state that their code calculates hydrogen generation from metal oxidation, but they do not elaborate on how their code addresses this issue. Neither code treats the oxidation of beryllium or carbon, or allows oxidation of heat structure surfaces within a control volume. Both codes use the same model for hydrogen and carbon monoxide combustion, that of the HECTR code.²² This model, which should be adequate for ITER applications, predicts ignition conditions and burn rates of hydrogen-carbon monoxide-steam-air-mixtures.

4.2 Merits of CONTAIN & MELCOR Thermal Hydraulic Models

Table 4 compares the capabilities of the CONTAIN & MELCOR codes in terms of the modeling requirements called out in Table 2. Based on this evaluation, we have drawn the conclusions that: (a) the MELCOR code is the more sophisticated of the two codes both in terms of thermal hydraulics and numerics, (b) the MELCOR code offers more modeling flexibility, and (c) the MELCOR code should be the preferred code for ITER hypothetical accident thermal hydraulic analyses. MELCOR allows for multiple flow paths between control volumes, two-phase flow modeling, and thermodynamic non-equilibrium calculations, while CONTAIN does not. Some of MELCOR's ESF models are less sophisticated than those of the CONTAIN code, for example the containment spray, ice condenser, and fan cooler models. However, aside from perhaps the CONTAIN ice condenser model, these ESF will either not be part of ITER, or will not be directly applicable to ITER because of differences between fission and fusion aerosol behavior. One specific deficiency of the MELCOR code is that it does not calculate radiative heat transfer between structures. The MELCOR authors claim that work is in progress to add this feature to their code.

Both MELCOR and CONTAIN have hydrogen combustion models that should be applicable to ITER conditions, but neither code allows oxidation of heat structures, or considers beryllium or carbon oxidation. Neither MELCOR or CONTAIN have versions that address all of the coolants being proposed for ITER, which are: water, cryogens, and liquid lithium. Neither MELCOR or CONTAIN addresses freezing of water, or condensing of gases that these codes presently consider to be non-condensibles.

Given the limited safety resources of ITER and time available for producing the ITER ESECS and PHAR documents, we propose that the ITER JCT use a modified version of MELCOR. MELCOR is best suited to model water spills and air ingress accidents. Models for cryogen spills, liquid lithium spills from test modules, radiative heat transfer between structures, beryllium and carbon oxidation, water freezing, and air condensation and freezing will have to be added to the MELCOR code.

Table 4. Thermal hydraulic comparison of the CONTAIN and MELCOR hypothetical accidents codes.

Phenomena	MELCOR	CONTAIN	Comment
Number of Conservation Equations solved for coolant (H ₂ O)	Six	Three	MELCOR solves conservation equations for both the vapor and liquid phases. This allows MELCOR the option of treating the vapor and liquid phases in a non-equilibrium fashion. CONTAIN assumes that these phases are always in equilibrium.
Liquid phase treatment			
Pool level tracking	Yes	No	
Pool heat transfer	Yes	Yes	CONTAIN only treats heat transfer between the pool (liquid phase) and one structure, and only if the lower cell model is invoked.
Number of enclosures	not limited	limited	Convergence speed of CONTAIN solution procedure limits the number of allowed enclosures through computer time constraints
Number of flow paths between enclosures	not limited	one	Only the vapor phase is allowed to flow in a CONTAIN flow path (no liquid transport between enclosures), both phases are allowed in MELCOR (interphase drag calculated)
Choking	Yes	Yes	CONTAIN-Ideal compressible gas formula MELCOR -Ideal compressible gas formula Henry-Fauske subcooled liquid Moody saturated liquid
Number of heat structures per enclosure	not limited	not limited	
Oxidation	Yes	Yes	In fission core models only, no Be oxidation
H ₂ /CO combustion	Yes	Yes	Same model
Interphase mass transfer	Non-equ.	Equilibrium	MELCOR considers heat transfer to pool surface for evaporation, equilibrium vapor formation within the pool, vapor escapes by virtue of a bubble rise model
Structure heat transfer			
Vapor phase			
Natural convection			
External	Yes	Yes	
Internal	Yes	No	
Forced convection			
External	Yes	Yes	
Internal	Yes	No	
Condensation	Yes	Yes	

Table 4. Thermal hydraulic comparison of the CONTAIN and MELCOR hypothetical accidents codes (cont.)

**Structure heat transfer
(cont.)**

Liquid phase			
Natural convection			
External	Yes	Yes	
Internal	Yes	No	
Forced convection			
External	Yes	No	
Internal	Yes	No	
Boiling			
Pool	Yes	Yes	CONTAIN only treats heat transfer from pool to one heat structure, and only in lower cell model
Film	Yes	Yes	
Radiation			
Atmosphere	Yes	Yes	
Pool	Yes	No	
Adjacent structures	No	Yes	CONTAIN has two radiation models, MELCOR development ongoing
Aerosol	No	No	
Inter-phase heat transfer	Yes	No	
Non-condensible transport	Yes	Yes	
Air condensation	No	No	
Pool scrubbing	Yes	Yes	
Suppression pool	Yes	Yes	MELCOR does not have a specific suppression pool model
Containment ESF's spray, filters, etc	Yes	Yes	
Ice condenser	Yes	Yes	CONTAIN model is more mechanistic

5. ITER LOCA TEST CASE FOR CONTAIN & MELCOR

As part of our assessment of the CONTAIN and MELCOR hypothetical accident analysis codes, we have developed an ITER relevant test problem to test these codes. The objective of this test problem is to: 1) compare predicted radioactive material confinement fractions of these two codes, 2) determine the anticipated confinement structure pressures for this type of accident, 3) assess the ease to which these codes can execute this type problem, and 4) identify modeling deficiencies of these codes. This section describes the model developed for and results of this test problem.

5.1 Input Model Description

Based on communications with safety personnel of the ITER Joint Central Team (JCT), we have adopted the following test problem: A break in the blanket that releases coolant into the vacuum chamber, pressurizes the vacuum vessel and vacuum pumping ducts, causes the vacuum pumping ducts to fail, allowing coolant into the cryostat. Figure 2 contains a schematic of how we believe this accident will occur.

There are a variety of modeling parameters that were required for this study. These included: quantity of dust to be suspended by the coolant, quantity of radioactive material to be mobilized by oxidation of the first wall, accident duration, temperature and volume of the blanket coolant, free-volumes of the vacuum vessel and cryostat, and failure pressure and cross-sectional area of the break in vacuum pumping ducts. Table 5 contains some of these parameters as given by the ITER JCT for this study.^{a,b,i}

Figure 3 contains a schematic diagram of the model we have developed for this test problem. This model has seven control volumes, seven heat structures, and eight flow paths. Two control volumes were used to model the blanket cooling system. This division reflects the fact that half of the coolant inventory will be at an elevated temperature (200 °C), having passed through the blanket, and half will be at a lower temperature (150 °C), having passed through the blanket cooling system heat exchangers. The flow paths that connect this cooling system to the blanket components inside the vacuum vessel are 70 m long, 0.63 m. diameter pipes. Form losses were added to these flow paths that resulted in a total loop pressure drop of 4×10^5 Pa. This pressure drop was based on friction losses in these pipes (fluid velocity 10 m/s) and within the proposed heat exchanger design (fluid velocity 8.6 m/s, pipe length 9.3 m, pipe

^aThese parameters are intended only for this illustrative comparison calculation, and should not be taken as, nor are they intended to be, results of a "design basis", or worst-case "design basis" sequence.

^bHans-Werner Bartels, Approximate Weights Table, ITER JCT Electronic FAX, April 14, 1994.

ⁱPrivate communication with S. J. Piet of ITER JCT, April 13, 1994.

diameter 0.15 m).^j Both flow paths connect to the top of the blanket components, as is the present ITER design. A simple pump model was added to the inlet flow path. This pump was tripped at the beginning of the accident, and had an assumed exponential e-folding decay constant of 10 s for the pump head. The initial pressure of the blanket cooling system was set at 2.2 MPa.

There is a single control volume modeling the water volume of the blanket components within the vacuum vessel. Its volume is 125 m³. A flow path, representing the blanket break, was placed between the bottom of this control volume and the control volume that depicts the plasma chamber. Within the plasma chamber are three heat structures, representing the inboard blanket, outboard blanket, and divertor components. Decay heat predicted by the REAC3 code was added to these blanket heat structures.^k

A flow path was added to model flow between the bottom of the plasma chamber and the region between the back of the blanket and the vacuum vessel, called out as the "inner zone" in Figure 3. The back surfaces of the blanket and divertor heat structures are attached to this inner zone control volume, along with two additional heat structures that represent the inboard and outboard surfaces of the vacuum vessel. These two additional heat structures were taken to be heat sinks at a constant temperature of 100 °C.

A flow path between the "inner zone" control volume and the vacuum duct control volume was added to reflect the flow path of the vacuum ducts themselves. The two remaining flow paths connect the vacuum ducts to the free-volume within the cryostat. These flow paths contain valves that open, and remain open, once the pressure within the vacuum duct control volume exceeds 2×10^5 Pa, simulating the rupture of bellows that connect the vacuum duct to the cryostat at the location of the divertor maintenance access ports. The lower flow path was included to allow for the possibility of liquid drainage.

The remaining two heat structures are located in the cryostat control volume. These heat structures model the thermal response of the magnets (toroidal field coils, central solenoid, and poloidal field coils), and magnet support structures. The surface area of these heat structures is approximated to be that of a right circular cylinder that is 14.5 m in diameter and 20 m high. One heat structure represents a pseudo surface for the magnets, and was made 0.01 m thick. The back surface of this heat structure was maintained at the maximum of the time-dependent surface temperature of the second magnet heat structure or 0 °C, while heat transfer to the front surface was determined by the standard heat transfer package of the CONTAIN or MELCOR code. The second heat structure is of the required thickness so as to account for the entire magnet and magnet structure masses.^l The back surface of this heat structure was assumed adiabatic, while the front surface had the time-dependent heat flux experienced by the pseudo magnet surface applied to it. This rather awkward modeling approach was taken to

^jH. Yoshida, Current Reference HX Design, JCT Electronic FAX, April 14, 1994.

^kGenn Saji, Ed Cheng, Initial Power Distribution and Decay Heat Data for Safety Design and Analysis (Rev.1), JCT Electronic FAX, April 16, 1994.

^lPrivate communication with D. F. Holland, April 25 1994.

Figure 2. Schematic of severe accident test problem for CONTAIN and MELCOR application

Figure 3. Schematic of model developed for CONTAIN and MELCOR severe accident test problem

Table 5. Modeling Parameters for CONTAIN and MELCOR Test Case.

Duration of accident	1 day
Blanket coolant	
Volume - Temperature	350 m ³ - 200 C 350 m ³ - 150 C
Mass of tokamak dust	~10 kg
Mass of oxide mobilized from first wall (in 1 hr)	~3 kg
Vacuum chamber free volume	3,650 m ³
Divertor	
Mass	7.8x10 ⁵ kg
Surface Area (~ value for one side only)	265 m ²
Cryostat	
Free volume	20,300 m ³
Surface area	1980 m ²
Blanket/first wall	
Surface area	
Plasma side (inboard - 400, outboard - 800)	1200 m ²
VV side	1200 m ²
Break area	.02 m ²
Vacuum ducts	
Free-volume	750 m ³
Cross sectional area	300 m ²
Pressure at which vacuum duct fails	0.2 MPa
Break area	.02 m ²
Magnet/support structure	
Surface area	6040 m ²
Surface temperature	0 C
Mass	2.34x10 ⁷ kg
Vacuum Vessel	
Surface area	1800 m ²
Temperature	100 C

allow the standard heat transfer packages of these codes to predict condensation of the steam that enters cryostat during this test problem, since these heat transfer packages will not allow temperatures that are below the freezing point of water.

All material properties for this calculation were taken to be those of stainless steel, with a surface emissivity of 0.3. All control volume elevations were determined from information in Reference 23.

The 10 kg of tokamak dust listed in Table 5 were input to the problem as monodisperse 3.25 μm diameter particles (section 8 of 10 sections^m of increasing particle diameters) and assumed to be present in the plasma chamber (control volume 4) at the start of the problem. Since only one aerosol particle density is allowed and the particles were expected to be mostly condensed water in this problem, a density of 1000 kg/m^3 was input for the particles in spite of the selection of concrete (class 15) as the most representative aerosol particle material and the fact that the dust would actually be denser. The suspended dust corresponds to an initial particle number density of approximately 1.5×10^{11} particles/ m^3 .

The 3 kg of volatilized oxide mobilized from the first wall in one hour shown in Table 5 was represented by a 8.33×10^{-4} kg/s source of 0.13 μm diameter particles (section 1) in the plasma chamber. The small size is typical of primary particles nucleated from vapor. After one hour, when a total of 3 kg of small particles had been added to the plasma chamber, the source rate was set to zero. The total particle number density added to the plasma chamber by this source was 9×10^{13} particles/ m^3 , a number density that would not be achieved because of rapid coagulation (At this concentration, the particle number density would typically be reduced by a factor of two in twenty seconds.²⁴ page 239)

5.2 Results from ITER Test Case

We have divided this section into four sub-sections. The first sub-section presents the thermal hydraulic results from the MELCOR code for this test case. The second sub-section describes the thermal hydraulic results obtained from the CONTAIN code. In the third sub-section, we present the aerosol transport results as predicted by the MELCOR code. And finally, the last sub-section compares the results of MELCOR and CONTAIN, and discuss the performance of these codes.

5.2.1 MELCOR thermal hydraulic results

Figure 4 contains MELCOR predicted blanket cooling system pressures for the first two hours of this test case. Three control volume pressures have been plotted, that of: 1) the blanket components inside of the vacuum vessel (bktcool), 2) the cold leg of the blanket cooling system (coolsy1), and 3) the hot leg of the blanket cooling system (coolsy2). Following the break in the blanket components, the pressure rapidly drops to 1.0 MPa, which is the saturation pressure at the mean blanket cooling system temperature. A slower pressure drop follows as the blanket coolant is expelled into the plasma chamber. After about 1000 s, the liquid inventory in the blanket volume dries up, resulting in only vapor being expelled from the blanket break. From this point on, the pressure in the cooling system decays exponentially in time. Figure 5, which contains the liquid mass in the blanket cooling system, confirms these conclusions.

^m The word "section" is used here to describe a range of particle sizes treated as one representative size, as it is in MELCOR documents. Other codes use the term "bin" to describe the same concept.

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Figure 4. MELCOR pressures for first two hours of ITER test case.

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Figure 5. MELCOR mass inventories during first two hours of ITER test case.

At 1000 s the liquid mass within the blanket reaches zero. By this time the hot leg of the blanket cooling system has lost nearly 80% of its coolant inventory, while the cold leg has lost only 27% of its coolant inventory. The average mass flow rate out of the break during this period of time was about 360 kg/s.

Figure 6 contains predicted pressures for the plasma chamber (plaschr), the region between the back of the blanket and vacuum vessel (the "inner" zone - inrzone), the vacuum ducts (vacduct), and the cryostat (cryosta). The pressure within the plasma chamber reaches 3×10^5 Pa. This pressure is primarily sustained by water vaporization produced from quenching the divertor component. This pressure occurs even though the vacuum ducts were assumed to fail once the pressure exceeds 2×10^5 Pa. The cryostat pressure for this test case did not exceed 2×10^4 Pa. Figure 7 presents the liquid mass within these same components. By 1100 s, the liquid mass within the plasma chamber has completely vaporized, and by 2000 s this liquid has either drained or vaporized from the vacuum ducts. The vapor masses within these components are presented in Figure 8. Comparing this figure with the results of Figure 7, it can be concluded that most of the liquid expelled from the blanket drains through to the cryostat, because in this test case there are no condensing surfaces within the vacuum ducts and the liquid mass greatly exceeds the water vapor mass in this volume. Figure 8 also shows how the magnets pump down the plasma chamber as the water vapor condenses within the cryostat.

ITER Test - blanket blowdown

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MELCOR IBM-RISC

Figure 6. MELCOR pressures for the first two hours of the ITER test case.

Figure 7. MELCOR liquid mass inventories during first two hours of ITER test case.

Figure 8. MELCOR vapor mass inventories during first two hours of ITER test case.

Four hours into this test case the pressures become very sub-atmospheric, and MELCOR starts to have problems with timestep size selection (i.e, less than 1.0×10^{-3} s). This trouble is the result of pressure oscillations in the solution that are not felt to be realistic, but rather an artifact of the explicit heat transfer treatment of the MELCOR code. Figure 9, shows these pressure oscillations. As can be seen, intermittent pressure spikes occur in the plasma chamber, inner zone, and vacuum duct pressures. These pressures have decreased to 8 kPa in magnitude by 7 hours, and continue to drop to nearly 2.5 kPa by 19 hours. Since pressure change per timestep is a MELCOR timestep size control criterion, these pressure spikes cause MELCOR to take small timesteps. The cryostat pressure held relatively steady over this time period, at about 0.7 kPa.

At 21 hours, MELCOR terminates the calculation with an error message that states the water vapor temperature inside the cryostat had dropped below the freezing temperature. This marked the end of a steady decline in water vapor temperature over this period of time, which started at about 100 s with a maximum of 325 K ($\sim 50^\circ\text{C}$). This maximum temperature was sustained for the first 2000 s of the transient. The liquid temperature in the cryostat followed this same trend. Long-term water vapor temperatures in the plasma chamber followed those of the blanket components which experienced a gradual rise in temperature to about 575 K ($\sim 300^\circ\text{C}$). The magnet temperature had only reached 19 K by 21 hours.

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Figure 9. MELCOR long-term pressures for ITER test case.

5.2.2 CONTAIN thermal hydraulic results

Based on our experience with applying the MELCOR code to the test case, we developed a more simplified model for our CONTAIN thermal hydraulic assessment. This model consists of all volumes and flow paths used by the MELCOR assessment, but had only one heat structure, that representing the magnet surface held at 1 °C. This simplification could be made because only water vapor is allowed to flow in CONTAIN flow paths, eliminating the need for flashing calculations to be made as water impacts the divertor/first wall components,^a and because MELCOR results demonstrated that the long-term flow pattern is driven by evaporation of the blanket coolant and condensation (water vapor pumping) in the cryostat. In addition, no time dependent flow paths were used in the CONTAIN model (i.e., the break in the vacuum duct to cryostat flow path is assumed to happen at time zero) because this happens rather early in the transient.

Figure 10 shows the pressures for each of the seven control volumes. From the inset graph, one can see that all the blanket volumes reach about the same pressure shortly after the transient begins. These volumes maintain approximately the same pressure until the end of the

Figure 10. CONTAIN pressures for ITER test case.

^aThis calculation could be accomplished by the CONTAIN code lower cell model if water were to somehow be transferred from the blanket cooling system into the plasma chamber.

one day transient. Likewise, the plasma chamber volume, the blanket/vacuum vessel volume and vacuum ducts follow very similar transient pressure curves. With the near freezing heat structure in the cryostat volume, this volume's pressure does not rise much above 40 kPa and reaches a quasi-steady pressure of about 12 kPa along with the rest of the non-blanket volumes at the end of the transient. The blanket volumes are at about 25 kPa at one day and are still decreasing.

Figure 11 shows the cell temperatures for this test case. The temperature curve for the cryostat looks very similar to the pressure curve. After some initial temperature spikes, which are thought to be due p-v work, the temperature drops to 325 K and slowly decreases approaching the magnet heat structure of 274 K (1°C) at the end of the transient. The blanket volume temperatures remain the highest after the initial blowdown of water vapor, dropping to about 335 K at the end of the one day transient. As with pressure, the rest of the non-blanket volumes follow each other in temperature, rapidly dropping to just under 400 K after the initial spike and slowly decreasing but remaining above the cryostat temperature.

The final figure, Figure 12, displays the predicted liquid inventories for this test case. The plasma chamber volume, inner zone volume (e.g. blanket/vacuum vessel gap volume) and vacuum duct volumes acquire only small amounts of liquid due mainly to expansion cooling of the water vapor. As expected, the liquid inventories of the blanket volumes decrease by evaporation while the cold cryostat volume collects liquid by condensation. However, even after one day, the liquid inventory in the cryostat is only about 125 Mg with about 575 Mg (about

Figure 11. CONTAIN temperatures for ITER test case.

Figure 12. CONTAIN liquid inventories for ITER test case.

80%) of the original blanket cooling system liquid inventory still remaining in the blanket system volumes.

5.2.3 MELCOR/CONTAIN thermal hydraulic performance comparison

The most dramatic difference between the predictions of these two codes has been the treatment of the liquid phase of the coolant. By 1000 s, MELCOR predicts that nearly 60% of the blanket coolant inventory has left the blanket cooling system, and by 5 hrs (after the hot leg becomes voided) nearly 70% of the coolant inventory has left the cooling system. In contrast, CONTAIN predicts that by the end of one day almost 80% of the coolant inventory still remains inside the blanket cooling system. This would have a significant impact on the predicted coolant corrosion product and tokamak dust transport, because the coolant corrosion product mobilization is proportional to the water inventory release, and because the tokamak dust would be swept away with the water as it drains into the cryostat. Since the break was assumed to occur at the bottom of the blanket for this comparison calculation, and since the bottom of the blanket represents a low point in the blanket cooling system, the MELCOR prediction is the more correct of these two results.

From this test case it appears that CONTAIN executes more stably during sub-atmospheric conditions. However, CONTAIN did not predict pressures as low as those

predicted by MELCOR. For instance, MELCOR predicted that the plasma chamber pressure would become 8 kPa by 7 hrs, whereas CONTAIN never predicts the cryostat pressure to drop below 12 kPa (MELCOR predicts the cryostat pressure to be as low as 0.7 kPa). MELCOR did not start to have timestep problems until pressures fell below 12 kPa. We expect that the primary reason MELCOR predicts lower pressures is due to the increased condensation surface area provided by the liquid pool at the bottom of the cryostat. Nonetheless, a major reason for examining this test case was to determine how well these codes would perform in a low temperature, evacuated fusion environment such as the cryostat. Based on these results, modifications will have to be made to the MELCOR code to allow more stable execution during sub-atmospheric conditions, and to correct the code crash that occurs when water freezes.

5.2.4 MELCOR aerosol transport results

Figure 13 shows the total aerosol mass in the gas phases of the plasma chamber (plaschr), the vacuum ducts (vacduct) and the cryostat (cryosta) for the first two hours of the test case. The non-volatile component^o of the aerosol particles mass in the gas phases is shown in Figure 14. After the first several minutes (180 s), the non-volatile component becomes the dominant part of the aerosol particle mass in the plasma chamber, vacuum ducts, and cryostat

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Figure 13. Total aerosol mass in the vapor phases calculated by MELCOR for ITER test case.

^o This component is the dust and oxide that was volatilized at the hot wall surface. In the cooler gas phase, the vapor pressure of these species is negligible.

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Figure 14. Nonvolatile component of aerosol mass in the vapor phases calculated by MELCOR for ITER test case.

because the lines in the two figures are indistinguishable.

Figure 15, which shows the radionuclide mass of water and non-volatile material present as particles in the gas phases and as part of the liquid phases (summed over all volumes), illustrates the rapid condensation of water vapor. One second after the start of the problem, 1.658 kg of the aerosol particles mass in the gas phase is water and 10 kg of the aerosol particles mass in the gas phase is non-volatile material. At 30 s, the water and non-volatile masses in the gas phase are 25.27 and 9.923 kg, respectively. By 500 s, 4.5 and 1.26 kg of water and non-volatile material remain in the gas phase particles while 9,715 and 8.999 kg of water and non-volatile material are in the liquid phase.

The release fractions of non-volatile material implied by Figures 13, 14, and 15 are very small. Table 6 shows the ratio of non-volatile material present as particles to the total non-volatile mass mobilized as a function of time. Even if all of the non-volatile material present as particles were to be released from the confinement, the potential release fraction decreases to 0.00000021 by 2 hours.

Table 6. Ratio of non-volatile material present as particles to total mobilized.

Time (s)	Particle Mass / Mobilized Mass
1.0	1.000
1.5	1.000
30	0.989
500	0.1208
1003	0.0339
1503	0.0314
2003	0.0336
2503	0.0313
3003	0.0291
3503	0.0301
3603	0.0299
4605	0.0015
5608	0.000052
6608	0.0000017
7207	0.00000021
9676	0.000000000033

Figures 16 and 17 show the calculated total and non-volatile mass of "aerosol" (really former aerosol) particles in the liquid phases of four control volumes as a function of time. The non-volatile mass and condensed water move with the liquid phase from the plasma chamber to the cryostat.

Figure 15. Radionuclide mass of water and nonvolatile material summed over all volumes.

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Figure 16. Total aerosol mass in the liquid phases calculated by MELCOR for ITER test case.

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Figure 17. Nonvolatile component of aerosol mass in the liquid phases calculated by MELCOR for ITER test case.

The mass median diameter^p and geometric standard deviation^q of the aerosol particles in four control volumes are shown in Figures 18 and 19. The larger particles present during the initial 1000 s of the problem settle into the liquid phase and/or leave with the convecting gas phase, leaving only very small particles after 1000 s.

The slope of the curves after 3600 s in Figures 13 and 14 shows that gravitational deposition is not the dominant mechanism removing the very small particles that remain after the first hour. If gravitational settling were the dominant mechanism controlling the removal of aerosol particle mass from the atmosphere, the mass of the airborne particles in a monodisperse aerosol would be given by the expression^{24 page 58}

$$m(t) = m(0) \exp\left(-\frac{V_{TS}t}{H}\right) \quad (1)$$

where

m	=	mass of particles in atmosphere (kg)
t	=	time (s)
V _{TS}	=	terminal settling speed (m/s)
H	=	height of the atmosphere (m).

Using 4×10^{-3} kg at 4000 s and 2×10^{-4} kg at 5000 s as representative points to determine the slope of the plots of the aerosol mass in the atmosphere yields a ratio of H over V_{TS} equal to approximately 333 s, resulting in a settling speed of approximately 5×10^{-2} m/s for a height of 17 m. This settling speed corresponds to particles on the order of 40 μ m diameter^{24 page 407}, not to the 0.2 μ m mass median diameter of Figure 18.

The 333 s time constant probably represents the rate at which particles left in the plasma chamber are diluted by the removal of part of the gas phase from the plasma chamber through

^p The mass median diameter is the mass weighted average diameter,

$$d_{\text{mass median}} = \frac{\sum_i m_i d_i}{M}$$

where m_i is the mass of the i th particle and d_i is the diameter of the i th particle.

^q The geometric standard deviation of the particle diameter is the exponent of the standard deviation of the log of the aerosol particle diameters with respect to the log of the geometric mean particle diameter, d_g ,

$$\ln(\sigma_g) = \left\{ \frac{\sum_i [\ln(d_i) - \ln(d_g)]^2}{N - 1} \right\}^{\frac{1}{2}}$$

Normally this geometric standard deviation is used with the geometric mean particle diameter. We do not understand why the MELCOR plot package offers only the mass mean particle diameter and the geometric standard deviation of the diameter.

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Figure 18. Mass median diameter of aerosol particles calculated by MELCOR for ITER test case.

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Figure 19. Geometric standard deviation of aerosol particles calculated by MELCOR for ITER test case.

the other volumes to the cryostat. For short residence times in the volumes downstream from the plasma chamber, a constant aerosol particle mass density would be expected in all volumes and the total aerosol mass present in each volume would be proportional to the volume of each control volume as is the case in Figures 13 and 14 after 3600 s. The information provided by the MELCOR output for the test problem is not sufficient to determine why the gas phase (vapor and aerosol particles) residence time in the cryostat is short, but steam condensation with particle deposition by diffusiophoresis is a reasonable guess.

Careful inspection of Figures 13 and 14 shows that condensation of water vapor onto aerosol particles is not a major contributor to particle deposition in this test problem. The volatile aerosol mass in the vapor phase implied by the difference in the total and non-volatile aerosol masses in the first few hundred seconds is in the cryostat where a water fog forms. The vapor in the plasma chamber is apparently too hot to allow significant condensation on the large particles initially present. Based on Figure 16 which shows aerosol mass in the liquid phase of the cryostat only from 300 to about 1299 s, we believe that 10 kg of relatively large particles present in the plasma chamber at the start of the problem settles into the liquid phase concurrently with being carried toward the cryostat by convection.

From 500 to 3600 s, the aerosol mass in the gas phases (Figures 13 and 14) approaches steady-state values defined by the oxide source rate and the inter-volume gas flow to and from each control volume. After 3600 s when the oxide aerosol source stops, the aerosol mass decreases exponentially (straight lines in the semi-log graphs of Figures 13 and 14) as would be expected for approximately constant fractional loss rates due to particle deposition and gas flow. The rapid change to straight lines at 3600 s shows the gas residence time in volumes between the plasma chamber and the cryostat is too short to allow transient storage of aerosol particles in these volumes.

In summary, the general features of the MELCOR aerosol particle transport calculation results in the test problem appear reasonable. Experience with the test problem also suggests that optional printing of information about the relative contribution of the various deposition mechanisms (time constants for each mechanism in each volume) would facilitate interpretation of the calculations.

We have not done CONTAIN aerosol calculations because CONTAIN and MELCOR have basically the same aerosol models but significantly different thermal hydraulics. Since the aerosol behavior analysis is complex and MELCOR has the more sophisticated and accurate thermal hydraulics (Section 4.2, page 21.), we chose to examine the aerosol models with MELCOR in greater detail than we could by spending our resources on analyses with both codes.

6. CONCLUSIONS AND RECOMMENDATIONS: PRIORITIES

Based on our observations given in the preceding sections and in Appendix B, we would conclude that several modifications would have to be made to CONTAIN and/or MELCOR to make these codes applicable for LOVA and LOCA analysis in ITER. This is especially true with respect to specialized approximations to support the aerosol transport model numerical solution method, materials properties of the gas phase that assume fission reactor containment gas properties, fission product decay heats, and electromagnetic effects on aerosol behavior. These rather extensive needs are balanced by a number of advantages of the CONTAIN and MELCOR codes; recognition in the fission community, coupled thermal-hydraulic and aerosol behavior models, and integration schemes that are efficient, at least under hypothetical accident conditions for fission power plants.

Based on our thermal hydraulic assessment of the CONTAIN and MELCOR codes, we have concluded that the MELCOR code is the more thermal hydraulic and numerically sophisticated of the two codes, that the MELCOR code offers more modeling flexibility, and that the MELCOR code should be the preferred code for ITER hypothetical accident thermal hydraulic analyses. Given the limited safety resources of ITER and time available for producing the ITER ESECS and PHAR documents, we propose that the ITER JCT use a modified version of MELCOR. MELCOR is best suited to model water spills and air ingress accidents. Models for cryogen spills, liquid lithium spills from test modules, radiative heat transfer between structures, beryllium and carbon oxidation, water freezing, and air condensation and freezing will have to be added to the MELCOR code.

Table 7 is a summary of the changes that we recommend after considering fusion modeling requirements (Section 2) and current capabilities (Sections 3, 4, and 5). In general, we recommend that the addition of fusion-relevant models to CONTAIN/MELCOR be preceded by simplifications intended make the code more characteristic of the state-of-the-art of fusion reactor analysis. Recommendations of "remove or inert" are associated with models for mechanisms not present in fusion confinements. The Priority column contains an estimate of the priority (H = high, M = medium, L = low) of the need for the model.

It should be noted that these priorities are only the current priorities for development of a confinement analysis tool. A number of experiment requirements have been identified²⁵ to clarify the relative importance of aerosol mobilization and transport mechanisms and to assess the completeness of the mechanisms we have identified. Resolution of the questions addressed by experiments are likely to alter the priorities in Table 7. These unresolved questions to be determined by experiments are:

1. What are the values of the important mobilization parameters? These parameters are the chemical species of the mobilized material (both activated isotopes and any structural material that becomes mobile in quantities on the order of kilograms of mass or more) and the mass rate of release versus time of each species. An estimate of the initial particle size formed during mobilization is needed but the details of the initial particle size distribution are less important than the species identification and mass release rate information.

2. What evidence can be presented to show that existing fission product transport data and mechanisms are applicable to fusion confinements?
3. Are there unique, fusion-specific effects (e.g. mobilization from large and distributed surface areas instead of hot volumes, mobilization into a vacuum for some paths, geometry, the possible presence of cryogenics, relatively long accident times, thermo hydraulic effects, or unique materials properties) that require experiment verification?

Based on experience with the implementation of mass transport modules in fission product behavior codes, it is also recommended that all but the most minor (e.g. constant changes) modifications to extend CONTAIN and/or MELCOR for analysis of fusion machine confinements be tested in a stand-alone driver module before they are implemented in CONTAIN or MELCOR. The stand-alone module (e.g. the PULSE analysis tool²⁶) would run on a personal computer and accept input tables of approximate thermal-hydraulic conditions. It would be used to assess (1) the impact of proposed models on containment behavior, (2) the accuracy of the module results, (3) the resources necessary to run the module prior to implementing the proposed model in large codes like CONTAIN or MELCOR. The stand-alone tool would also be useful as a supplement to full-capability models in the development of experiment specifications.

The details of the additions and modifications listed in Table 7 have been discussed in preceding sections or the appendices and the third column provides brief comments where appropriate. Some additional discussion of the high priority modifications and the aerosol transport models follows.

The first three modifications are the removal of approximations that are not appropriate for fusion confinement analysis. The fourth is part of the task of addressing the fact that the materials, gas pressures, and temperatures in fusion reactors are not the same as those in fission reactors. In addition to changing the properties, it is simply good code structure practice to place the materials properties in an easily-accessed module so that they can be revised as better data for ITER-relevant materials become available.

Structure-to-structure radiant heat transfer is especially important when some structures are at cryogenic temperatures. We have also indicated the need for at least an approximate model to account for the effect of non-transparent aerosols on radiant heat transfer. While there is some treatment of the effect of aerosol and gas emissivity of radiant heat transfer in CONTAIN, revision of both CONTAIN and MELCOR will be required to include all of the effects of the gas and aerosol composition for the fusion environment.

It would be best if volatilization models are be part of CONTAIN/MELCOR so that the coupling between wall temperature, vapor flow, and mobilization can be addressed. During the initial stages of modifying the code it may be necessary to use input to specify mobilization.

The model for aerosol particle nucleation from the vapor is needed to replace the specialized water vapor/containment dust model in CONTAIN or the assumed-fog-generation model of MELCOR with a model appropriate for the fusion environment. This model is expected to allow consideration of the possibility of immediate condensation of plasma-vaporized material.

The model for resuspension of Tokamak dust and spalled oxide completes all of mobilization models except for the model for injection of spalled oxides. The spalled oxide injection model currently has lower priority because of the need for additional data from large-scale surfaces.

The complex nature of the transport of aerosol particles suggests that development of these models should start early. However, a high priority for these models is not appropriate at the present time for two reasons. First, general-purpose models for many of the mechanisms listed are already present in CONTAIN and MELCOR so it should be possible to invoke or modify those models in a relatively short time. Second, some parts of a large, all-inclusive effort to validate or add aerosol behavior models could be wasted for many aerosols. (e.g. If the particles are all large, only a deposition by gravity model is needed to show they deposit.) When relevant experiment data are available, it may turn out that many of the mechanisms considered in classic aerosol behavior models have such small effects in ITER that they are not worth the cost of installing, maintaining, and running them. If existing models do not impact code running times significantly, they can be left in place but the addition of complex models should be delayed until more complete experiment data make it clear that these models are needed. At the present time, the best models for the transport of less-volatile activated isotopes would be a few simple models describing those aspects of aerosol particle behavior that are expected to have major effects on the transport of aerosol particles. These are evaporation/condensation from/to particles, deposition due to gravity, deposition due to inertial effects, the effects of curved paths and/or electric/magnetic effects, and agglomeration.

Table 7. Summary of CONTAIN/MELCOR Modifications to Extend them for Fusion Confinement Analysis and Current Priorities.

Modification	Priority	Comment
Inert the model for automatic addition of aerosol seeds "as needed" (i.e. whenever critical saturation occurs?)	H	This model may not be appropriate for ITER because it is based on the assumption that the environment is typical air near one atmosphere and near 100% humidity
Remove the factor that artificially reduces water evaporation from aerosols close to dryout	H	This factor is only for hygroscopic seeds and water vapor
Remove, inert, or generalize the coding that limits condensed layers to 0.0005 m for all condensing materials	H	This feature is appropriate only if the condensate is liquid or two phase
Add materials properties needed to assess transport of non-volatile activated elements. Begin the process of separating all materials properties into an easily-accessed module	H	The transport of these elements needs to be assessed as part of the structural materials determination. Considerable development time may be required to prepare new models for mechanisms or regimes not present in fission containments.
Add structure-to-structure radiant heat transfer, including effects of possible obstruction of radiation by aerosol particles	H	Capability is required for long-term temperature trends to be correctly predicted. Radiant heat transfer is the predominant mode for transfer of decay heat to vacuum vessel cooling system.
Add beryllium and carbon oxidation models to heat structures	H	Predominant source of hydrogen generation. For beryllium, also an important heat source for first wall and divertor components.
Add oxide spalling model	H	The timing of oxide spalling may be important.
Add volatilization models	H	

Table 7. Summary of CONTAIN/MELCOR Modifications to Extend them for Fusion Confinement Analysis and Current Priorities (cont.).

Modification	Priority	Comment
Add model for aerosol particle nucleation from the vapor	H	Models implemented in the PULSE code ²⁶ do not cause numerical difficulties.
Improve MELCOR stability during sub-atmospheric conditions	H	Required for cryostat pressurization calculations.
Add model(s) for resuspension of Tokamak dust and spalled oxide	H	
Add air condensation models	M	Air condensing on cryostat walls or particles has the potential to affect particle transport.
Revise aerosol models for decay heating	M	Fission decay heating of aerosols needs to be changed to represent fusion
Extend condensation model to consider adsorption or absorption of hydrogen gas on or in aerosol particles	M	Adsorption and solution need to be assessed as part of the structural materials determination. The large surface area of aerosols make this a potentially significant transport phenomena that may depend on the particle species.
Add water vapor deposition/freezing model	M	Correct pressure predictions for water injected into cryogenic temperature confinement volumes will be required by these codes.
Revise model for evaporation from and condensation onto particles (both rate expressions and particle size models)	M	Large surface areas of aerosol particles make calculations sensitive to particle size distribution and concentration.
Revise model or user input values for decay heat to make energy deposition characteristic of ITER	M	Current models are either user input or default to typical LWR structure partitioning.
Add cryogenic helium properties	M	Helium pressurization is an important cryostat issue.
Replace diffusiophoresis model with a more general version	M	The current model may give incorrect answers.
Add model for injection of spalled oxides	L	

Table 7. Summary of CONTAIN/MELCOR Modifications to Extend them for Fusion Confinement Analysis and Current Priorities (cont.).

Modification	Priority	Comment
Add model for breakup of spalled oxide or Tokamak dust particles to sizes that are mobile	L	This model will be important only if significant spalled oxides are injected.
Extend condensation model to consider radiation heat transfer to cryogenic material condensates	L	This Modification is Important Only if the Potential for Condensation of Cryogenic matter is identified.
Add models for isotopic exchange between elemental gas and water vapor or condensed water	L	An out-of-code scoping analysis should be Water carried out to bound the order-of-magnitude of this effect before the model is added to the computer code.
Add models for centripetal inertial deposition and the contribution of different radial speeds on particle agglomeration	L	These models will supplement the deposition and agglomeration rates due to gravity. They will be significant only if larger particles are significant.
Generalize models for gravitational settling to include well mixed and non-Stokes settling	L	
Add Non-linear time step option	L	This change is justified only if the code runs too slow due to particle size change models.
Add models for the effects of charged particles or dipole moments fusion aerosols	L	This effect has not been shown to be important for fusion aerosols yet.
Add model for oxidation of a plasma-vaporized vapor (vapor phase chemical reactions	L	A general, mechanistic model is available from our fission modeling efforts but this model has not been tested.
Add models for biological conversion of hydrogen (tritium)	L	Models should wait for of Hydrogen (Tritium) development of a specific conversion.
Add liquid lithium models	L	Liquid lithium blanket option is not the primary ITER blanket option.

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Appendix A
CONTAIN and MELCOR Aerosol Models

APPENDIX A CONTENTS

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FIGURES

Figure A-1. A schematic diagram showing the use of twenty particle size classes and the mass per unit gas volume of each chemical species in each size class to represent the particle size and chemical species distribution. A-5

The CONTAIN and MELCOR aerosol behavior models have been critically reviewed for relevance to fusion reactor confinements. The CONTAIN review is based on a current CONTAIN 1.1 reference manual¹ and earlier or alternate descriptions of the models referenced in the current manual^{2,3}. The MELCOR review is based on a description of MELCOR 1.8.0.⁴ Since both CONTAIN and MELCOR aerosol dynamics models are based closely on the MAEROS models⁵, they differ only in some of the simplifications made to improve running time. Details of the review follow.

Transport of Steam/Water with Tritium

The discussion of the models for the transport of steam/water is divided into mechanisms that apply to the vapor phase and models of the evaporation and condensation of steam.

Thermodynamics and Inter-Cell Flow Features Relevant to Aerosol Behavior

CONTAIN and MELCOR have the ability to describe the flow and temperature of gas/liquid mixtures. They are basically control-volume/junction (Eulerian) codes that allow for an arbitrary arrangement of the volumes and flow path connections.^{1 p. 1-7} Both implicit and explicit (pressure versus time or initial pressure) flow solution options are available and either option can use inertial, quasi-steady, and/or critical flow models. When the inertial model is used, flow is modeled as turbulent.^{1 p. 3-7} When the quasi-steady flow model is selected, the inertia of the material in the flow path is neglected. An additional option that is available is the use of a user-specified mass or volumetric flow rate.

These fluid behavior models are adequate for aerosol behavior modeling, except for three features that should be added or revised:

1. The radius of curvature of the fluid flow path needs to be added to the information available to the aerosol models (for the particle centripetal inertial deposition model).
2. The gas phase composition is assumed to be constant.^{1 p. 4-6 and 4 p. 3-52} A few (four is typical) calculated values of the coefficients used for aerosol dynamics are determined in the constant-composition gas and interpolated as a function of the time-dependent temperature and pressures. In hypothetical ITER accidents, evaporation of material frozen on cold surfaces or reaction of water vapor with hot surfaces is likely to cause significant changes in gas properties such as viscosity and density that affect aerosol dynamics significantly.
3. The third feature that may have to be changed is the cell-to-cell transport of aerosol particles with a large velocity relative to the fluid speed. In the explicit flow option of CONTAIN, aerosol slip is not considered. With the implicit flow option,^{1 p. 3-38} "aerosols are considered to flow at the sum of the hydrodynamic gas convective velocity and the component of the aerosol settling velocity *along the flow path axis*." Taken literally, this description means aerosol do not move from cell to cell unless a gas flow does. In fact, large particles can be carried from cell to cell by any external force like gravity or by the lack of an external force when the gas is not

flowing in a straight line. This cell-to-cell transfer without fluid flow may be a key part of the deposition of large particles of spalled oxide containing activated material. In MELCOR⁴ p. 3-47, the model does include the transfer of particles from one control volume to another by gravity. However, the possible transfer from one control volume to another by the radial speed relative to the fluid is not included.

Evaporation and Condensation

The CONTAIN and MELCOR models for the evaporation and condensation of steam onto aerosol particles are discussed below as part of the general discussion of the evaporation and condensation of any vapor onto aerosol particles. Models for the evaporation and condensation of steam onto walls or heat structures are discussed as part of the discussion of volatile activated isotopes.

Oxide Spalling

Neither CONTAIN nor MELCOR has models for the spalling of oxides from wall surfaces. This information will have to be provided by user/other-code input or by new models added to CONTAIN for the purpose of calculating the time, chemical species, mass, and size distribution of any oxides released from surfaces.

Breakup of Mechanically Spalled Oxides

Neither CONTAIN nor MELCOR has models for the resuspension of spalled oxides or for the possible production of small, mobile aerosol particles from spalled material during time spans when fluid flows at high speeds. This information will have to be provided by user/other-code input or by new models added to CONTAIN or MELCOR for the purpose of calculating the time, chemical species, mass, and size distribution of any oxides released from surfaces.

Adsorption and Absorption of Hydrogen or Steam on Aerosol Particles

CONTAIN has a model for the adsorption and absorption of steam on aerosol particles (hygroscopicity)¹ pp. A-5 and 4-12 but no model for hydrogen adsorption. The hygroscopicity model consists of a correlation that reduces the evaporation rate of water from a drop (Equation (14) on page A-15 of this document) when the mass fraction of water is small and/or new models for solubility and Kelvin effects. The details of the new models are not presented in Reference 1 so it is not possible to determine what solubilities (or user inputs) are employed from this reference. The MELCOR model for the evaporation has two versions⁴ p. 3-13, either assume equilibrium is attained in a very short time, or calculate rates using the same (Mason) equation employed in CONTAIN⁴ p. 3-53. Apparently Equation (14) is not employed in MELCOR. "Instead, the mass of liquid water in the atmosphere (fog mass) calculated by the CVH (control volume hydrodynamics) package is distributed over the aerosol sections in the RN (Radionuclide Behavior) package for consistency in the overall calculation scheme."

The expressions necessary to model hydrogen absorption or the absorption of any other vapors are part of the expressions presented in the discussion of the evaporation of any vapor from or condensation of any vapor onto particles in the discussion of potential modifications to

CONTAIN or MELCOR in Appendix B. The most difficult part of the implementation of models for adsorption and absorption of vapors is the addition of the accounting necessary to keep track of the amount of hydrogen isotopes in particles of each size class.

Transport of Any Volatile Activated Isotopes

There is no model for this but all that is needed is a capability to keep track of the location of the gas.

Transport of Non-Volatile Activated Isotopes

Models that may be relevant to the description of the transport of non-volatile activated isotopes include an aerosol nucleation model, some approach to tracking the aerosol size distribution, a description of particle agglomeration, and models for the evaporation/condensation of vapors from or onto aerosol particles. Since many of these models are also required for fission reactor behavior studies, many of the CONTAIN models for these behaviors are complete.

Aerosol Nucleation Model

The CONTAIN model for aerosol nucleation is simply a provision for providing "seed" nuclei when needed^{1 p. 4-13} and MELCOR introduces a fog of the vapor in excess of saturation^{4 p. 3-53}. The lack of a mechanistic nucleation model is acceptable for analysis of fission reactor containments because water vapors present at concentrations above saturation will condense on pre-existing particles present as dust or liquid drops in these systems. However, nucleation of particles directly from a vapor is likely to occur when temperatures are lowered or fluids are injected rapidly into relatively clean environments like a tokamak vacuum vessel, and this behavior is likely to change the transport of the condensing species significantly^a. The possibility of a leak of cryogenic fluids into a vacuum volume is a candidate for a situation with nucleation of large numbers of small particles so it is likely that such a model will be required for a complete description of tokamak accidents. While the need for inclusion of a complete nucleation model is debatable, the existence of simplified time-integrated models like the one in developed for the PULSE code^{6,7} means that most of the features of nucleation can be considered without having to repeat the development of aerosol nucleation models that do not seriously impact computer code running times. Experience with the PULSE nucleation model has indicated that it is useful if only to prevent the inadvertent assumption of physically impossible supersaturations during computer code calculations.

Aerosol Size Distribution

Aerosol particle behavior is strongly dependent on particle size. This dependence forces computer models to adopt some method for representing the size distribution of particles present in the system being analyzed. In CONTAIN, the aerosol size distribution is described by a set of discrete particle sizes that represent the behavior of a domain of sizes in a neighborhood around each size by the behavior of the average size as illustrated in Figure A-1. This method has been

^a The larger number of smaller particles typically caused by nucleation are less likely to be deposited than fewer numbers of larger particles.

reasonably successful in the QUICK⁸, TRAP-MELT⁹, and MAEROS⁴ computer codes. The method is more general than approaches that impose an assumed log normal distribution of particle size yet does not have the high cost of working with non-discrete size distribution representations. In CONTAIN 1.1, only one population of particle species is considered (i.e. all particles of a particular size are assumed to have the same composition) but the method could be extended to represent more than one population of particle species if necessary. (For example, an aerosol made up of spalled oxide particles and of injected liquid helium drops would be represented as a collection of particles with oxide and liquid helium present on any particle in the size range where both the oxide and the liquid are represented.)

Figure A-1. A schematic diagram showing the use of twenty particle size classes and the mass per unit gas volume of each chemical species in each size class to represent the particle size and chemical species distribution.

The representation of two separate aerosol populations is not needed after the aerosol particles have been present in a volume for times longer than those required for particle agglomeration/coagulation to mix the two populations. Since these times are inversely proportional to the particle number density squared and the effects of small populations of particles are negligible, the limitation is not expected to limit the relevance of the CONTAIN aerosol behavior models to fusion confinements. MELCOR can be run with more than one aerosol particle population but that approach is discouraged.^{4 p. 3-52}

Particle Agglomeration

Reference 1 does not reproduce the detailed equations but simply states that the expressions for the effects of Brownian motion, differential gravitational settling, turbulent shear and turbulent inertial impaction are employed. Since the detailed expressions are not given

in the current version of the user's manual, the best published version of the expressions used to describe the rate of particle agglomeration or coagulation is the description of the precedent computer codes^{3,5}. The expressions for the rate of agglomeration are given in terms of collision frequency functions for each agglomeration mechanism, $\beta_{\text{mechanism}}$ ^a.

From Reference 5, the expression used for the sectional coagulation coefficient due to Brownian motion is

$$\beta_B = \frac{2\pi [D_i + D_j] [\gamma_i d_{p_i} + \gamma_j d_{p_j}]}{\frac{d_{p_i} + d_{p_j}}{d_{p_i} + d_{p_j} + 2\sqrt{g_i^2 + g_j^2}} + \frac{8 [D_i + D_j]}{\bar{v}_{i,j} [d_{p_i} + d_{p_j}]}} \quad (1)$$

where

- D_i = particle diffusivity¹⁰ of particles of size class i (m^2/s)
- γ_i = agglomeration shape factor¹⁰
- d_p = particle diameter (m)
- v_i = average speed of a particle of size i subject to Maxwell-Boltzmann statistics ($[8kT/\pi m_i]^{0.5}$ m/s)
- g_i = the steady-state distribution function for particles relative to a stationary particle of size class i in the fluid¹¹ given by the expression

$$g_i = \frac{1}{3 d_{p_i} \lambda_{p_i}} \left\{ [d_{p_i} + \lambda_{p_i}]^3 - [d_{p_i} + \lambda_{p_i}]^{\frac{3}{2}} \right\} - d_{p_i} \quad (2)$$

- λ_{p_i} = particle mean free path, given by

$$\lambda_i = \frac{8 D_i}{\pi v_i} \quad (3)$$

One advantage of Equation (1) is that it is valid for the continuum (gas molecule mean free path much less than the particle diameter), transition, and free molecule (gas molecule mean free path

^a The collision frequency functions can be used to find the number of collisions per unit volume per unit time between particles of different sizes. To find this rate, the collision frequency function is multiplied by the number density of each of the colliding particle sizes. To describe the agglomeration of a distribution of particle sizes, the expression for the rate of agglomeration of size i and size j must be integrated over the distribution of both size i and size j . When a set of discrete particle sizes is used instead of an integral expression, the integral becomes a sum over the sizes. Apparently out of concern due to this difference and the (theoretical) need to average β over the "bin width" of each particle size, the authors of CONTAIN change the usual name for β from collision frequency function to "sectional coagulation coefficient".

much less than the particle diameter) regimes.¹¹ For cases not in the transition region, the equation is unnecessarily complicated. For example, the factor with the γ 's in the numerator and the denominator reduces to the sum of the two particle radii in the continuum environment. Also, the advantage of having an equation valid for all regimes is largely lost if the particle shape factors, the sticking probability when particle collide (contained in one of the two expressions Reference 11 offers for the particle diffusivity) is not known, or the appropriate expression for the gas mean free path is not known because the gas is a mixture.

The expression used for the sectional coagulation coefficient due to differential gravitational settling is

$$\beta_{grav} = Col_g \frac{\pi}{4} [\gamma_i d_{p_i} + \gamma_j d_{p_j}]^2 |v_{s_i} - v_{s_j}| \quad (4)$$

where

$$\begin{aligned} \gamma_i &= \text{agglomeration shape factor}^{10} \\ Col_g &= \text{collision efficiency factor, the square of the smaller particle diameter divided by the square of the sum of the diameters of the two colliding particles} \\ v_{s_i} &= \text{terminal settling speed of a particle in size class } i \text{ (m/s). (The equation used for this speed is given in the section that discusses the deposition of particles due to gravity.)} \end{aligned}$$

The expression used for the combined effects of the shear and inertial turbulent contributions is the square root of the sum of the squares of the shear and inertial contributions,

$$\beta_T = \sqrt{\beta_{T1}^2 + \beta_{T2}^2} \quad (5)$$

The turbulent shear contribution, β_{T1} , is given by

$$\beta_{T1} = \sqrt{\frac{\pi e_T}{120 \nu}} [\gamma_i d_{p_i} + \gamma_j d_{p_j}]^3 \quad (6)$$

where

$$\begin{aligned} \nu &= \text{gas kinematic viscosity (m}^2/\text{s)} \\ e &= \text{turbulent energy dissipation rate (m}^2/\text{s}^3) \end{aligned}$$

The turbulent inertial contribution, β_{T2} is calculated with the equation

$$\beta_{T2} = \frac{0.04029 \rho_g^{\frac{1}{4}} e_T^{\frac{3}{4}}}{\eta^{\frac{5}{4}}} [\gamma_i d_{p_i} + \gamma_j d_{p_j}] \left| \frac{\rho_i C_i d_{p_i}^2}{\chi_i} - \frac{\rho_j C_j d_{p_j}^2}{\chi_j} \right| \quad (7)$$

where

ρ_g	=	gas density (kg/m ³)
ρ_{pi}	=	density of the condensed phase that forms particles in the i th size class (kg/m ³ of condensate)
η	=	gas viscosity (kg/ (m s))
C_m	=	the Cunningham slip correction ¹⁰
χ_i	=	dynamic shape factor (unitless). ⁵

There is one other particle agglomeration mechanism that may be significant for an accurate description of aerosol behavior in fusion confinements. The high electric fields expected in fission reactor containments might cause particle or gas ionization and associated electrostatic effects. Models for these effects are not in CONTAIN or MELCOR. For a fusion machine, the possible inclusion of an electrostatic precipitator, the possible formation of ions by high electric fields, and the possible presence of aerosol particles with permanent electric or magnetic dipole moments (some iron oxides are ferromagnetic) may require consideration of charge and (in the absence of significant static charging of the particles) dipole forces on agglomeration rates. According to Fuchs¹² page 310-315, the fact that agglomerating dipoles can increase the dipole moment of the agglomerate represents a potential positive feed-back situation where the formation of some agglomerates increases the rate of agglomeration of the particles. Until aerosol behavior data more characteristic of ITER materials, dimensions, and time become available, it is difficult to judge the need for models for the effect of electric or magnetic fields on agglomeration. Initial models for these effects are discussed in Appendix B.

Evaporation from and Condensation onto Particles

In fission reactor containments, water vapor is the species that dominates evaporation from and condensation onto aerosol particles. The CONTAIN and MELCOR codes have a corresponding emphasis on water as the condensing species. In CONTAIN, only one species is allowed to evaporate or condense in any control volume and that species is water/steam unless the user over-rides that default^a.² Except for removal of gaseous iodine species by containment spray system, the evaporation/condensation of gaseous material other than water is not considered.

The expression used to calculate the rate of evaporation/condensation of steam from/to an aerosol drop in CONTAIN¹ Equation 4-8 is^b

^a The authors have been unable to find a concise statement of this limitation in Reference 1. However, the conclusion is strongly implied by Section 2 of Reference 2, by the form of the expression for the rate of particle deposition by diffusiophoresis, and by paragraph one of Section 4.2.2 of Reference 1.

^b The units of the two terms in the denominator of Equation (1) are not consistent. The latent heat of vaporization should be squared.

$$\xi = \frac{2 \pi d_p [SSat - 1]}{\left[\frac{M_{H_2O} h_{H_2O}}{k_{gas} R T^2} \cdot \frac{1}{\rho_{steam} D_{steam}} \right]} \quad (8)$$

where

ξ	=	mass condensation rate on particles (kg/s)
SSat	=	supersaturation, partial pressure of condensing or evaporating species divided by the equilibrium partial pressure of the species over a flat surface (no units)
M_{H_2O}	=	molecular mass of water (kg/kg-mole)
h_{H_2O}	=	latent heat of vaporization of water (J/kg)
k_{gas}	=	gas thermal conductivity (W/m-K)
R	=	gas constant, $8.314 \cdot 10^3$ J/kg-mole-K,
T	=	bulk temperature of fluid (K)
ρ_{steam}	=	saturated steam density (kg/m ³)
D_{steam}	=	steam diffusivity (m ² /s)

The term in the denominator that contains the latent heat of vaporization (squared) accounts for the fact that the heat of vaporization must be provided by transport to the drop. Substitution of typical values for the material properties shows that the heat transfer term dominates for species whose equilibrium vapor pressure is large (a major fraction of one atmosphere) at the temperature of the aerosol, especially for species like water where the latent heat is large.

When one or more species is evaporating and/or condensing onto particles, the differential equations that describe the movement of particles and their associated condensed mass between size classes often become very stiff.⁴ p. 3-53 In particular, it is difficult to avoid extremely severe Courant-like limits on the time step size of the solution caused by the exit^a of some species from some aerosol size classes. Not only are the equations stiff, but there can be large discontinuities in the rate of loss of a species from a size class when the last bit of a rapidly decreasing species is gone. In CONTAIN, these stiffness and "dry-out" problems are addressed in part with an artificial reduction of the evaporation rate¹ page 4-12 and in part by allowing only one vapor species, usually steam, to evaporate or condense.² Section 2 If temperatures below ambient room temperatures are considered or if details of the aerosol size distribution formed by volatilization are considered, it is likely that more than one species of vapor will condense. To consider aerosol behavior realistically, the single-volatile-species and slow evaporation approximations made in CONTAIN will have to be replaced with more appropriate models for the effect of evaporation/condensation on particle size distribution.

The MELCOR description says the change in aerosol size distribution is handled by the

^a This exit is usually thought of as evaporation and referred to as "dry-out", but a species may also be lost rapidly from a size class when particles grow or shrink rapidly. This loss by size-shift is every bit as troublesome numerically as the direct loss by evaporation when several species are present.

same equations as in the MAEROS condensation/evaporation model^{4 p. 3-53} but no description of these equations has been found. The fact that neither the MAEROS method nor the rate equations of CONTAIN are used suggests that a rather arbitrary distribution is used, for example a distribution weighted by the particle surface area or by the particle radius (because of a factor of r in the diffusivity). This approach is unacceptable because it will generate or destroy particle number density in contrast to the physical behavior which preserves the particle number density.

Experience developing the PULSE analysis tool has led to the development of one model that conserves not only chemical species mass but also particle number densities when several species of vapor are evaporating and/or condensing at the same time and place. With appropriate implementation, running time is not seriously impacted by the size-change model. This model is discussed in Appendix B as one of the potential modifications and additions to CONTAIN or MELCOR.

Particle Deposition

The expressions used in CONTAIN and MELCOR to describe the rate of particle deposition consider the effects of gravitational settling, diffusion to surfaces, thermophoresis, and diffusiophoresis. In all cases, the models are expressed in the form of a deposition velocity which is the flux of particles to a surface divided by the bulk average particle concentration. With the exception of the possible need to allow variations in gas compositions with time and include properties helium or nitrogen gas as well as air (the default gas species considered by the CONTAIN and MELCOR aerosol models), the basic expressions should apply to fusion confinements as well as fission containments. Changes recommended to the models are based not on the belief that the models are wrong, but rather that they may contain approximations not appropriate for fusion environments.

Gravity. The expression used for the deposition velocity due to gravity is

$$v_s = \frac{d_p^2 \rho_p g C_m}{18 \mu \chi} \quad (9)$$

where

v_s	=	the terminal settling speed (m/s)
ρ_p	=	the density of the particle (kg/m ³)
g	=	the acceleration of gravity (9.8 m/s ²)
C_m	=	the Cunningham slip correction ¹⁰
χ	=	the particle dynamic shape factor ¹⁰ .

This expression is restricted to the Stokes-law region where the particle Reynold's numbers^a are

^a The particle Reynolds number is the condensed phase density times the particle diameter times the particle speed relative to the fluid all divided by the fluid viscosity¹⁰.

much less than one. If a subcode is developed (or incorporated^a) to consider non-stokes regions for electrostatic precipitators (discussed below) or large pieces of spalled oxide, it should be applied to generalize this expression. Also, the direct application of this expression implied by the CONTAIN description is appropriate to the case of tranquil settling only. If the confinement is stirred in order to filter aerosols as proposed by Brereton et. al.¹³, generalization to include this stirring will be required.

Centripetal Inertial Deposition. Neither CONTAIN nor MELCOR has a model for particle deposition due to non-linear fluid flow. If the centripetal acceleration of fluid moving in curved paths during a fusion accident is a major fraction of the acceleration of gravity, the transport of aerosol particles to walls on the outside of curved stream lines may be an important particle deposition mechanism, especially for large particles that can stick to walls. A simple model for this deposition is presented in the Appendix B. At this point, the need for the model is difficult to assess because the size of aerosol particles present in fusion machines and the fluid speed are not well characterized.

Diffusion to Surfaces. The deposition velocity due to diffusion to surfaces is calculated in CONTAIN with the equation

$$V_{diff} = \frac{kT c_m}{3 \pi \mu d_p \Delta} \quad (10)$$

where

v_{diff}	=	diffusion deposition velocity (m/s)
k	=	the Boltzmann constant, $1.38 \cdot 10^{-23}$ J/(sm ² K ⁴)
μ	=	viscosity (kg/(m s))
Δ	=	diffusion boundary layer thickness (m).

In CONTAIN, the diffusion boundary layer thickness must be specified by the user^{1 p. 4-15}. The use of a user-specified diffusion boundary layer thickness amounts to allowing user-adjusted answers so the current model will not be satisfactory if diffusion is an important contributor to deposition. Expressions for the diffusion boundary layer thickness are discussed in Appendix B. The input requirements of MELCOR include a diffusion boundary layer thickness that defaults to 1.0e-05 m.

Thermophoresis. The expression used for the thermophoretic deposition velocity in CONTAIN is calculated with the classic Brock equation¹⁴ for the force and the definition of particle mobility,

^a A subroutine for this purpose based on tables from Fuchs¹² has been developed and implemented in both the TRAP-MELT⁹ and PULSE⁶ computer codes.

$$V_{therm} = \frac{1.5 \mu C_m \left[C_t Kn + \frac{k_{gas}}{k_p} \right] \nabla T}{\chi \rho_{gas} T_w \left[1 + 3 C_m Kn \right] \left[1 + 2 C_t Kn + \frac{k_{gas}}{k_p} \right]} \quad (11)$$

where

- Kn = the Knudsen number, $2\lambda/d_p$ where λ is the mean free path of gas molecules
 k_{gas} = thermal conductivity of gas (W/(m K))
 k_p = thermal conductivity of particle (W/(m K))
 ∇T = temperature gradient toward the wall near the wall surface (K/m)
 C_t = thermal accommodation coefficient.

Deposition by thermophoresis is most important when there are large temperature gradients and the particles are small. When the wall is colder than the gas phase, the deposition velocity is positive but when the wall is hotter than the gas phase, the thermophoresis force on particles is away from the wall. Since both very cold and very hot walls may exist during fusion machine accidents, this deposition mechanism may be important if small particles are present. The mechanism is not likely to be important for particles above 10 μm in diameter.

In fission reactors, thermophoresis is not an important contributor to particle deposition because in these reactors locations with large temperature gradients are also locations where large amounts of vapor are condensing. In this situation, particles increase rapidly in size due to condensation and deposit by other means. The mechanism may be more important in some fusion machine accidents because they can last for days and may have high temperature gradients in the absence of condensing vapors.

Diffusiophoresis. Particle deposition by diffusiophoresis is calculated in CONTAIN¹ p. 4-16 (and, presumably, in MELCOR) with the equation,

$$V_{diffus} = \left[\frac{\gamma_1 \sqrt{M_w}}{\gamma_1 \sqrt{M_w} + \gamma_2 \sqrt{M_w}} \right] \left[\frac{\frac{dm_v}{dt}}{\rho_w A_{ap}} \right] \quad (12)$$

where

- M_w = kg-mole weight of water (kg / (kg-mole))
 dm_v/dt = mass rate of water vapor condensed/evaporated to/from the *aerosol particle surface* (kg/s).
 A_{ap} = outer surface area of an aerosol particle (m^2)
 ρ_p = density of water film boundary immediately adjacent to the aerosol particle (Kg/m^3)
 γ_1, γ_2 = aerosol intermediate factors, defined as

$$\begin{aligned} \gamma_1 &= P_{\text{sat}}(T_{\text{sp}}) / P_{\text{gas}} \text{ and } \gamma_2 = 1 - \gamma_1 \\ P_{\text{sat}} &= \text{water saturation pressure evaluated at the aerosol temperature} \\ P_{\text{gas}} &= \text{gas phase pressure (Pa).} \end{aligned}$$

The rather convoluted form of Equation (12) (the first factor on the right hand side is simply γ_1) is apparently the result of the partial simplification of a more general expression to the special case of the deposition of water particles by condensing water. In addition to this, the application of this expression to evaporation and condensation from the surface of a spherical particle is difficult to understand. If Equation (12) was derived considering the condensation/evaporation of water vapor onto/from water particles as a supplement to the classical expression for deposition velocity due to condensation/evaporation on a wall¹⁵, the symmetry of the particle should cause the first order terms of the classical expression to cancel, leaving only a term dependent on the concentration gradient of the vapor not condensing on the particle. Equation (12) has the same form as the classical expression for the condensation/evaporation on a wall but the vapor flux to the wall has been changed to a vapor flux to a particle.

In a fusion reactor, the aerosol particle and/or the condensing vapor may not be H₂O so the CONTAIN source code expressing Equation (12) should at least be revised to the form for arbitrary species of vapor and particles if diffusiophoresis is determined to be a potentially significant particle deposition mechanism. In addition to this, there should be only an expression for the effect of vapor transport to a wall until a defensible derivation for the effect of vapor transport to and from particles is produced. Incidentally, according to Horst (Reference 15), the form of Equation (12) applies only to the free molecule regime, i.e. when the gas molecular mean free path is much greater than the particle radius. More general forms of Equation (12) for fusion containments are presented in Appendix B.

In fission reactors, diffusiophoresis is an important particle deposition mechanism in containments because of the significant condensation of water vapor on relatively cool containment walls. In fusion machines, diffusiophoresis may not be as important as it is in fission reactor containments because there may not be as much hot water in the confinement to provide a large vapor flux to the walls.

Precipitators. CONTAIN has no model for the removal of aerosol particles by precipitators. If electrostatic precipitators are employed, expressions for the removal of aerosol particles by these devices will have to be added to the other deposition mechanisms considered by the CONTAIN and/or MELCOR codes.

Containment Spray and Scrubbing. Models for particle deposition by containment spray and by aerosol scrubbing do not apply to fusion confinements so they should be removed or deactivated before CONTAIN is applied to fusion problems.

Isotopic Exchange Between Elemental Gas and Water Vapor or Condensed Water

CONTAIN and MELCOR do not have models for isotopic exchange. If analysis cannot be used to show isotopic exchange is never an important consideration, these will have to be identified or developed and added to the code.

Chemical Reactions of Hydrogen

The CONTAIN/MELCOR model for chemical reactions of hydrogen was designed to consider the possibility and effects of deflagrations if hydrogen builds to sufficient concentrations for a burn. The model presumes a deflagration is initiated when minimum threshold concentrations of combustible gas and oxygen are exceeded or when a burn can propagate from an adjacent burning cell. Flame speed is calculated using a matrix of correlations, with the particular correlation used selected based on the concentration of hydrogen, oxygen, and water vapor. There is no provision for hydriding of condensed phases.

With the exception of a need to generalize the existing model to lower pressures and include the possibility that helium gas may also be present, the model should be adequate to analyze hydrogen burns.

Dynamics (Numerical Solution Methods)

After all of the particle agglomeration, deposition, external sources, and coupling to the vapor rates are defined, any aerosol behavior model is faced with the difficult task of integrating rate equations of the form

$$\begin{aligned} \frac{dQ_{l,k}}{dt} = & \frac{1}{2} \sum_{i=1}^{l-1} \sum_{j=1}^{l-1} [{}^1a\overline{\beta}_{i,j,l} Q_{j,k} Q_i + {}^1b\overline{\beta}_{i,j,l} Q_{i,k} Q_j] \\ & - \sum_{i=1}^{l-1} [{}^2a\overline{\beta}_{i,l} Q_i Q_{l,k} - {}^2b\overline{\beta}_{i,l} Q_l Q_{i,k}] \\ & - \frac{1}{2} {}^3\overline{\beta}_{l,l} Q_l Q_{l,k} - Q_{l,k} \sum_{i=l+1}^m {}^4\overline{\beta}_{i,l} Q_i + {}^1\overline{G}_{l,k} Q_l \\ & \sum_{i=1}^{N_a} [{}^2\overline{G}_{l,i} Q_{l,k} - {}^2\overline{G}_{l-1,i} Q_{l-1,k}] + {}^3\overline{G}_{l-1,k} Q_{l-1} \\ & + \overline{S}_{l,k} - \overline{\mathcal{R}}_{l,k} \end{aligned} \tag{13}$$

where

$dQ_{l,k}/dt$	=	time rate of change of aerosol mass of component k (per unit volume) in particle size class l
k	=	index specifying the chemical species
l	=	index specifying the particle size class
$Q_{l,k}$	=	mass of species k in size class l
G	=	gas-particle conversion ($m^3 s^{-1}$)
β	=	sectional coagulation coefficient ($m^3 s^{-1} kg^{-1}$)

Integration of these equations is carried out under simplifying assumptions in CONTAIN. Many of these approximations are imposed to avoid time-consuming re-calculations of the coefficients β_{ij} , G_{ij} , and $\mathcal{R}_{ik}$. The approximations are

- The ratio of adjacent particle size class average sizes is forced to be greater than two^{1 p. 4-5}. This limits the numbers of size classes coupled by a single agglomeration event
- The aerosol material density is assumed to be the same for all components.^{1 p. 4-6}
- The aerosol shape, as modeled by the dynamic and agglomeration shape factors, is independent of aerosol composition.^{1 p. 4-6}
- The medium in which the aerosol processes are assumed to occur has fixed composition and this composition is taken to be that of air.^{1 p. 4-6}
- The degree of turbulent agglomeration is fixed throughout the problem.^{1 p. 4-6}
- Other parameters that control deposition rates do not depend on particle composition. For example, the ratio of the thermal conductivity of air to that of the aerosol material is fixed.^{1 p. 4-6}
- When the water mass in an aerosol size class becomes comparable to the dissolved solid mass, the rate of evaporation is reduced artificially by a factor,

$$1.037 \tanh(2 \text{ mass fraction water }) \quad (14)$$

to eliminate the sudden change in the rate of water vaporization that occurs at particle dry-out and causes difficulty with the Runge-Kutta integrator used in CONTAIN.^{1 p. 4-12}

A Runge-Kutta integration scheme is implied by the last assumption. Based on the indication, it is assumed for this assessment that a Runge-Kutta integrator is used in CONTAIN. While this is certainly a reasonable choice, the Courant-like limits associated with the growth or shrinking of particle sizes during the evaporation/condensation of multiple species may force the development of additional approximations to keep the Runge-Kutta method efficient or it may force the use of some of the newer techniques that have been developed since Runge-Kutta¹⁶.

The modifications required to extend CONTAIN for fusion confinement analysis are fairly extensive because of fusion/fission differences. Along with these changes will come changes to the limits and approximations imposed to support the integration schemes of CONTAIN and MELCOR. In fact, the schemes themselves may have to be tailored to optimize them for the most important fusion models. In addition to these, the fact that fusion confinement design is still changing rapidly means that either (1) the models in the fusion confinement analysis computer code will have to be changed frequently as the design and materials of the confinement evolve or (2) a more inclusive integration approach will have to be employed.

Decay Heat (Fusion Product Behavior Models)

The CONTAIN¹ pp. 5-1 to 5-15 and MELCOR⁴ p. 3-56 models for fission product behavior are designed for fission product decay heating and LWR structures. This fact and the fact that the decay heat is assumed to be deposited directly into the "host" material (i.e. if the species is deposited on an aerosol particle, the decay heat is assumed to be contained in the particle.) or a user-input partitioning between host materials means that the fission product behavior models or at least the user-input partitioning of CONTAIN or MELCOR will have to be modified to consider isotopes and depositions appropriate to fusion machines. In addition, the assumption that the decay heat will be deposited in the host materials at fixed ratios will have to be re-justified for the fusion environment or the model will have to be changed to a more general analysis.

Materials Properties

The materials properties used in CONTAIN are embedded in the code. This may be acceptable for the relatively fixed nature of fission reactor containments at the present time, but the uncertainty about which materials will finally be employed in fusion machines implies that the materials properties should be moved to a separate module to facilitate analysis with varying materials.

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Appendix B
Potential Aerosol Model Modifications

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FIGURES

- Figure B-1.** The concept used to model particle size changes during evaporation/condensation. f_u is the fraction of the final particle volume and/or species mass that is placed in size class i_u B-7

In the critical review of CONTAIN and MELCOR aerosol modeling capabilities, a number of needs to extend the code model fusion reactor confinements were cited. This appendix describes modifications that would address the needs identified.

Resuspension

Models for the resuspension of particles deposited during normal operation are to be determined.

Injection of Spalled Oxides from Surfaces

There are currently no models available to describe the injection of spalled oxides from surfaces into the fluid phases of a tokamak. A task to produce at least preliminary models has been identified and these models will have to be added to CONTAIN to produce a complete analysis if the task shows that these spalled oxide may contribute significantly to the transport of activated isotopes.

Breakup of Mechanically Spalled Oxides

A correlation for the rate of small particle production that could be used to produce a model has been produced by an analysis of measurements¹. This correlation relates the rate of small particle production to the rate of impact and the impact stress on particles that hit walls,

$$y = 1.074 \times 10^{-10} \sigma_{\text{impact}}^2 + 3.497 \times 10^{-7} \sigma_{\text{impact}} \quad (1)$$

where

- y = small particle yield (ratio of the mass of small particles produced to the mass of large particles striking the wall)
- σ_{impact} = particle impact stress (Pa). The calculation of this stress is discussed in Reference 1.

The method used to derive Equation (1) is sufficiently general that it should also be applicable to resuspended tokamak dust.

Adsorption and Absorption of Hydrogen or Steam on Aerosol Particles

Models for the solution of either hydrogen or steam in aerosol particles consist of means of providing numerical values of the activity of steam or hydrogen (γ_c in Equation (20) and keeping track of the mole fraction of steam or hydrogen in the condensed phase (x_c in Equation (20)). The activity of steam for fusion-relevant aerosol particle materials is 1.0 and the activity of hydrogen for fusion-relevant aerosol particle materials is to be determined.

Transport of Non-Volatile Activated Isotopes

Aerosol Nucleation Model

The nucleation of particles from the vapor phase is typically a very fast process that causes difficulties with the solution of the very stiff differential equations that describe the process. Because of these numerical problems, it is proposed that aerosol formation be modeled with two approximations, one to limit the rate of condensation of vapor used in the nucleation and the other to limit the rate of particle agglomeration caused by the formation of just-nucleated particles. The approximate model is based on a source code developed by D. A. Petti² in response to difficulties encountered in modeling fission product behavior in a series of fission severe accident tests has been successfully used to model the test results.

In this model, the rate of particle formation and the critical size to prevent re-evaporation of transient particles are calculated using the classical nucleation theory discussed below. Often, the rate of consumption of vapor is so rapid that the differential equations for transfer of mass from the vapor to particles are extremely stiff with respect to both the transport of mass out of the vapor state and the rate of agglomeration of the large numbers of small particles nucleated from the vapor.

Problems with solving the stiff equation for the vapor mass are avoided by checking the start-of-step rate times the time step size being used in the analysis to see if the approximate vapor consumption implied would lower the species vapor concentration below saturation. If it would, the nucleation is assumed to stop at saturation during the time step. If the approximate vapor consumption is not excessive, the rate of formation is assumed to continue throughout the time step.

Problems with the stiff nature of the equations that consider the rate of agglomeration of the particles formed by the nucleation process are avoided by checking to see if the agglomeration rate implies most of the particles increase to a larger size classification during the time step. This check is carried out by assuming the mass of aerosol particles formed by nucleation appears in the size class corresponding to the larger of the critical size and the smallest size class used in the analysis and comparing the agglomeration time constant (a parameter determined assuming agglomeration is the only mechanism removing particles from a particular size class) to the time step size. If the time constant for agglomeration out of the trial size class is less than the time step size, the aerosol mass corresponding to the initial particles is moved to the next larger size classification and the test is repeated until the time constant for agglomeration out of the size classification is larger than the time step size.

The rate of formation of aerosol particles is calculated following Petti's suggestions,²

$$J = \left[\frac{P}{kT} \right]^2 \left[\frac{2\sigma m}{\pi} \right]^{\frac{1}{2}} \frac{S^2}{\rho_p} \exp \left(- \frac{4\pi}{3} \frac{\sigma r^{*2}}{kT} \right) \quad (2)$$

where

J	=	rate of formation of aerosol particles (particles/(m ³ s))
P	=	vapor pressure of nucleating species (Pa)
σ	=	surface tension of condensed phase (M/m)
m	=	mass of an atom of the condensing vapor (kg)
S	=	supersaturation ratio (unitless)

- r^* = the radius of particles formed in the absence of ions (m)
 $2\sigma / [\rho_p R T \ln(S)]$
 R = the gas constant, $8.314 \cdot 10^3 \text{ kg m}^2 / (\text{s kg-mole K})$.

The rate of nucleation is increased when ions are present in the vapor phase because the ions attract clusters to a common location. The additional rate due to ions is given by

$$J_{ion} = \frac{4 \pi r_k^2 P}{[2 \pi k T m]^{\frac{1}{2}}} \left[\frac{4 \pi \sigma r_k^2 - [1 - e^{-1}] \left[\frac{e^2}{4 \pi \epsilon_0 r_k} \right]}{9 \pi k T n_k^2} \right]^{\frac{1}{2}} S N_a \exp \left(\frac{-\Delta G_0}{k T} \right) \quad (3)$$

where

- J_{ion} = rate of nucleation of vapor as a result of ions (particles/ (m³ s))
 ϵ = dielectric constant of condensing species
 e = charge of the electron, $1.6 \cdot 10^{-19}$ coulomb
 n_k = number of atoms in a cluster of radius r_k
 N_a = number of ions/volume (ions/ m³)
 r_k = the larger of two roots of the radial derivative of the change of free energy (or Gibbs function) in the condensation process.

In order to use this result, a value of r_k must be determined. This is done by writing the equation that expresses the change in the free energy in the condensation process, taking the derivative of this expression with respect to the radius of the cluster formed, and setting this derivative equal to zero. The equation to be solved for r_k is

$$\frac{\partial [\Delta G(r_p)]}{\partial r_p} = -k T \ln(S) + \frac{2 \sigma V_m}{r_p} - \frac{e^2 V_m}{8 \pi r_p^4 [4 \pi \epsilon_0]} \left[1 - \frac{1}{\epsilon} \right] = 0 \quad (4)$$

where

- r_p = particle radius (m)
 V_m = molecular volume of condensing species (molecules/m³)

The FORTRAN subroutines used to find the roots of Equation (18) and the rate of nucleation^a are available from newer versions of the PULSE computer code.³

Evaporation from and Condensation onto Particles

Equation (8) in Appendix A is a version of the Mason Equation. Mason's version⁴ includes

^a Subroutines AERO, IONNUC, HMNUC, NEWTON, and function DELTAG plus the agglomeration time constant from subroutine DERV.

additional terms that account for the effects of the temperature gradient on the gas diffusivity, the activity of the vapor species, and the Kelvin effect on the equilibrium vapor pressure over a curved surface,

$$\xi = \frac{2 \pi d_p \left\{ SSat - 1 - \frac{4 \sigma M_{H_2O}}{\rho_{H_2O} R T d_p} + \frac{64 \cdot 6 m}{M_1 d_p^3} \right\}}{\left\{ \frac{h_{H_2O}}{k_{gas} T} \left[\frac{M_{H_2O} h_{H_2O}}{R T} - 1 \right] + \frac{1}{D_{steam}} \left[\frac{1}{\rho_{steam}} = \frac{R T}{P_{steam} M_{H_2O}} \right] \right\}} \quad (5)$$

where

- ξ = mass condensation rate on a particle (kg/s)
- m = mass of dissolved salt (g)
- M_1 = molecular weight of the salt (g)
- ρ_{H_2O} = density of water (g/cm³)
- σ = surface tension of condensed phase (dynes/cm)
- P_{steam} = partial pressure of steam (dynes/cm²).

(The equal sign in the bracket at the right hand end of the denominator represents alternate forms obtained by using the ideal gas law to write the density of steam in terms of the partial pressure of steam.)

The numerator of Mason's expression is an approximate form derived by assuming that the solute (salt) is diluted a great deal by the solvent (water). The derivation of Mason's equation can be carried out without using the dilute-solute approximation to show that

$$\xi = \frac{2 \pi d_p \left\{ SSat - \gamma_c x_c e^{\frac{4 \sigma M_c}{\rho_c R T d_p}} \right\}}{\left\{ \frac{h_c}{k_{gas} T} \left[\frac{M_c h_c}{R T} - 1 \right] + \frac{R T}{P_{cv} D_{cv} M_c} \right\}} \quad (6)$$

where

- γ_c = condensing species activity
- x_c = mole fraction of condensing species in the condensed phase
- c = denotes whatever chemical species is condensing (not just H₂O)
- cv = denotes the vapor of the condensing chemical species.

If the aerosol particles contain cryogenic condensates, both conduction and radiation can be important heat transfer mechanisms for the latent heat of vaporization. Repeating the derivation of the Mason equation with radiation heat transfer to/from a drop that "sees" a heat structure at temperature T_w adds a factor of

$$\left[1 - \frac{L M}{R T^2} \frac{d_p}{s} \frac{5.677 \cdot 10^{-8} \frac{J}{m^2 K^4} [e_w T_w^4 - e_p T_p^4]}{2 [SSAT - 1]} \right] \quad (7)$$

where

e_w = emissivity of the wall
 e_p = emissivity of particle surface
 T_w = wall temperature (K)
 T_p = temperature of particle surface, $\approx T$, (K)
 to Equation (6) .

The factor that accounts for radiation heat transfer always represents a negative contribution to the rate of change of particle radius when the heat structure temperature is greater than the aerosol temperature. For cryogenic materials like liquid helium and perhaps liquid nitrogen, the evaporation/condensation rate equation is biased toward evaporation by radiation heat transfer. Aerosol droplets formed by helium spray will evaporate but condensation will be inhibited by the need for a large temperature gradient away from the drop surface in order to allow the heat transfer needed for condensation.

For fusion reactor confinements, the addition of both the activity factor for hydrogen isotopes and (if cryogen spills are to be modeled) some form of the radiation heat transfer term will be needed. The activity will allow for improved analysis of the range of hydrogen/tritium adsorption effects and the radiation heat transfer will avoid erroneous calculations of the condensation of cryogenic vapors.

It was mentioned in Appendix A that the equations for particle size changes often become very stiff and present severe Courant-like restrictions when several species of vapor may be evaporating and/or condensing at the same time and place. One way to model the change in particle size is to replace the use of rates of each material in and out of each size class by the use of the net size change during a time span^a. With this approach, particles can pass through several size classifications during a time step without causing any instabilities in the solutions of the particle equations. Of course, this method does not account for the effects of particle size change on the evaporation/condensation rate during the time step so the method is not exact. It is, however, more accurate than the current practice of completely ignoring the effect of the size change.

Figure B-1 illustrates the concept used in the derivation of the expression for the change in particle size required to model evaporation/condensation from/to aerosol particles. The gray vapor species, species 1, is shown evaporating from particles of size class 1 (i.e. radius r_1 and volume V_1) while a larger amount (more condensed phase volume) of the white vapor species, species 2, is condensing onto the particles. Since there is a net increase in particle volume, some mass will have to be shifted to a larger size class in this example. In general, the amount shifted is found by calculating the volume per particle of particles initially in size class 1 after a time-step of Δt

^a This approach is analogous to the use of the impulse instead of the rate of change of momentum to describe impacts like the striking of a ball by a bat.

Figure B-1. The concept used to model particle size changes during evaporation/condensation. f_u is the fraction of the final particle volume and/or species mass that is placed in size class l_u .

seconds by adding the condensed volume of all the species:

$$V_{final}(\Delta t) = V_i + \frac{1}{N_i} \sum_k \left[\frac{\frac{dm_{k,i}}{dt}}{\rho_k} \right] \Delta t \quad (8)$$

where

V_{final}	=	volume per particle of particles that were initially in size class l (m^3)
N_i	=	number of particles in size class l
$dm_{i,k}/dt$	=	average rate of condensation of vapor species k onto all particles of size class l during time step (kg/s)
ρ_k	=	condensed phase density of k th chemical species (kg/m^3),
Δt	=	the time-step increment (s).

In order to be consistent with the discrete particle size approach to describing aerosol particles and be consistent with the fact that the number of particles does not change during

evaporation from or condensation onto particles (except in the case that all condensed phases evaporate), V_{final} is divided into the next-smaller and next-larger size classes using the constraint that the number of particles doesn't change. If l_u is the next-larger size class, $l_u - 1$ is the next smaller size class, fu is the fraction of each particle originally in size class l to be placed into size class l_u , the constraint that the divided V_{final} still represents one particle can be written^a.

$$1 = \frac{[1 - fu] V_{final}}{V_{l_u - 1}} + \frac{fu V_{final}}{V_{l_u}} \quad (9)$$

where

V_l = volume associated with size class l .

Solving for fu yields

$$fu = \frac{1 - \text{RATIO} \frac{V_{l_u}}{V_{final}}}{1 - \text{RATIO}} \quad (10)$$

where

RATIO = ratio of l th size class volume to $l+1$ th class volume.

The mass of each species that remains as part of the particles is also partitioned between the l_u and $l_u - 1$ size classes using the fraction fu .

An alternate approach, using the instantaneous rate of shift from size class l to $l+1$ or $l-1$ is possible but the approach requires a Courant-like limit on the time step size that is often very restrictive, as mentioned earlier in the discussion of CONTAIN models.

Particle Charge Distribution and Magnetic Dipole Moments

Aerosol particle charge distribution is an important consideration because electrostatic forces are much greater than the other forces that cause agglomeration and deposition if the particles are highly charged. Even the forces associated with magnetic dipoles could be significant if the particles have permanent dipole moments. Models for the effects of charge and magnetic dipole moment on agglomeration and particle deposition are discussed below. These models require the charge and magnetic dipole moment distribution among the particles. The major uncertainty about the effects of electromagnetic interaction come from uncertainty in the particle charge and magnetic dipole moment distributions.

There are four classes of mechanisms by which aerosol particles charge: static electrification,^{9 p. 292} diffusion charging,^{9 p. 292} field charging,^{9 p. 292} and charging due to radioactive decay of particle material⁵. Static electrification occurs when particles are separated from surfaces. Of

^a Conservation of mass is guaranteed by dividing the V_{final} into fractions fu and $1-fu$.

the several static electrification mechanisms discussed by Hinds, the most relevant is contact charging during the separation of dry nonmetallic particles from solid surfaces (e.g. resuspended graphite tokamak dust). This mechanism is driven by the flow of electrons to equalize the Fermi levels of the materials constituting the dust and the surface when the particle is resting on the surface. When the particles are resuspended, there is an excess or deficiency of electrons on the particle, leaving the surface and the particle charged. According to Hinds this is not a reliable mechanism for aerosol charging. If this effect is to be modeled, we will have to develop tables of the difference in Fermi energy levels or correlations for specific pairs of particles and surfaces. We have not done this because we think a more appropriate first step would be preliminary observations of tokamak dust removed from surfaces to see if they are actually charged. At present, the main conclusion about this mechanism of particle charging is that dust resting on a surface of the same composition as the particle will not charge by contact charging because the Fermi levels of the particle and surface will be the same.

Diffusion charging is the charging of particles mixed with ions by random collisions between the ions and the particles. This process is most important for small particles (less than $0.2\text{ }\mu\text{m}$ diameter) mixed with unipolar ions. An expression for the rate of particle charging by the smaller and smaller fraction of ions that have sufficiently high velocities to overcome the force of repulsion of the increasingly charged particle is given by Hinds (his Equation (15.24)). It is our judgement that this mechanism will not be an important source of particle charging because the ingress of air or steam will produce ions of both positive and negative charge so that a net particle charge is only a second order effect. The reason we expect both positive and negative charge is the probable mechanism of gas ion charging is corona discharge by nonuniform electric fields (discussed by Hinds in his section 15.5). In corona discharge, electrons accelerated by high electric fields impact neutral ions creating positive ions. If an electronegative gas like oxygen is present, the electrons move out of the very high field region, slow down and attach to neutral gas molecules to form negative ions. Thus, air and water will tend to have both negative (oxygen, hydroxide) and positive (hydrogen, deuterium, tritium, metals) ions, preventing the build-up of excess charge of either sign on aerosol particles by diffusion.

Field charging is charging by unipolar ions in the presence of a strong electric field. The presence of the strong electric field directs ions along the field lines into particles, especially particles with high dielectric constants, like water. As in the case of diffusion charging, the presence of positive and negative gas ions prevents the accumulation of significant amounts of either charge on particles. Positively charged ions moving down the electric field lines will be mostly cancelled by negative charges moving up the electric field lines.

The fourth mechanism for particle charging is a build-up of charge on larger particles because beta particles emitted due to radioactive decay are more likely to escape from smaller particles. Clement has worked out detailed expressions for the net charging of particles due to this mechanism and charged gas ions⁵. While it should be possible to apply his expressions, the results will depend on aerosol particle composition because the rate of electron or positron emission will depend on the isotopes present in the aerosol particles. Even if the particles do charge by this mechanism, the bipolar gas ions caused by air or steam and high electric fields will severely limit the amount of charge that can build up on an aerosol particle.

The brief survey of the four classes of particle charging mechanisms just given leads to the conclusion that there are a number of ways the aerosol particles can acquire charge in tokamaks.

However, there is also a strong negative feed-back mechanism when both positive and negative ions are present in the gas. Particles that are initially charged will attract oppositely charged ions and repel like-charged ions. Calculations discussed in Hinds' section 15.7 show that the average particle charge is typically less than eight electrons for particles 10 μm in diameter or less. In the absence of measurements with ITER-relevant particles in ITER-relevant environments, the expressions given by Hinds are recommended for use in calculations to scope the possible effects of particle charging on agglomeration and deposition.

Most of this section has dealt with electrostatic charging effects because Coulomb effects dominate magnetic effects when particles have macroscopic charges. In the absence of these charges, the dominant electromagnetic effect on aerosol particles may be the interaction of ferromagnetic dipole moments of iron oxide or iron-rich particles. If ferromagnetism is present in aerosol particles, it should be easily observable and it will enhance agglomeration to large particle sizes. We recommend modeling the effect of particle magnetic dipoles on aerosol only if ferromagnetic particles are observed in tokamaks.

Particle Agglomeration

The effect of Coulomb forces on particle agglomeration is discussed by Friedlander¹⁰ Sections 7.4 and 7.6 who finds that the presence of a charge distribution on particles modified the agglomeration coefficient due to Brownian motion (This coefficient is Equation (1) of Appendix A.) by causing the appearance of a denominator, W , in the expression. This denominator is given by the expression

$$W = \frac{1}{y} [\exp^y - 1] \quad (11)$$

where

$$y = \frac{2 q_i q_j}{\epsilon kT [d_i + d_j]}$$

and where

q_i	=	charge on the i th particle (coulomb)
ϵ	=	permittivity of gas (coulomb ² /(kg m ³ s ²))
k	=	Boltzmann's constant, 1.38×10^{-23} J/(s m ² K ⁴).

Implementation of this result for the general case will be complicated by the need to deal with the two dimensional distribution over particle size and charge. Before this is attempted in a large code like MELCOR we recommend that a sensitivity study be conducted with either simplified analytical calculations or a smaller stand-alone aerosol behavior code and a series of charge distributions based on Table 15.7 of Hinds.⁹

Derivation of the agglomeration coefficient due to magnetic dipole moments will require a slight generalization of the results of Friedlander for Coulomb (potential proportional to $1/r$) and van der Waals forces (potential proportional to $1/r^6$) to dipole-dipole interactions (potential

proportional to $1/r^3$).

Particle Deposition

Gravity. In the discussion of Appendix A, it is mentioned that the expression for the terminal particle settling speed in the Stokes region, Equation (9), might require modifications for application to the non-Stokes region and/or for application to a stirred volume. One way to modify the particle speed to account for the non-Stokes region is to use the function SETTLE from either the PULSE³ or TRAP MELT⁶ computer code. This function interpolates Table 5 from Fuchs⁷ to return the particle Reynolds number (which is proportional to the settling velocity). If the fluid in a volume is well mixed, the simple motion of particles toward the bottom of the volume that is characteristic of tranquil settling is replaced by a fractional removal of the particles that can be visualized by thinking of the entire homogeneous field of particles as shifting relative to the physical volume. In the tranquil process the rate of removal of particles is given by^{9 page 57}

$$J = \begin{cases} v_s n(0) & \text{for } t < \frac{h}{v_s} \\ 0 & \text{for } t \geq \frac{h}{v_s} \end{cases} \quad (12)$$

where

J = flux of particles striking a bottom surface normal to gravity (particles/(m² s))
 $n(0)$ = aerosol particle number density introduced into the volume at the start of the settling process (particles/m³).

In the well-mixed process, the rate of removal of particles by gravity is given by

$$J = -v_s n(t) \quad (13)$$

Models for situations between well-mixed and tranquil would require some means of treating the spacial dependence of the particle number concentration in the volume (e.g. smaller control volumes) and the mixing rate within the volume. These models may or may not be needed, depending on the fluid conditions found from thermal hydraulic analysis of hypothetical accidents.

Centripetal Inertial Deposition. If fluids move in curved paths, aerosol particles must be acted on by a force in the radial direction to move with the fluid. From elementary physics, a circular path requires a force equal to the particle mass times the tangential velocity squared divided by the radius of curvature,

$$F_{centrip} = -m_p \frac{v_{fluid}^2}{r_{bend}} \hat{r} \quad (14)$$

The centripetal force must be provided by a drag force which, in turn, must be provided by particle

motion toward the outside of the bend

$$F_D = \frac{V_{radial}}{B} = m_p \frac{V_{fluid}^2}{r_{bend}} = F_{centrip} \quad (15)$$

where

B = the particle mobility.

Solving for the radial velocity yields

$$V_{radial} = B m_p \frac{V_{fluid}^2}{r_{bend}} \quad (16)$$

This radial velocity corresponds to the terminal settling speed obtained when the force acting on the particle is gravity. In fact, if the expression for the particle mobility is substituted into Equation (16), the expression that results for the radial velocity is the expression for the terminal settling speed, Equation (9), with the acceleration of gravity replaced by the centripetal acceleration

$$V_{radial} = \frac{d_p^2 \rho_p \left[\frac{V_{fluid}^2}{r_{bend}} \right] C_m}{18 \mu \chi} \quad (17)$$

Diffusiophoresis. According to Horst (Reference 8), the form of Equation (12) of Appendix A for particles in a gas with a condensing vapor and a noncondensing component is

$$V_{diffus} = \left[\frac{\gamma_v \sqrt{M_v}}{\gamma_v \sqrt{M_v} + \gamma_n \sqrt{M_n}} \right] \left[\frac{J_v}{\rho_v} \right] \quad (18)$$

where

- V_{diffus} = the deposition speed, the flux of particles to the surface divided by particle concentration (m/s)
- M_v = kg-mole mass of the condensing vapor (kg / kg-mole)
- M_n = kg-mole mass of the noncondensing vapor (kg / kg-mole)
- J_v = mass flux of vapor condensing on the surface on which the aerosol particle is being deposited (kg/s). The mass rate should be negative for evaporation from the surface.
- ρ_v = density of vapor in the gas mixture (kg/m³)
- γ_v = mole fraction of the condensing vapor in the gas phase

$$\gamma_n = \begin{matrix} \text{mole fraction of the noncondensing part of the gas phase,} \\ 1 - \gamma_v \end{matrix}$$

The equation shows that the particle is carried in the direction of the vapor flux but at some fraction of the velocity of the vapor molecules*. Equation (18) is derived for the free molecule (gas molecule mean free path much less than the particle diameter) regime. For later comparison to results in the continuum (gas molecule mean free path much less than the particle diameter) regime, Horst expresses the deposition speed as a function of the gradient of the mole fraction of the condensing species,

$$v_{diffus} = - \left[\frac{\gamma_v \sqrt{M_v}}{\gamma_v \sqrt{M_v} + \gamma_n \sqrt{M_n}} \right] \frac{1}{\gamma_n} D_{v,n} \nabla \gamma_v \quad (19)$$

where

$D_{v,n}$ = diffusivity of the vapor in the vapor/noncondensable mixture (m^2/s)

From Equation (19), it is apparent that the particle deposition velocity is independent of particle size in the free molecule regime.

For the continuum regime, two expressions for the velocity of a particle are given in Horst's review⁸. One is

$$v_{diffus} = - \left[1 + \sigma_{v,n} \gamma_n \right] \frac{D_{v,n}}{\gamma_n} \nabla \gamma_v \quad (20)$$

where the "diffusion slip factor," $\sigma_{v,n}$ was fit to data with the expression

$$\sigma_{v,n} = 0.95 \left[\frac{M_v - M_n}{M_v + M_n} \right] - 1.05 \left[\frac{d_v - d_n}{d_v + d_n} \right] \quad (21)$$

where

d_v = diameter of the condensing vapor gas molecule (m)
 d_n = diameter of the noncondensing vapor gas molecule (m)

The competing expression for the particle deposition velocity in the continuum regime is

$$v_{diffus} = - \frac{\rho_v}{\rho} \frac{D_{v,n}}{\gamma_v} \nabla \gamma_v \quad (22)$$

* The velocity of the vapor molecules is the flux of the vapor divided by the density of the vapor.

where

$$\begin{aligned}\rho_v &= \text{mass density of the condensing vapor (kg / m}^3\text{)} \\ \rho &= \text{mass density of the gas (kg / m}^3\text{)}.\end{aligned}$$

Electric Field Effects on Charged Particles. The fundamental expressions for deposition of a charged particle due to an electric field are like those for gravity but the force of gravity, i.e. the particle mass times the acceleration of gravity, is replaced by the electric force, i.e. the particle charge times the electric field. Obtaining a solution for the motion of the particle requires knowledge of the spacial variation of the electric field and thus can not be easily implemented in general. We recommend that implementation of general models for particle deposition due to electric fields be preceded by sensitivity studies with typical electric fields and particle charge distributions.

Magnetic Field Effects on Charged Particles. If the magnetic field remains on during an event, charged particles will experience forces perpendicular to their velocity and the magnetic field. This will tend to delay deposition because the magnetic force will tend to cause the particle to orbit around the magnetic field lines. While it is easy to write the equations of motion for a charged particle in a magnetic field and the spacial variation of the magnetic field is known, obtaining a solution for the motion of the particle requires knowledge of the motion of the particle due to fluid flow and thus can not be easily implemented in general. We recommend that implementation of general models for particle deposition due to magnetic fields be preceded by sensitivity studies with typical magnetic fields, particle charge distributions, and fluid velocity fields to determine the importance of this effect before trying to implement general models in a large code like MELCOR.

Precipitators. For a properly-designed laminar-flow precipitator, 100% of the particles in the aerosol are deposited.^{9 pp.305-309} If (as is usually the case) the flow in the precipitators is turbulent, the collection efficiency of the device is given by the Deutsch-Anderson Equation,

$$Eff = 1 - \exp\left(-\frac{v_{TE} A_c}{Q}\right) \quad (23)$$

where

$$\begin{aligned}Eff &= \text{efficiency of the precipitator, that is the fraction of the} \\ &\quad \text{particles entering the device that are removed} \\ v_{TE} &= \text{deposition velocity due to electrostatic fields (m/s)} \\ A_c &= \text{area of the collection surface in the precipitator} \\ Q &= \text{volume flow rate through the precipitator.}\end{aligned}$$

The electrostatic field deposition velocity is derived using an analysis very similar to the analysis for gravitational deposition but with the gravitational field replaced by the electrical field^{9 p. 288}. However, the fact that the typical electrical force is much larger than the force of gravity on a particle means that the electro-static analysis will probably be required to include non-stokes behavior.

Diffusion to Surfaces. Equation (10) of Appendix A results from using the Stokes-Einstein expression for the coefficient of diffusion^{10 pp. 24-31} with the assumption that the deposition of particles is driven by diffusion from a region of full particle concentration outside the boundary

layer to zero concentration at the surface. If it turns out to be necessary, basic diffusion theory could be generalized to particles and applied to yield results for particle deposition that would be as defensible as the analogous heat and vapor transport results. The development of an improved expression to replace Equation (10) is necessary only if diffusion is an important mechanism for particle deposition and this is usually the case only for very small particles, those 0.3 μm or less in diameter. In the event that diffusion does turn out to be a key deposition mechanism, it will probably be possible to adopt analyses like those of Epstein and Hauser¹¹ or Wood¹².

Isotopic Exchange Between Elemental Gas and Water Vapor or Condensed Water

A model for isotopic exchange between elemental gas and water vapor is to be determined. A paper published recently by J. M. Simonson¹³ may be helpful.

Dynamics (Numerical Solution Methods)

One common cause of difficulties in obtaining a solution to the aerosol behavior equations is the very stiff nature of the equations for the increase or decrease of particle size when vapors are evaporating from or condensing onto particles. Even with the removal of the Courant-like limit by allowing particles to change by more than one size class in a time step, large particle surface areas often make rates of vapor-to-particle mass transport very fast compared to rates of mechanisms like chemisorption on walls. Time constants on the order of 1 μs for the particle condensation/evaporation compared to minutes for the other aerosol time constants are common. One simple but effective approach to modeling this process is to use a non-linear sequence of time steps, beginning with a very short time span when the supersaturation or subsaturation is large and increasing the step as the vapor pressure of the species being transported approaches saturation and the process slows.

This approach has been implemented with considerable improvement of running times in the PULSE code by determining the time step size without considering particle size changes and determining the shortest time in which any particle will change size by one size class. The ratio of these two numbers (rounded up) is the number of equal-duration time steps imposed by particle size changes, NS. If NS is greater than ten, ten or less of the smaller time steps are used. If more than ten would be needed, the long step is divided into smaller time intervals with lengths in the ratio 1 : 2 : 3 : 4 : 10 : 30 : 50 : 100 : 300 : 500 : 1000 : 3000 : 5000 : ∞ so that

$$NSV = 1 + 3 \log_{10} (NS) \quad (24)$$

instead of NS steps are needed.

Decay Heat (Fusion Product Behavior Models)

Models for fusion product decay heat are to be determined.

Materials Properties

In addition to the need to develop a separate module for materials properties discussed in the section about aerosol modeling capabilities in CONTAIN, there is a need to develop the capability to extend the capability of the code to consider bulk fluids other than air. Many of the needed subroutines for mixtures of up to ten gases were developed as part of the MATPRO package¹⁴ and need "only" be implemented.

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