

Current status of MELCOR 2.2 for fusion safety analyses

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Abstract

MELCOR is an integral code developed by Sandia National Laboratories (SNL) for the US Nuclear Regulatory Commission (USNRC) to perform severe accident analyses of Light Water Reactors (LWR). More recently, MELCOR capabilities are being extended also to analyze non-LWR fission technologies. Within the European MELCOR User Group (EMUG), organized in the framework of USNRC Cooperative Severe Accident Research Program (CSARP), an activity on the evaluation of the applicability of MELCOR 2.2 for fusion safety analyses has been launched and it has been coordinated by ENEA. The aim of the activity was to identify the physical models to be possibly implemented in MELCOR 2.2 necessary for fusion safety analyses, and to check if those models are already available in MELCOR 1.8.6 for fusion version, developed by Idaho National Laboratory (INL). From this activity, a list of modeling needs emerged from the safety analyses of fusion-related installations have been identified and described. Then, the importance of the various needs, intended as the priority for model implementation in the MELCOR 2.2 code, has been evaluated according to the technical expert judgement of the authors. In the present paper, the identified modeling needs are discussed. The ultimate goal would be to propose to have a single integrated MELCOR 2.2 code release capable to cover both fission and fusion applications.

Keywords: MELCOR; Fusion reactor safety; advanced reactor safety.

Abbreviations

ACP	Activated Corrosion Product
BB	Breeding Blanket
CSARP	Cooperative Severe Accident Research Program
CF	Control Function
CVH	Control Volume Hydrodynamic
DCLL	Dual Coolant Lithium Lead
DTT	Divertor Tokamak Test
EDF	External Data Files
EMUG	European MELCOR User Group
EOS	Equation of State
FLIBE	LIF+BeF ₂ molten salt
HCLL	Helium-Cooled Lithium Lead
HCPB	Helium-Cooled Pebble Bed
HITEC	KNO ₃ + NaNO ₂ + NaNO ₃ molten salt
HTC	Heat Transfer Coefficient
IFMIF-DONES Source	International Fusion Material Irradiation Facility-DEMO-Oriented NEutron
IHTS	Intermediate Heat Transport System
INL	Idaho National Laboratory
ITER	International Thermonuclear Experimental Reactor
LOCA	Loss of Coolant Accident
LOVA	Loss of Vacuum Accident
MDH	Magnetohydrodynamic
MELCOR	Methods of Estimation of Leakages and Consequences of Releases
NCG	Non-Condensable Gas
PFC	Plasma Facing Components
SNAP	Symbolic Nuclear Analysis Package
SNL	Sandia National Laboratories
TMAP	Tritium Migration Analysis Program
USNRC	United States Nuclear Regulatory Commission
VV	Vacuum Vessel
VVPSS	Vacuum Vessel Pressure Suppressor System
WCLL	Water-Cooled Lead Lithium

1 Introduction

Several organizations worldwide are conducting research on the safety of nuclear fusion installations. MELCOR fusion version is being adopted as one of the reference codes to carry out deterministic safety analyses of fusion installations and related facilities.

Initially, MELCOR was developed by Sandia National Laboratories (SNL) for the United States Nuclear Regulatory Commission (USNRC) for the safety analyses of Light Water Reactors (LWR) [1]. MELCOR is a fully integrated code able to simulate the thermal-hydraulic phenomena in steady-state and incidental/accidental conditions, as well as core degradation and aerosol/vapor transport up to the outer environment during severe accident. MELCOR capabilities have been extended, for the past two decades by SNL, to analyze non-LWR fission technologies. The newest current available version is MELCOR 2.2.

The Idaho National Laboratories (INL) made fusion reactor specific modifications to MELCOR 1.8.2 (developed and validated through pedigree analysis for the use in International Thermonuclear Experimental Reactor (ITER) Safety Preliminary Report) and then introduced these modifications into MELCOR 1.8.6 [2],[3]. Currently, MELCOR fusion is adopted for the safety analyses of fusion reactors and fusion-related facilities, such as ITER [4], DEMO [5],[6] and, more recently, the IFMIF-DONES (International Fusion Material Irradiation Facility-DEMO-Oriented Neutron Source) accelerator neutron source [7]-[10], and it will be adopted for the Divertor Tokamak Test (DTT) facility [11].

The development of a common MELCOR version release, that also includes models for fusion safety analyses, would allow to use all the state-of-art features implemented in the code and the capabilities of SNAP (Symbolic Nuclear Analysis Package) [12] for the development of input-decks, post processing of the data, and uncertainty analysis. However, the current released version of the code, MELCOR 2.2, still has not yet implemented some models needed to carry out analyses of some specific phenomena occurring in fusion facilities.

At the European MELCOR User Group (EMUG), held in 2018 in Zagreb (Croatia), organized in the framework of USNRC Cooperative Severe Accident Research Program (CSARP), a session was dedicated to “GEN IV and Fusion Applications”. Afterwards, an activity has been launched and it has been coordinated by ENEA to identify the models necessary for fusion safety analyses possibly to be implemented in MELCOR 2.2, based on the feedback provided by several MELCOR users.

The present paper describes the code modeling needs to address fusion safety issues, ranking their priority for implementation according to the technical background and priorities of the participant organizations involved in fusion activities. In addition, it is described whether the models are already implemented in MELCOR 1.8.6 for fusion version [2], developed by INL, or if the physical phenomena of interest can be simulated through specific methodologies.

It should be underlined that experimental data are required to formulate models and validate the computational tools. The availability of adequate experimental data (and the related scaling issue [13][14]) or the need for new experiments is not addressed in the present paper. This contribution is intended as a first step toward the identification and ranking of the modeling needs for fusion applications, while the availability of data and the needs for new experiments should be furtherly investigated in other works.

2 Modelling needs to address fusion facilities safety issues

The models identified to be implemented in MELCOR 2.2 for addressing fusion safety issues are listed in Table 1. In the table, the priority for model implementation from 1 (low) to 3 (high) has been assigned according to the technical expert judgement of the authors. The following subsections provide additional details regarding each code modeling need, including their present availability in the fusion version of MELCOR code.

Table 1 List of identified code modeling needs

N°	Code modeling needs	Priority
1	Inclusion of additional working fluids with multiphase capabilities	3
2	Implementation of the possibility to use different fluids simultaneously in the same code input	3
3	Introduction of models for chemical reactions of selected working fluids	2
4	Introduction of model for steam oxidation of the PFC	2
5	Introduction of model for air oxidation of the PFC	2
6	Extension of MAEROS models for aerosols deposition with different carrying gases and mixtures	2
7	Implementation of model for aerosols resuspension	2
8	Extension of the aerosols deposition and resuspension modelling to consider remnant magnetization effects	1
9	Introduction of models for aerosols transport in multifluid (multi-working fluid) simulation	2
10	Implementation of specific heat transfer correlations for simulating Helium and other working fluids in the geometry of interest	2
11	Standard Scrubber model in FL Package for Helium	1
12	Inclusion of dissolved Non Condensable Gas (NCG) species within working fluids	2
13	Implementation of magnetic pump modelling and features (e.g. coast-down, etc.)	1
14	Inclusion of Magnetohydrodynamics (MHD) effects on heat transfer correlations and pressure drop evaluation	1
15	Extension of the water properties below the triple point	2
16	Implementation of model for air condensation onto cryogenic structures	2
17	Implementation of model for Helium condensation onto cryogenic structures	2
18	Inclusion of the possibility to work with low temperature operations (>3K) and cryogen working fluids	2
19	Extension of material physical properties to cryogenic range	3

2.1 Modeling need N. 1: Inclusion of additional working fluids with multiphase capabilities

In magnetic fusion technology, several materials can be used: the molten salt FLIBE (Li_2BeF_4) [15], metallic lithium, LiPb, solid ceramic lithium compound, etc. Different Breeding Blanket (BB) concepts adopting various materials as coolant and breeder are under discussion (e.g. $\text{H}_2\text{O}/\text{LiPb}$ [16], He/LiPb [17] in case of DEMO design, etc.). Molten salts [18] with lower melting point, e.g. HITEC and Solar salt, are also used as Intermediate Heat Transport Circuit (IHTS) fluid.

In order to analyze the complexity of the thermohydraulic behavior of fusion facilities during their normal operation and accident conditions, the use of different multiphase fluids should be implemented in the code. For example, in the cryostat of the ITER facility there are two different fluids (Helium and Nitrogen) that work as coolants. In particular, this system is composed by three liquid Helium refrigerators that operate in parallel to supply Helium and provide the required cooling power for coils and magnets. Likewise, an air separator produces liquid Nitrogen (LN_2) for the liquid Helium refrigerators [19].

It should be underlined that, to update the library of working fluids, it would be necessary to:

- extend the Equation Of State's (EOS) pressure field to low pressures (<300 Pa);
- include the possibility for users to add libraries for other fluids.

Examples of additional working fluids with multiphase capabilities which could be useful for fusion safety analysis are:

- Air,
- Lithium,
- LiPb,
- FLIBE (LiF+BeF₂) breeder material,
- Helium,
- KNO₃ + NaNO₂ + NaNO₃ molten salt (HITEC),
- Solar salt intermediate circuit fluid, heat storage.

Table 2 shows the priority for code implementation of different working fluids according to the technical expert judgement of the authors.

Table 2 Priority for code implementation for different fluids

Fluid	Priority
FLIBE	1
Air	2
Helium	3
HITEC	3
Lithium	3
LiPb	3
Solar salt	3

Some additional working fluids are already implemented in MELCOR fusion, in particular:

- MELCOR 1.8.2 allows Helium and air as a working fluid [20];
- MELCOR 1.8.5 allows Helium, Hydrogen, FLiBe, Lithium, Nitrogen, LiPb, etc. [21];
- MELCOR 1.8.6 allows Helium, LiPb [22] and, being a development of MELCOR 1.8.5, it allows also Hydrogen, FLiBe, Lithium, Nitrogen.

2.2 Modeling need N. 2: Implementation of the possibility to use different fluids simultaneously in the same code input

Implementation of the possibility to use different fluids in different circuits simultaneously during the same code calculation, such as:

- Lithium/H₂O,
- PbLi/H₂O,
- PbLi/He,
- He/H₂O,
- CO₂/FLiNaK,
- FLiBe/FLiNaK,
- Pb/H₂O.

Some of the above mentioned working fluids have been already implemented in MELCOR1.8.6 for fusion, e.g. H₂O, LiPb, He, etc.; however, only one working fluid can be considered in a single input deck. It is important to adopt fusion relevant working fluids in MELCOR 2.2 for performing

safety analyses of fusion installations and reproduce the fluid behavior and possibly interactions in mixture, especially in accident scenarios. In case of failure of the first wall or structural material in the breeding zone of the BB or divertor PFC, exothermic reaction may occur if the coolant (e.g. water) gets in contact with the PFC (e.g. tungsten/beryllium), breeding material (e.g. Lithium/LiPb) or neutron multiplier material (e.g. LiPb/beryllium). The reaction type will depend on the selected BB and divertor concepts.

Codes like TRACE [23] and RELAP5-3D [24] integrate the possibility of modelling circuits running with different fluids in separate systems of a common input deck. This code capability is useful, for example, for safety analyses applied to different BB concepts for DEMO. This is also important considering its possible application to the IHTS with molten salt as working fluid.

A methodology, suggested by INL in [25] with MELCOR 1.8.6 for fusion, to overcome this code limitation in MELCOR 1.8.6 for fusion consists of defining two different inputs (one for each different working fluids) and parallelizing [26] the calculations (to simulate, for example, blowdowns).

The coupling of the two working fluids is implemented in MELCOR 1.8.6 for fusion by means of an external script. This script shares some relevant information at the same time step with the two input decks. An exercise, using this methodology, was performed by the Sapienza University of Rome [27] to analyze an in-box LOCA of the WCLL blanket concept. Two different input decks were created: the first one to simulate a water circuit and the second one to simulate the LiPb system (Figure 1). In addition to MELCOR inputs, a Python script was developed with the aim of coupling the two simulations and obtain more reliable data. Even adopting this procedure for the analysis, intrinsic code limitations of MELCOR multicomponent capabilities remain since several simplifications have been made to be able to perform the simulation.

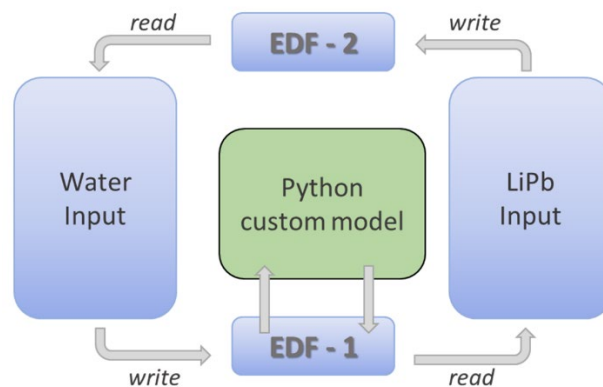


Figure 1 Scheme of the Python script [27]

2.3 Modeling need N. 3: Introduction of models for chemical reactions of selected working fluids

In a safety analysis involving BB or other experimental installations, it is important to model chemical reactions between working fluids, such as those between Lithium (and/or LiPb) with water, air and concrete [29][30].

Chemical reactions e.g. involving lithium and water can also generate H₂ and other gases/aerosols (e.g. NH₃, LiOH). For example, in the case of the Vacuum Vessel (VV) LOCA involving water and LiPb some oxidations, Hydrogen and other gases/aerosols production can occur. The physical hazard due to the energy and hydrogen release from exothermic reactions with consequent possible overpressure, deflagration or explosion events could also be worsened by the potential mobilization and release of an important population of toxic and corrosive aerosols. Moreover, in fusion facilities like IFMIF-DONES, the radiological source term (represented by T, Be7 and activation products), initially retained by the flowing liquid lithium in closed loops or in dedicated traps, could be mobilized upon lithium fire conditions.

Few chemical reactions are implemented in MELCOR v1.8.6 for fusion, in particular a Lithium-air reaction model is implemented in the code to simulate the reactions of lithium with nitrogen and oxygen [28][29]. In addition, with the same version, it is possible to simulate specific Lithium reaction products, i.e. Li_2O , Li_3N , through the standard MELCOR RN Package as two independent aerosol classes. A model for the Lithium – H_2O reaction has not been implemented in the code yet [31].

2.4 *Modeling need N. 4: Introduction of model for steam oxidation of the PFC*

Modeling of steam oxidation of the PFC following a blowdown transients. The consequences of the contact vary from material to material: e.g. Beryllium produces a strongly exothermic reaction, Tungsten a soft exothermic reaction, and Carbon an endothermic reaction.

A LOCA transient in the VV will generate hydrogen, and if a simultaneous Loss of Vacuum Accident (LOVA) occurs, there will be risk of a hydrogen explosion due to presence of oxygen in the vessel atmosphere. This could lead to the mobilization of radioactive dust and release of tritium and Activated Corrosion Products (ACPs).

A possible approach to simulate this phenomenon is to create a source term of Hydrogen and a sink term of steam in the Control Volume Hydrodynamic node (CVH) that encompasses the PFC heat structure. The hydrogen production reaction rate constant can be calculated through Control Functions (CF) and the temperature of the heat structure component. The amount of oxide generated and the Hydrogen source will depend on a CF; it will be correlated on the reaction rate constant, and the already reacted mass.

In MELCOR v1.8.2 and 1.8.6 for fusion it is possible to model the oxidation of PFC material in presence of steam [21].

2.5 *Modeling need N. 5: Introduction of model for air oxidation of the PFC*

Due to a LOVA, air can enter in the VV and can interact with PFC materials as Beryllium, Tungsten and Carbon. This determines material oxidation and energy production. As mentioned in subsection 2.4, this phenomenon could be involved in the release of radioactive material in the outer environment.

A possible approach to simulate this phenomenon is the same presented for modeling need N. 4.

In MELCOR v1.8.2 and 1.8.6 fusion adapted it is possible to model the oxidation of PFC material in presence of air [32].

2.6 *Modeling need N. 6: Extension of MAEROS models for aerosols deposition with different carrying gases and mixtures*

This is relevant for safety because it can influence the release of radioactive products.

Improvements were done in MELCOR fusion (v1.8.2) on aerosol deposition model by adding different carrier gases (e.g., air, steam, helium, gas mixtures, etc.) [20].

2.7 *Modeling need N. 7: Implementation of model for aerosols resuspension*

The erosion of the PFC components generates dust that can be mobilized again due to resuspension during the transient progression of an accident scenario (LOCA and LOVA).

This is relevant for safety because it can influence the release of radioactive products. The model should be validated against similar conditions expected in fusion facilities. Specific models should be developed to provide a better reproduction of resuspension phenomena occurring at low pressure (order of few kPa) and at higher pressure (order of >100 kPa).

Improvements were done in MELCOR fusion (v1.8.5) on aerosol deposition modelling [33]. Two models have been implemented:

- Vainshtein resuspension model;
- Reeks and Hall → Rock 'n Roll resuspension model.

MELCOR 2.2 already implements resuspension models [34] (they call the phenomenon “lift-off” instead of “resuspension”), but the suitability of the available models has to be tested. An attempt to introduce a resuspension model in MELCOR 1.8.6 using CFs was also done in the past showing promising results [35].

2.8 Modeling need N. 8: Extension of the aerosols deposition and resuspension modelling to consider remnant magnetization effects

The structural materials and the dust generated through the erosion of the PFC components might have a remnant magnetization after sitting in a magnetic field for some time. This phenomenon should be taken into account for deposition and resuspension.

Currently, no model is implemented in MELCOR fusion to cover this issue.

2.9 Modeling need N. 9: Introduction of models for aerosols transport in multifluid (multi-working fluid) simulation

In a transient progression involving BB technologies, it is important to model aerosol transport in different working fluids. For example, in the case of the VV LOCA involving water and LiPb, resuspension of dust and lithium-lead vapors and droplets can occur. This is relevant for safety because it can determine the release of radioactive products.

MELCOR 2.2 shall model these phenomena depending on the thermal-hydraulics boundary conditions simulated during the scenario in order to cover the transport of the dust and ACPs in presence of more than one working fluid.

Currently no model is implemented in MELCOR fusion to address this issue.

2.10 Modeling need N. 10: Implementation of specific heat transfer correlations for simulating Helium and other working fluids in the geometry of interest

Since Dittus-Boelter correlation applied in MELCOR for forced convection cannot be accurate enough in some conditions and geometry, other correlations (e.g. Gnielinski correlation [24][36]), can be implemented in the code to improve the accuracy of the calculated results. However, the applicability of such correlations outside the standard pressure range (e.g. below the atmosphere pressure) has to be verified. In order to obviate the problem, the users should have the possibility to modify certain correlations through sensitivity coefficients as allowed in other codes, e.g. in [37].

An approach to overcome the missing correlation would be to determine the Heat Transfer Coefficient (HTC) of a heat structure with CF based on properties such as temperature, density, viscosity, characteristic length, etc., which define specific non-dimensional numbers.

It is necessary to extend the correlations for HTC in MELCOR fusion due to different flow behavior in normal operation and accident case with different coolant.

2.11 Modeling need N. 11: Standard Scrubber model in FL Package for Helium

Pool scrubbing has been already developed for simulating steam/water containing aerosol. The model is present in MELCOR 1.8.6 for Fusion [38] (FL package → FLnnn02 – Flow path junction switches IBUBF= 1). Such model could be used for simulating the wash phenomenon of the activated product and tritium combination with water inside the suppression pool into the Vacuum Vessel Pressure Suppressor System (VVPSS). It would be interesting to benchmark its accuracy if Helium is used.

2.12 Modeling need N. 12: Inclusion of dissolved Non Condensable Gas (NCG) species within working fluids

Tritium is a relevant radioisotope and exists in a dissolved state within many working fluids (e.g. LiPb) and cannot be represented by a NCG or aerosol, as the gas can be transported within a working

fluid and later released without transport of a NCG species. For example, a release of liquid LiPb (only) would not automatically lead to a release of tritium in current models.

MELCOR fusion is being further developed to be coupled with the Tritium Migration Analysis Program (TMAP) code [39]. TMAP was developed to dynamically analyse the transport of hydrogen species (e.g. H₂, D₂, T₂, DT, HT) through structures, between structures and adjoining enclosures, and among enclosures. MELCOR-TMAP can also use multiple working fluids such as H₂O, PbLi, Sn, SbLi, FLiBe, Li, Na, cryogenic He, N₂ and O₂. Due to some open issues the code is not yet ready for release [40].

2.13 Modeling need N. 13: Implementation of magnetic pump modelling (for design) and features (e.g. coast-down, etc.)

As magnetic pumps are often used in fusion facilities, numerical models which take into account related effects (e.g. coast-down), can help to properly simulate and investigate transients in such design, and possibly improve the accuracy of the results and decrease related uncertainties.

Currently no models are implemented in MELCOR fusion to address this need.

2.14 Modeling need N. 14: Inclusion of Magnetohydrodynamics (MHD) effects on heat transfer correlations and pressure drop evaluation

Magnetic fields are captured in the Hartmann number of a fluid and can significantly affect heat transfer processes and pressure drop.

Currently no models are implemented in MELCOR fusion to cover this issue.

2.15 Modeling need N. 15: Extension of the water properties below the triple point

Simulation of cryogenic temperatures could be useful for safety analysis considering specific phenomena such as the water freezing in the cryostat of a fusion reactor during an accident scenario (e.g., LOCA). Specific modifications are present in MELCOR fusion (v1.8.2) covering three areas: EOS, transport properties, and ice film buildup on heat structure [20]. A freezing film model is also available in MELCOR fusion (v1.8.2) [20][28].

2.16 Modeling need N. 16: Implementation of model for air condensation onto cryogenic structures

Air entering into the cryostat during an accident progression (e.g., LOVA) may condense and freeze. Cryogenic temperature implementation could be useful for cryostat safety analysis considering the air condensation in the cryostat.

Some modifications to the air condensation model are present in MELCOR fusion (v1.8.2) [21][41]. This model is no longer available in more recent versions of MELCOR fusion, i.e. v1.8.5, v1.8.6.

2.17 Modeling need N. 17: Implementation of model for Helium condensation onto cryogenic structures

This is an important modelling need which allows simulating a LOCA transient in a helium superconductor cooling circuit.

The model is implemented in MELCOR fusion (v 1.8.2) [20].

2.18 Modeling need N. 18: Inclusion of the possibility to work with low temperature operations (>3K) and cryogen working fluids

Magnet systems present overpressure risks due to superconductor quench events, leading to rapid boiling of helium or nitrogen cryogen. Cryostat safety can be compromised by massive helium or nitrogen ingress during a quench event.

The model is implemented in MELCOR fusion (v 1.8.6).

2.19 Modeling need N. 19: Extension of material physical properties to cryogenic range

Since MELCOR for fusion handles cryogenic cooling, it is necessary to extend the range of material properties of the cryogenic fluids and the construction materials accordingly.

The model is partially implemented in MELCOR fusion (v 1.8.5).

3 Conclusions

Several organizations worldwide are actively involved in the research on safety analysis of nuclear fusion installations. In addition, several activities are in progress to design new experimental facilities, such as IFMIF-DONES in Spain and DTT in Italy. In the present paper, the main models to be implemented in MELCOR 2.2 to address fusion safety issues have been identified and ranked according to the technical expert judgement of several MELCOR users. The required models have been described, and their current implementation status in MELCOR fusion version has been highlighted.

In particular, the implementation of additional different working fluids and the possibility to use different fluids in different circuits should be further developed to perform more consistent safety analyses of fusion installations. In fact, the design of these plants is based on the use of different BB concepts using different materials for the breeder and coolant. Linked to that, the introduction of models for chemical reactions for different working fluids has been underlined. A refined modelling of steam oxidation and air oxidation of the PFCs is needed to study the risk of hydrogen explosion and material oxidation. The aerosol resuspension model to be implemented is highlighted considering also the possibility to introduce models for aerosols transport in multifluid. Implementation of specific heat transfer correlations for simulating new working fluids and the introduction of a standard scrubber model in FL for Helium could improve the accuracy of results. The possibility to implement NCG as working fluids could permit to develop further studies focused on Tritium transport. Implementation of magnetic pump modelling and MHD effects on heat transfer could be helpful.

Considering the cryogenic conditions present in fusion plants, the extension of water properties below the triple point could be useful to consider the water freezing phenomenon in the cryostat. In relation to the cryostat, the modeling of air and helium condensation in cryogenic structures should also be implemented in the code. Also related to the cryogenic conditions, allowance of low temperature operations, cryogenic working fluids and the extension of material properties to cryogenic range could permit to analyze transients scenarios involving magnet systems with possible overpressure due to superconductor quench events.

In conclusion, the development of a future common MELCOR version including fusion features is strongly recommended by the authors. This future version would allow to use all the state-of-art features already implemented in MELCOR 2.2 and would made the future code advances automatically available for the MELCOR fusion community. In addition, this would allow the use of SNAP by fusion users, which could be important to support the development of fusion safety analyses. This paper, based on the feedback of MELCOR code users in fusion application, represents a first contribution to identify the code modeling needs, which would be necessary to be implemented also in other deterministic codes (e.g. thermal-hydraulic system codes) to address specific fusion safety issues.

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