Development of Corium Property Library for Severe Accident Analysis

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1. Introduction

It is essential to accurately calculate the properties of corium for the interpretation of a highly reliable nuclear severe accident. Calculation of properties of materials depends on experiments. However, experiments in severe accident condition tend to rely on extrapolation due to a lack of data, which causes a large difference in properties according to the model.

During the development of the molten core-concrete interaction (MCCI) module in a project called 'Development of Computational modules for Risk-Significant Severe Accident Phenomena in Reactor Containment Building', we faced the problem of selecting appropriate corium property models.

To facilitate the calculation of corium properties, we implemented a corium property library based on the property models of the CORQUENCH code [1], which successfully simulates MCCI validation experiments such as CCI test.

2. Methodology

In this section the property models and the implemented library are described. The models are based on the CORQUENCH code, and the library is implemented using Excel automation module, 'xlwings'.

2.1 Corium properties

In the proposed library, properties are calculated through a weighted average for each constituent as shown in Table I.

When calculating corium density, the library uses solid and liquid density data from CORQUENCH. [1]

Liquidus and solidus temperatures are calculated for the oxidic phase and the metallic phase, respectively. In the case of oxidic phase, the properties are calculated using the phase diagram data of Roche et al. [2] and Lamberston and Mueller [3]. In the case of the metallic phase, the properties are calculated using Fe-Ni-Cr ternary phase diagram, assuming that the main component is stainless steel. [4] In the presence of other metallic constituents, the products of the properties and molar fraction of each constituent are added to the solidus (1) and liquidus (2) temperatures, where f_i is mole fraction of constituent i and $T_{sol,SS}, T_{liq,SS}$ are solidus and liquidus of stainless steel using Fe-Ni-Cr ternary phase diagram.

$$T_{sol,metal} = (f_{Fe} + f_{Cr} + f_{Ni})T_{sol,SS} + \sum_i f_i T_{sol,i} \quad (1)$$

$$T_{liq,metal} = (f_{Fe} + f_{Cr} + f_{Ni})T_{liq,SS} + \sum_i f_i T_{liq,i} \quad (2)$$

Effective thermal conductivity of corium is calculated using thermal conductivity of oxidic phase and metallic phase. Thermal conductivity of oxidic phase and metallic phase is calculated by volume weighting the thermal conductivity of each constituent. [1]

The effective viscosity of the corium is determined using the Ishii-Zuber model. [5] To calculate the effective viscosity, the viscosity calculation of each phase must precede. The viscosity of the metallic phase is determined using the De Andrada formula [6], and the viscosity of the oxidic phase is determined using the Shaw model. [7]

Corium specific heat is calculated by differentiating enthalpy, a function of temperature. Enthalpy is assumed to be in the form of a parabolic function for temperature in a solid state and a linear function for temperature in a liquid state. [1]

Corium surface tension is obtained by volume weighting the surface tension values of oxidic phase and metallic phase proposed by Kao and Kazimi [8], and corium emissivity is also obtained by volume weighting the emissivity values of oxidic phase [9] and metallic phase [10] in the same way.

Table I: Corium properties calculated in the library

Property	Weighting factor	Model
Density (kg/m^3)	Mass fraction	[1]
Liquidus/Solidus (K)	Mole fraction	[2], [3], [4]
Thermal conductivity (W/m·K)	Volume fraction	[1]
Viscosity (Pa ·s)	Mole fraction	[5], [6], [7]
Specific heat (J/kg·K)	Mole fraction	[1]
Surface tension (N/m)	Volume fraction	[8]
Emissivity	Volume fraction	[9], [10]

The library calculates the properties of the corium consisting of 22 constituents as shown in Table II, and the data of the corresponding constituents are embedded.

Table II: Corium constituents considered in the proposed library [1]

Index	Constituent	Index	Constituent
1	Na_2O	12	Ni
2	TiO_2	13	Zr
3	SiO_2	14	ZrO_2
4	CaO	15	B_2O_3
5	MgO	16	U
6	Al_2O_3	17	B_4C
7	FeO	18	Si
8	Fe_2O_3	19	SiC
9	Fe_3O_4	20	Cr_2O_3
10	Fe	21	NiO
11	Cr	22	UO_2

2.2 Corium property library

The library is based on the Excel automation module 'xlwings', which enables the interworking of Excel macros and Python. Previously, corium properties were calculated in a Python file while performing MCCI analysis, which has a limitation that corium properties can be calculated only during MCCI analysis. This library is a program that provides input to the Python file when the input is entered to the Excel sheet, and outputs the calculated properties to Excel.

This program takes the mass of each constituent of corium and the temperature of corium as inputs, and provides the following outputs: total mass of corium, solidus temperature, liquidus temperature, specific heat, density, thermal conductivity, emissivity, surface tension, viscosity, and specific enthalpy of corium.

3. Results

The program's execution screen is shown in Figure 1. After entering the input, clicking the 'Calculate!' button on the right will display the corium properties.

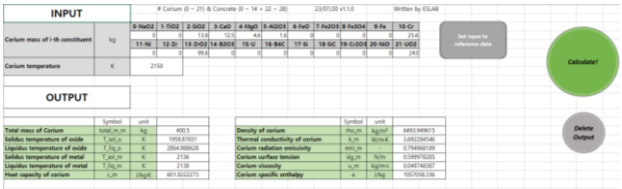

Fig 1. Corium property library program run screen

A plotting system, allowing the observation of changes in output values corresponding to variations in input values, is also integrated within the program, as shown in Fig 2. By selecting the input value for the x-axis and the output value for the y-axis, and defining the range of input values, the program provides a graph of output values for the range.

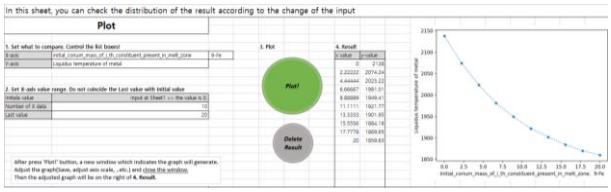

Fig 2. Corium property plotting system

The figures below show the change in property according to the change in the mass of one corium constituent. These results are based on the corium composition of the CCI-2 test [11], while keeping the remaining values same and varying only the mass of the constituent corresponding to the x-axis.

Fig 3 shows the corium viscosity according to the mass of Ni in the corium. An increase in mass of Ni leads to a decrease in corium viscosity. Fig 4 shows the liquidus temperature of the oxidic phase relative to the mass of Zr. As the mass of Zr increases, the oxidic liquidus temperature decreases and is consistent with the trend of Lamberston-Mueller phase diagram data. Fig 5 shows the solidus temperature of the metallic phase according to the mass of Ni.

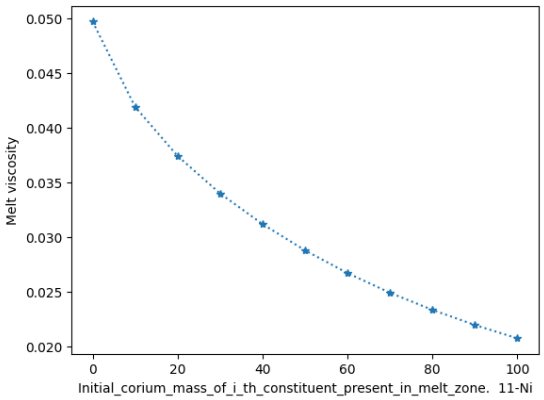

Fig 3. Corium viscosity according to Ni mass

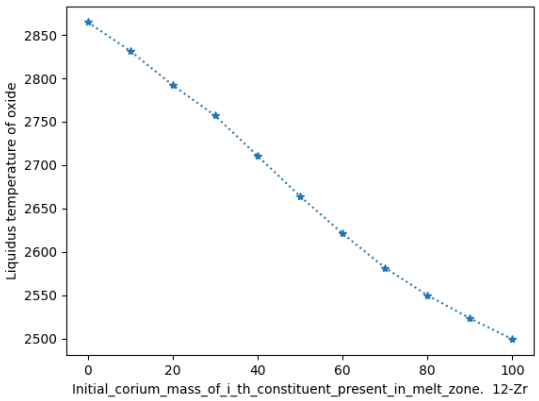

Fig 4. Corium liquidus temperature of oxidic phase according to Zr mass

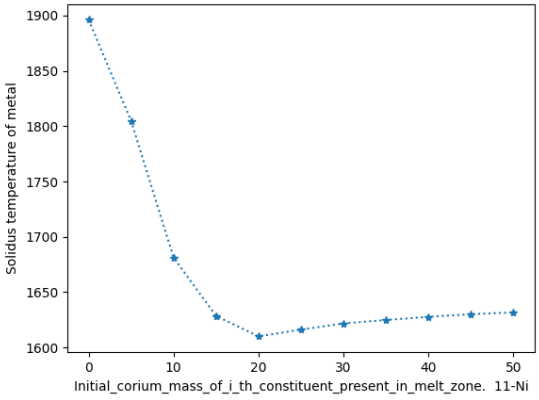

Fig 5. Corium solidus temperature of metallic phase according to Ni mass

4. Conclusions

In this paper, we developed a library that outputs properties when inputting the temperature of corium and the mass of each constituent. Using the proposed corium property library, easier access to the corium property in a high temperature condition is possible. In addition, when only one component is changed, the change trend of the property can be visualized. This helps to understand the effect of changes in composition on corium. The proposed library is expected to serve as a database that can be easily used in various analysis that require corium properties as well as MCCI analysis.

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