Seminar

Institute for Plasma Research

Title : A consistent approach for coupling lumped-parameter and phase-field models for in-vessel corium to thermodynamic databases

Speaker: Dr. Vaishnvi Tiwari
University of Paris-Saclay, France

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Abstract :

This Ph.D. thesis is focused on ensuring a thermodynamically consistent representation of in-vessel corium (a high temperature mixture of molten reactor core and structural materials, described as a U-O-Zr-steel system) in the coupled thermohydraulic-thermochemical models. These models are used for performing Severe Accident (SA) analysis of nuclear Light Water Reactors (LWRs).

Considering the nuclear core meltdown and the mitigation strategy consisting of retaining the molten materials (aka. corium) at the bottom of the Reactor Pressure Vessel, the knowledge of in-vessel corium behaviour and the associated risk of vessel failure are matters of prime interest. Corium represents a complex thermodynamic system whose behaviour is dependent on the associated thermo-chemical and thermo-hydraulic phenomena. Modelling the kinetics of such a complex multicomponent system requires coupling between the thermochemical models and the thermal/thermo-hydraulic models, which is closely related to the thermodynamic inputs. In this context, the use of a thermodynamic database obtained by the CALPHAD method seems relevant by providing closures and inputs to the thermohydraulic and thermochemical models respectively. These databases consist of models for Gibbs energy functions of the possible phases for a system that can be used to obtain the equilibrium thermodynamic description for the system as well as material thermodynamic properties for out-of-equilibrium conditions.

Through this work, a systematic approach for ensuring extensive utilization of CALPHAD data in the coupled models was developed, and the associated questions were answered for 'mock-up' macroscopic and mesoscopic models developed for describing some of the phenomena pertaining to in-vessel corium behavior.

As a first step, the feasibility of using CALPHAD data for the coupled thermochemical-thermohydraulic model developed using lumped-parameter approach was tested. Considering the ternary U-O-Zr system, the model describes 1-D plane front solidification process at the boundary of a molten corium pool. Such integral thermal models consist of mass and energy conservation equations that require inputs related to thermochemical properties of the materials, which are closely related to the thermodynamic state

variables. In particular, the closure of energy conservation equations requires enthalpy-temperature relations. Following the approach of keeping a general formulation of energy conservation equations in terms of specific enthalpies of the phases, CALPHAD based Gibbs energy functions were used for calculation of phase change temperature, the composition of the solid phase forming at the solidification interface, the closures to the energy conservation equations and to obtain functions associated with other thermodynamic properties. The feasibility of using CALPHAD based closures (in the form of enthalpy-temperature relations and local equilibrium conditions) for a consistent thermodynamic representation of the systems throughout the model was shown.

The second part of the work focused on the development of a general formulation for diffuse interface models under the phase-field approach, which can be used to simulate the kinetics of various thermochemical processes under non-isothermal conditions such as solidification and phase segregation. For this, a phase-field model was developed by adopting a rather general formulation in Grand Potential. This choice of using the grand potential is favourable in terms of performing numerical simulations as the bulk and interface properties can be adjusted independently. When it comes to treating the case of non-isothermal solidification, the incorporation of the energy equation is necessary. The thermodynamic closures to the developed model can be obtained from CALPHAD databases. The closures for this non-isothermal model were studied in details, in particular, the constraints associated with the use of CALPHAD data. Further, the effect of 'up-scaling' the interface thickness on the kinetics of the phase-field model was studied. In particular, the constraints related to the maximum choice of interface thickness, and consequently its impact on the choice of the phase-field mobility parameter were discussed and the numerical results were discussed for binary U-Zr and U-O systems under isothermal conditions.