Multi-physics approach for nuclear reactor analysis using thermal-hydraulics and neutron kinetics coupling methodology

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Abstract: In this paper, a realistic thermal-hydraulics of nuclear reactor was visualized by adopting multi-physics approach. Multi-dimensional thermal-hydraulics in the reactor core was calculated by coupling the reactor kinetics code. Thermal-hydraulics were obtained by the CUPID code which is aimed for the analysis of transient two-phase flows in nuclear reactor components. For neutron kinetics behavior, two different codes were taken into account: MASTER code based on neutron diffusion code and the DeCART code to consider transport effect. In addition, different methodologies for multi-physics simulation according to which neutron kinetics code is applied were explained in detail. Steady state power distribution of nuclear reactor was considered for the preliminary calculation.

Keywords: Numerical Algorithms, Computational Fluid Dynamics, Turbulence Modeling, Aeroacoustics.

1 Introduction

Since various physical phenomena such as thermal-hydraulics, neutron kinetics, nuclear fuel structure, and water chemistry in the nuclear reactor are deeply related with one another, a need to investigate multi-physics analysis have been raised. Multi-physics analysis with thermal-hydraulics and neutron kinetics has been investigated for decades. The neutron kinetics of the reactor core is quite sensitive to temperature of nuclear fuel rod and density of coolants. That is, the thermal-hydraulics and neutron kinetics is strongly coupled with each other. These multi-physics simulations have been used to make it possible to visualize the nuclear reactor core more realistically in terms of safety margin. Thus, the coupled calculation between thermal-hydraulics and three-dimensional neutron kinetics is essential and necessary to obtain the realistic solution.

The consortium for advanced simulation of light water reactors (CASL) has developed a multi-physics simulation platform named VERA (virtual environment for reactor analysis) [1, 2]. From the CASL project, the neutron kinetics codes were improved for high-performance computing (HPC) environment and co-simulated with high-fidelity thermal-hydraulics codes [3]. Safety issue due to the CRUD in nuclear fuel is numerically revealed by multi-physics calculation with thermal-hydraulics, neutron kinetics, and water chemistry [4, 5]. CRUD generation and deposition were resolved by water chemistry code, MAMBA, and moderator feedback as a boundary condition was provided by the CFD codes. Another program for multi-physics analysis called NEAMS (Nuclear Advanced Modeling and Simulation) was launched, from which high-fidelity platform, MOOSE (multiphysics objects oriented simulation environment) has been developed [6].

Korea Atomic Energy Research Institute (KAERI) has been developing a component-scale thermal-hydraulics code, CUPID [1]. The objectives of the development is to support a high-resolution for the thermal hydraulic issues regarding the transient multi-dimensional two-phase phenomena which can
be raised in an advanced light water reactor. For the numerical closure, it adopts a three-dimensional, transient, two-phase and three-field model, and includes physical models and correlations of the interfacial mass, momentum, and energy transfer. By adopting governing equations for both the open medium and the porous medium, it can be used as either a typical CFD code or a component code, i.e., porous CFD code, depending on the length scale of phenomena that need to be resolved. With respect to the neutron kinetics analysis, three-dimensional neutron kinetics codes have been also developed by the KAERI: MASTER and DeCART. The MASTER code is three-dimensional reactor kinetics code, which is a two-group, three-dimensional neutron diffusion code for microscopic depletion, xenon dynamics, on-line departure of nucleate boiling (DNB) analysis and kinetics calculation. It has been utilized for multi-physics calculation with system-scale thermal-hydraulics codes [7]. The DeCART code is developed for heterogeneous whole core transport calculation [8]. It is capable of directly generating 3D sub-pin level power distributions and core reactivity with thermal feedback for the pressurized water reactor (PWR) cores. During the core calculation, it accesses a fine group cross-section library which is generally the master library for the lattice physics calculations to generate homogenized few-group constants.

In this paper, multi-physics simulation coupled with thermal-hydraulics code and neutron kinetics codes is conducted. Two different methodologies are utilized to couple. Firstly, an explicit coupling method is considered by compiling neutron kinetics code, MASTER, into dynamic link library (DLL). Since the MASTER code is based on the diffusion equation of neutron, it can calculate with relatively less number of meshes. Thus, coupled simulation with the MASTER code is generally run in Windows system. However, the DeCART code requires huge memory size and computation time. That is, the supervisory program should be organize the coupling procedure, and the thermal-hydraulics code, CUPID, and DeCART code are coupled by socket methodology. For preliminary simulation, the Korean nuclear reactor (OPR1000) is taken into account for normal operation condition.

2 Numerical Methodology

2.1 Thermal-hydraulics code, CUPID

2.1.1 Governing equation

To describe two-phase flows, a transient two-fluid three-field model is adopted in the CUPID code. The three fields represent a continuous liquid, an entrained liquid (i.e., droplets), and a vapor field. In the three-field model, the mass, energy, and momentum equations for each field are established separately and, then, they are linked by the interfacial mass, energy, and momentum transfer models. The continuity equation for k-field is;

$$\frac{\partial}{\partial t} (\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k u_k) = \Omega_k$$

(1)

where $$\Omega_k = \Gamma_v + \Gamma_{wall} = -\Omega_l$$.

(2)

The momentum equation for the k-field is;

$$\frac{\partial}{\partial t} (\alpha_k \rho_k u_k) + \nabla \cdot (\alpha_k \rho_k u_k u_k) = -\alpha_k \nabla P + \nabla \cdot [\alpha_k \tau_k + \tau^T_k] + \alpha_k \rho_k g + M_{ik}$$

(3)

where $$M_{ik}$$ is the interfacial momentum transfer term. $$M_{ik}$$ includes the interfacial drag, the momentum exchange due to the interface and wall mass transfer, and various non-drag forces such as the virtual mass force, lift force, wall lubrication force and turbulent dispersion force. $$M_{ig}$$ is written
as,

\[ M_{gl} = F_{gl} + \Gamma_u u_{gl} + \Gamma_{wa} u_{gl} + F_{nd} = M_{sl} \quad (4) \]

where \( F_{gl} \) and \( F_{nd} \) are the interfacial drag force and non-drag forces respectively. The interface velocities, \( u_{gl} \), are needed to obtain the interfacial momentum transfer due to the interface mass transfer. These are determined using a donor formulation concept.

It is assumed that the continuous liquid and droplet fields are in a thermal equilibrium. Then, the energy equations for the gas and liquid fields are;

\[
\frac{\partial}{\partial t}(\alpha_g \rho_g c_g) + \nabla \cdot (\alpha_g \rho_g c_g u_g) = -P \frac{\partial}{\partial t} \alpha_g + E^D - PV \cdot (\alpha_g u_g) + Q_{lg} - Q_{lg} + q_{wg},
\]

\[
\frac{\partial}{\partial t}[(1 - \alpha_g) \rho_e c_e] + \nabla \cdot [(\alpha_i u_i + \alpha_d u_d) \rho_e e_e] = -P \frac{\partial}{\partial t} (1 - \alpha_g) + E^D - PV \cdot (\alpha_i u_i) - PV \cdot (\alpha_d u_d) + Q_{il} + Q_{lg} + q_{wl}.
\]

where \( E^D \) includes the conduction, turbulent energy source, and viscous dissipation that are represented in terms of a diffusion. \( Q_{lg} \) and \( Q_{il} \), are the interfacial energy transfer terms. \( Q_{gl} \) is the sensible heat transfer rate per unit volume at the non-condensable gas-liquid interface.

For a mathematical closure, the equations of the states and the constitutive relations for the interfacial drag force, the interfacial heat transfer and the wall boiling model are necessary. The governing equations take into account the porosity concept to model the two-phase flows at the component scale. However, for simplicity, the explanation of the porosity concept is omitted in this paper [9, 10].

CUPID adopts RANS turbulence models such as standard \( k-\varepsilon \), low Reynolds number \( k-\varepsilon \), RNG \( k-\varepsilon \), realizable \( k-\varepsilon \), and SST \( k-\omega \) models. The LES turbulence model has not yet been implemented since the applications of CUPID are focused on the practical simulation of thermal hydraulic issues related to light water nuclear reactors.

The CUPID code provides two different numerical schemes: semi-implicit scheme and implicit scheme. The semi-implicit scheme has been adopted in system-scale thermal-hydraulics codes for decades in order to take into account mass change considerably in nuclear society [11]. Since the mass and energy changes due to phase change rather than the momentum jump should be calculated accurately, the mass and energy equations are implicitly coupled while the momentum equations are discretized explicitly. An implicit method is implemented in the CUPID code for fast computation of steady state problems. Although the semi-implicit method is well suited for simulating fast transients, its time step size is limited by the CFL number. For a mild transient or a steady state problem, the computation time can be reduced by using time steps greater than the CFL limit. In the implicit method, the time step size can be larger than the CFL limit since all the convection and diffusion terms appearing in the governing equations are calculated implicitly. The implicit method is available only when the energy decoupled method is used.

### 2.1.2 Porous media approach

Since it is impossible to model real geometry due to its complexity of nuclear reactor, a porous media approach is utilized in many application to simulate reactor thermal-hydraulics. In general, a single OPR1000 fuel assembly contains 16×16 fuel rods lay-out including control rods and spacer grid. Even though the radial reflector region surrounding the reactor core can be modeled as multiple channels according to their location, a single channel in this simulation is utilized under the assumption that the reflector channel has usually same thermal-hydraulic condition.

Generally, a composition of the fuel rod and corresponding control rod in the fuel assembly is slightly different according to where to be located. Since the purpose of this study, nevertheless, is the coupling between the thermal hydraulics code and neutron kinetics code and its preliminary
calculation, the porosity and permeability is simply obtained by assuming that the fuel assembly is packed with 16×16 fuel rods. Porosity is a measure of the void space in an arbitrary medium. The definition of porosity in a fuel assembly is obtained as follows.

\[
\gamma = \frac{V_{\text{fluid}}}{V_{\text{total}}} = 1 - \frac{(\pi D^2 / 4) \times \text{No. of rod}}{L \times L}
\]  

(7)

where \( D \) is the outer diameter of the fuel rod and \( L \) is the width of the unit fuel assembly. Permeability, as known as area porosity, is a measure of an ability for fluid to transit through cell faces, and is achieved through the assumption that the fluid flows freely in between cells horizontally, but is partially constrained in the axial direction by the array of rods.

2.1.3 1D conduction for fuel rod

For obtaining the temperature fields of the fuel rod in the porous zone, the simple conduction equation for only radial direction is considered. Since dimension of a single fuel rod is 9.7 mm outer diameter and 3.81 m height, an axial heat transfer is assumed to be negligible. In addition, the heat source from the neutron kinetics code is assumed to be distributed uniformly at each plane so that an azimuthal variation is not also taken into account. Thus, radial temperature profile needs to be obtained. Each porous cell has the heat transfer area, which is defined as the ratio of the overall contact surface of the fuel rods to the provided cell volume. Since a heat generation distribution for all fuel rods of each porous cell is assumed to be uniform, a representative fuel rod can be considered. General one-dimensional heat conduction equation is adopted as follows;

\[
\rho C_p \frac{\partial T}{\partial t} = \nabla (k \nabla T) + q^*
\]  

(8)

Nuclear fuel rod is consisted of pure element called pellet and clad material outside. For radial discretization of the fuel rod, both pellet and cladding are taken into account. Thin gap is assumed to be existed in between them. In general, the gap region can be numerically treated by two way; i) conductor with gap thickness having finite thermal conductivity, \( k_{\text{gap}} \) and ii) convective boundary condition with equivalent heat transfer coefficient, \( h_{\text{gap}} \) as thermal resistance parameter [12].

2.1.4 Cross flow modeling (turbulent mixing)

Since the porous media approach is employed to resolve the subchannel including fuel rod, an additional pressure drop model should be taken into account. Especially for the subchannel between fuel rod, numerous pressure drop models have been developed. In order to consider the radial flow dispersion, turbulent mixing models are derived. The turbulent mixing between neighboring subchannel can be occurred due to the turbulent fluctuation and the flow disturbance by structures such as grid spacer mixing vane. In adiabatic single-phase flow, no net mass transfer occurs between adjacent subchannels but momentum and energy can be distributed. This fluid exchange mechanism is modeled by Equal Mass exchange model (EM model). EM model acts only in the lateral directions to reduce the velocity difference between adjacent subchannels. EM model applied to momentum conservation equation is given as follows;

\[
\overline{M_k}' = - \sum w_j \left( U_i - U_j \right)
\]  

(9)

In adiabatic two-phase flow and heated flow condition, mass and energy transfer as well as momentum transfer can occur between adjacent subchannels. Thus, equal volumes of fluid and void are exchanged, as opposed to mixing equal masses of fluid. These flow mixing mechanisms are modeled as Equal Volume exchange and Void Drift model (EVVD model). The turbulent mixing
terms are modeled by simple diffusion approximation using mixing length theory [13]. The turbulent mixing and void drift of mass, energy and momentum transfer are as follows;

\[
\bar{M}_e = \epsilon \frac{s}{z} \left( \rho_f - \rho_g \right) \theta \left[ \alpha_{v,j} - \alpha_{v,i} - (\alpha_{v,j} - \alpha_{v,i})_{\text{equil}} \right], \tag{10}
\]

\[
\bar{M}_h = \epsilon \frac{s}{z} \left( \rho_f h_f - \rho_g h_g \right) \theta \left[ \alpha_{v,j} - \alpha_{v,i} - (\alpha_{v,j} - \alpha_{v,i})_{\text{equil}} \right], \tag{11}
\]

\[
\bar{M}_k = \epsilon \frac{s}{z} \left( \rho_f v_f - \rho_g v_g \right) \theta \left[ \alpha_{v,j} - \alpha_{v,i} - (\alpha_{v,j} - \alpha_{v,i})_{\text{equil}} \right]. \tag{12}
\]

2.2 Coupling methodology

The thermal-hydraulics and neutron kinetics of the reactor core is intimately coupled by the feedback effect between the moderator and fuel rod. Especially, neutron kinetics is strongly spatial dependent so that a three-dimensional analysis should be required. Thus, the thermal-hydraulics / neutron-kinetics coupled calculation is needed in order to represent the thermal-hydraulic behavior realistically.

The CUPID code is consisted of hydrodynamic model (HDM) for thermal-hydraulic behavior and heat structure model (HSM) for fuel rod conduction. These two models are explicitly coupled. The CUPID code uses thousands of computing mesh for the core, whereas the reactor kinetics model (RKM) uses more detailed mesh system. And, in terms of RKM, the reactor fuel region as well as the reflector region should be considered. The reflector region is subdivided into top/down and radial
direction. Figure 2 shows a schematics of information transfer for the interface variables among the hydrodynamic model (HDM), heat structure model (HSM) and reactor kinetics model (RKM). The RKM calculates the core power and transfers to the HSM. Meanwhile, the HDM and HSM provide the moderator density and fuel rod temperature, which are utilized for reactivity feedback calculation.

2.2.1 Explicit coupling based on dynamic link library (DLL)

The coupling procedure between CUPID and MASTER is achieved under the Windows operating system so that the dynamic link library (DLL) feature could be used and the resulting code can be executable on personal computers. At first, the MASTER code is compiled into a dynamic link library. Then, CUPID calls the MASTER DLL and calculates the heat source prior to calculating the HSM. This coupling methodology has been used in system scale thermal-hydraulics code coupling [14].

Figure 3: Network socket communication with MPI
2.2.1 Network socket communication

The DeCART code performs the sub-pin level three-dimensional whole reactor core transport calculation and generates the equivalent parameters of homogenized group constants and surface discontinuity factor. DeCART code needs huge memory that coupled simulation with the CUPID code is not able to be run in Windows operating system. Thus, alternative methodology should be considered.

In order to run two codes simultaneously, network socket are utilized. The variables to be delivered between CUPID and DeCART are directly transferred from one to the other through a network socket. The independent supervisory program controls the data transfer. The coupling procedures by the socket are shown in Fig 2. The supervisory program is ready for the socket and stands by. The coupled variables are transferred from each code to the server program as soon as the two codes are ready. The CUPID and DeCART starts to execute the calculation separately after the transfer of the coupled variables from server program is completed. If either or both codes are converged or reached at limited iterations, the code waits for the other to be converged or reach limited iterations. After each iteration of the two codes is completed, the common variables to be coupled are updated by the server program through the network socket, and these procedures are repeated.

3 Results and Discussion

3.1 Reactor core modeling

The resolution of two neutron kinetics codes, MASTER and DeCART, is different from each other. With respect to the simplicity of mapping procedure, the grid system of the thermal-hydraulics analysis is adjusted to those of neutron kinetics codes. Figure 4 shows a schematic of a computational domain. In this study, only the fuel assemblies and surrounding reflector area are taken into account. In Fig. 4, yellow region is the reactor core and outer green zone is the reflector area. The reactor core considered here is consist of 177 fuel assemblies, each of which includes 16×16 fuel rods.

![Computational geometry of the reactor core of OPR1000](image)

For the CUPID-MASTER coupling, each fuel assembly is assigned to employ a single computational cell. That is, in the horizontal plane, the computational domain for fuel assemblies is divided into 177 cells in order to match each one to a single fuel assembly, and additional 64 cells are needed to consider the outer reflector region. In the axial direction, 25 cells for both fuel assembly and reflector are assigned. The number of cells along axial direction is identical for both thermal-hydraulics and neutron kinetics calculation to guarantee the one-to-one correspondence without additional mapping algorithm. Thus 6,025 meshes are employed for the thermal-hydraulic analysis using the CUPID code. However, radial mesh distribution differs between two codes. Figure 5 shows a quarter of whole...
radial computational cells for both codes. For minimizing an effort to generate mapping algorithm, the radial cell configuration is divided according to the fuel assembly unit. As explained above, the CUPID code employs single cell per single fuel assembly. The MASTER code employs more resolved computing cell configuration; 4 computing cells for each fuel assembly as well as surrounding reflector channel. That is, 964 radial cells are assigned for neutron kinetics calculation.

For CUPID-DeCART co-simulation, more resolved grids are employed. In DeCART calculation, fuel assembly as well as outer reflector area are also modeled. However, CUPID takes into account only fuel assembly region. For radial discretization, every single cell is assigned to model each fuel rod. Thus 45,312 grids are used for CUPID and 61,696 for DeCART. To avoid complexity of general mapping between two codes, the number of axial mesh are identical. Overall 26 meshes are adopted along reactor height. Totally 1,178,112 and 1,604,096 meshes are assigned for CUPID and DeCART code, respectively.

Since the DeCART code generates the rectangular mesh manually, an order numbering grids is always fixed. However, the CUPID codes is based on the independent pre-processing program such as SALOME [15], the order of cell is arbitrarily determined. Therefore, the mapping algorithm should be needs to match both independent grid system. Since the cell order of the DeCART code is fixed, the mapping file is generated to match the grids of CUPID into those of DeCART according to the coordinates of grids. Figure 6 shows the snapshot of the mapping file for fuel assembly. Once the mapping file is generated explicitly, the supervisory program reads it, and allocates the buffers for variables to be communicated such as liquid temperature and heat generation.

Figure 6: Mapping file for CUPID-DeCART coupling
3.2 Domain decomposition for parallel computing

Since the CUPID-MASTER coupling with DLL method is based on the Windows operation system, a serial computation is enough to obtain the results. Multi-physics calculation by CUPID-DeCART needs millions of grids and correspondingly large memory. Thus, parallel computing should be done. The DeCART code has a capability to run OpenMP/MPI hybrid computing. Every radial plane is assigned to be parallelized with MPI communication. Because the grids are generated manually in the code, the subdomains along the axial direction can be easily decomposed. Within each plane, parallel computing with the OpenMP can be conducted. Since 26 radial planes, in this study, is accumulated axially, the 26 processors are assigned for MPI communication.

The CUPID code is parallelized based on MPI communication. An overall geometry is arbitrarily divided into subdomains with METIS library [16]. Figure 7 shows domain decomposition of computational grids for CUPID calculation. The number of subdomains is 26 and each subdomains are assigned into each processors. Thus, supervisory program is run independently, and both CUPID and DeCART utilize 26 processors, respectively.

![Figure 7: Domain decomposition for CUPID calculation.](image)

3.3 Steady state power distribution

![Figure 8: Nominal power distribution: left is liquid temperature and right is volumetric heat source.](image)

In this study, normal operation condition for reactor core full assembly is calculated in conjunction with whether the EVVD model is adopted or not. Problem time is set to 100 sec during which data for coupled simulation are transferred according to iteration number of CUPID calculation. The duration for data transfer is determined in input for supervisory program and set to be every 1,000 iteration of CUPID calculation. Fig. 7 shows contours of heat generation and liquid temperature without additional pressure drop model. The left side is liquid temperature and right side is volumetric heat generation which is output is DeCART results. From the shape of power output distribution, the
multi-physics calculation is properly performed. When the turbulent dispersion model is not adopted, the liquid temperature is not radially mixed and then relatively high liquid temperature is obtained. The power distribution of a single fuel assembly is presented in Fig. 9. Within the fuel assembly, the local maximum and minimum can be easily comprehended: local maximum for hot channel is colored in red; waterhole in blue.

By adopting EVVD model, however, radial mixing phenomena is clearly observed. Figure 10 shows power distribution and liquid temperature for null transient until 100 sec. as time goes by, an effect of flow dispersion due to the turbulent mixing model occurs. Due to the mixing effect, lower liquid temperature range is obtained, compared with those of Fig. 8.

Figure 9: Power ratio from DeCART result: Red positions are local maximum
Figure 9: Contours of power distribution and liquid temperature: left column is power distribution; right column is liquid temperature

### 3 Conclusion and Future Work

In this study, a multi-physics simulation of thermal hydraulics and neutron kinetics was attempted. The component thermal hydraulic analysis code CUPID was coupled with three-dimensional neutron kinetics code, MASTER and DeCART. OPR1000 reactor core was taken into account for coupled simulation. Porous media approach was adopted to simplify the complicated reactor core geometry for thermal hydraulic analysis. The MASTER code was compiled as a dynamic link library (DLL) feature and then, both codes were able to run simultaneously. In order to link the data required for both codes, heat structure module for was derived; fuel rod including outer cladding is radially solved by using general conduction equation. The CUPID-DeCART co-simulation was controlled by supervisory program which calls two codes with MPI communication. For thermal-hydraulics analysis, porous media approach was adopted and corresponding pressure drop models such as friction and turbulent mixing were considered. Steady state of normal operation for OPR1000 reactor was taken into account.

### References


