Research Article

Code Development in Coupled PARCS/RELAP5 for Supercritical Water Reactor

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The new capability is added to the existing coupled code package PARCS/RELAP5, in order to analyze SCWR design under supercritical pressure with the separated water coolant and moderator channels. This expansion is carried out on both codes. In PARCS, modification is focused on extending the water property tables to supercritical pressure, modifying the variable mapping input file and related code module for processing thermal-hydraulic information from separated coolant/moderator channels, and modifying neutronics feedback module to deal with the separated coolant/moderator channels. In RELAP5, modification is focused on incorporating more accurate water properties near SCWR operation/transient pressure and temperature in the code. Confirming tests of the modifications is presented and the major analyzing results from the extended codes package are summarized.

1. Introduction

The supercritical water reactor (SCWR) is a generation IV nuclear reactor concept characterized by its system simplification and high thermal efficiency. Due to its higher operating pressure and temperature, separated moderator and coolant channels, and a strong coupling between power (neutronics calculation) and moderator temperature (thermal-hydraulic (T/H) calculation) because of a large density variation of water (100 to 700 kg/m³), existing LWR codes are not capable of analyzing SCWR design without appropriate modifications [1]. Yamaji et al. have shown coupled neutronics and T/H analysis of high temperature supercritical-pressure light water reactor (SCLWR-H). The code package includes SRAC code system (neutronics) from Japan Atomic Energy Research Institute (JAERI) and SPROD code (T/H) from University of Tokyo. Buongiorno and Macdonald presented and analyzed the U.S. reference SCWR design using RELAP5 with a point kinetics model [2, 3]. The current study developed a neutronics and T/H coupled analysis capability for the U.S. reference design by extending existing LWR analysis code package, that is, the core simulator PARCS and the T/H code RELAP5, which have been verified for analyzing PWR and BWR in coupled mode and are easily accessible

for academic purposes [4]; this paper discusses the codes modifications and presents the preliminary tests confirming the major extensions in code coupling module and nuclear cross section feedback module in PARCS and water property module in RELAP5. The SCWR analyzing results using the extended code package are summarized here and the details are discussed in another paper [5].

2. Existing Coupling Mechanism

Current study analyzes the SCWR using extended code package PARCS/RELAP5.

PARCS [6] is a 3D reactor core simulator developed in Purdue University. It solves the steady state, time-dependent, and multigroup neutron diffusion equation and SP3 transport equation to predict the dynamic response of the reactor to reactivity perturbations. PARCS is applicable to both PWR and BWR and can be coupled directly to the T/H system code RELAP5.

RELAP5 [7] is a T/H code designed for best-estimate transient simulation of light water reactor system. It was developed at the Idaho National Lab for the U.S. Nuclear Regulatory Commission. It is capable of modeling coupled

FIGURE 1: PARCS/RELAP5 coupling mechanism.

behavior of the reactor coolant system and core for accidents and transients using eight field equations. The version used in current study is RELAP5/MOD3.3.

In order to simulate the feedback between the thermal-hydraulics and the neutronics, the field equations of RELAP5 can be coupled to either a built-in point kinetics model or a 3D neutronics code PARCS. By using the 3D kinetics code we can calculate power distribution in a new type of reactor design such as SCWR instead of appealing to typical LWR parameters like in point kinetics model.

To couple PARCS/RELAP5, in the point of view of PARCS, is to replace the internal thermal hydraulics solver in PARCS with an external T/H code, which is RELAP5 in this case (Figure 1). As the solving scheme of a steady state problem shown in Figure 2, PARCS performs neutronics calculation to generate new power profile with nuclear cross section information based on the temperature data from RELAP5; then RELAP5 receives the updated power profile from PARCS and performs T/H calculations to generate the new temperatures of fuel, moderator, and coolant and passes the temperature information back to PARCS. The coupled simulation will be ended when the iteration in PARCS converges.

The RELAP5 data map routine (RDMR) module in RELAP5 is designed to communicate with neutronics code PARCS through a general interface (GI) module in PARCS. The PARCS-specific data map routine (PDMR) module in PARCS is the counterpart to RDMR in RELAP5, and it functions as an interface between PARCS and external T/H codes, such as RELAP5 and TRAC-M, through the GI module. PDMR is designed to maintain consistency with the requirements of both the GI and the RDMR while preparing data to be transferred to RELAP5. A space-dependent variable mapping input file read by PDMR module defines the corresponding nodes between PARCS and RELAP5 models. The parallel virtual machine (PVM) code is utilized to control the communications between two codes.

The U.S. reference design is essentially a light water reactor (LWR) operating at higher pressure and temperature with a direct cycle. Comparing to a normal PWR, the major difference is that SCWR uses light water as moderator and

FIGURE 2: Solving scheme for steady state eigenvalue problem in PARCS.

coolant in separated channels as shown in Figure 3; the feed water temperature is 280°C and outlet temperature is 500°C at pressure of 25 MPa [2, 3].

3. Modifications on PARCS

Because the SCWR reference design has higher operating pressure and temperature and utilizes the new cladding material and separated coolant and moderator channels [8], in order to analyze it the following modules in PARCS need to be modified:

- (i) water and cladding thermophysical property functions or tables are modified accordingly;
- (ii) variable mapping input file and PDMR module need to be modified to deal with information from extra flow channel, in order to model separated coolant and moderator flow channels;
- (iii) the nuclear macroscopic cross section updating module in PARCS should be extended to include the feedback based on not only fuel and coolant but also moderator thermophysical properties; the accessory modification in PARCS also includes the new input lines for SCWR specially in the input files and the new variable storage file for SCWR problem in source files.

FIGURE 3: The cross sections assembly of U.S. reference design [2].

3.1. Modification of Thermophysical Properties of Water and Cladding. In coupled simulation mode (PARCS/RELAP5), the thermophysical properties will be supplied by T/H solver RELAP5; however, in the initialization process in PARCS the functions describing thermophysical properties of water and cladding material functions are still called. Therefore the modifications in these functions are needed for SCWR analysis.

The thermophysical properties of water are originally described by simple polynomial equations as a function of temperature or enthalpy under PWR or BWR operating pressure. Therefore a water density function under supercritical pressure is added. Because of the dramatically changing water density near the pseudocritical point, a more sophisticated scheme specifying water density under 25 MPa based on NBS/NRC steam tables [9] is adopted using lookup tables and data are arranged in uniform intervals of temperature (0.1 K) or enthalpy (1 K/Kg) and can be searched by direct index.

Because MA956 is used as cladding material in SCWR reference design instead of zircalloy for ordinary PWRs or BWRs in original PARCS, the polynomial functions of the conductivity and thermal capacity of MA956 based on tabulated data are implemented in the code for SCWR design [10].

3.2. Modification in Nuclear Cross Section Feedback Module. SCWR reference design has separated coolant and moderator channels, so water flowing in the separated channels has different temperatures and densities. Therefore the neutronics cross section feedback mechanism in PARCS should be able to handle the moderator and coolant thermophysical properties separately.

The original PARCS can update the macroscopic cross section based on fuel temperature, coolant temperature, control rod positions, and burnable poison concentration, and the modified PARCS can also update the cross section based on moderator density and temperature. As shown in (1) underlined parameters are newly added, term $\frac{(\partial\Sigma/\partial T_m)\Delta T_m}{\partial\sqrt{T_f}}$ represents the cross section feedback due to the moderator temperature change, and term $(\partial\Sigma/\partial D_m)\Delta D_m + (\partial^2\Sigma/\partial D_m^2)(\Delta D_m)^2$ represents cross section feedback due to the moderator density change; notice that the dependence of moderator temperature is modeled as linear, and dependence of moderator density is quadratic. There are two parts involved in the modification: firstly a new option is added into cross section feedback module in PARCS; secondly the cross section data file is updated to store the cross section information from different combinations of moderator and coolant thermophysical properties, fuel temperature, and control rod position; the data file is generated using GenPMAXS code based on calculation results from lattice code HELIOS [11]:

$$\begin{aligned} \Sigma(\alpha, T_f, T_m, T_c, D_m, D_c) = & \Sigma_r + \alpha \Delta \Sigma_{cr} + \frac{\partial \Sigma}{\partial \sqrt{T_f}} \Delta \sqrt{T_f} \\ & + \frac{\partial \Sigma}{\partial T_m} \Delta T_m + \frac{\partial \Sigma}{\partial T_c} \Delta T_c \\ & + \frac{\partial \Sigma}{\partial D_m} \Delta D_m + \frac{\partial^2 \Sigma}{\partial D_m^2} (\Delta D_m)^2 \\ & + \frac{\partial \Sigma}{\partial D_c} \Delta D_c + \frac{\partial^2 \Sigma}{\partial D_c^2} (\Delta D_c)^2. \end{aligned} \quad (1)$$

3.3. Modifications in Variable Mapping File and Coupling Module. PARCS is coupled to RELAP5 using PDMR module based on mapping rules defined in the space-dependent variable mapping input file. Because the SCWR reference design has separated moderator and coolant channels, extended mapping rules should be supplied in the variable mapping input file and corresponding modifications are needed in both PARCS and RELAP5.

As shown in Table 1, an original mapping input file contains four cards: "Trip," "DOPL," "Table 1," and "Table 2." The "Table 1" card defines the mapping rule between hydrodynamic volumes in RELAP5 model and neutronics nodes in PARCS model. "Table 2" card defines the mapping rule between heat structures in RELAP5 model and neutronics nodes in PARCS model. These two cards have multiple input lines in the same format.

In some cases the number of neutronics nodes in PARCS and the number of hydrodynamic volumes/structures in RELAP5 used to represent same physical region are different. The weighting factors are used to lump adjacent nodes or volumes/structures to make the mapping possible.

These mapping tables are sufficient for ordinary PWR/BWR designs, but not for the current SCWR design. The separation of moderator and coolant in SCWR instead of

TABLE 1: PARCS/RELAP5 mapping input file.

* %Table 1		
*RELAP volume number	PARCS node number	Weighting factor
335010000	1	1
335020000	2	1
335030000	3	1
⋮	⋮	⋮
335880000	88	1
335890000	89	1
335900000	90	1
* *Heat structure to node table		
* %Table 2		
*RELAP structure number	PARCS node number	Weighting factor
3360001	1	1
3360002	2	1
3360003	3	1
⋮	⋮	⋮
3360088	88	1
3360089	89	1
3360090	90	1

* Data ignored from the original table. And the “⋮” means the more similar input lines are ignored.

the combined moderator/coolant flow in PWR/BWR means for each neutronics node in SCWR PARCS model, there will be two corresponding hydrodynamic volumes in RELAP5: one representing coolant flow and the other moderator flow. Using the tables described above only one hydrodynamic volume can be matched to each neutronics node.

Therefore both the variable mapping file and related subroutines in PDMR module in PARCS are extended to solve this problem. In the new mapping input file, a fifth card, “Table 3,” is added to map hydrodynamic volumes representing moderator flow to neutronics nodes. The original “Table 1” card now only manages the mapping between hydrodynamic volumes representing coolant flow and neutronics nodes.

Appropriate modifications in PDMA module are introduced to receive data from the newly added mapping table “Table 3” and integrate these data to a permuted matrix together with the mapping information from “Table 1” and “Table 2” then send the matrix to RELAP5 together with the newly added control options for SCWR simulation in coupled mode. And the error checking subroutine is also updated for new mapping table “Table 3” and moderator thermal properties.

FIGURE 4: Density versus pressure in isotherm from original and modified water tables of RELAP5.

4. Modification on RELAP5

There are two modifications needed in the current version of RELAP5/MOD3.3 in the point of view of analyzing SCWR: RELAP5 is not stable at pressure above 25.9 MPa where the SCWR transients usually happen, because a coarse grid in supercritical point region is used in water property table; the error checking routine in the module RDMR (RELAP data mapping routines) in RELAP5 treats the water density below 0.35 g/cm^3 as an error, but the water density can reach 0.1 g/cm^3 crossing pseudocritical point in SCWR.

4.1. Modification in Water Property Table. In RELAP5, the grid of the water property table is calculated by input temperature and pressure values. The original temperature values consist of 157 points with 15 points covering the supercritical temperature range 645 K–675 K and 14 points covering the higher temperature region (700 K–6000 K), and the pressure values consist of 116 points with 10 points covering the pressure range from 20.9 MPa to 30.0 MPa and 5 points covering higher pressure region (30.0 MPa–99.9 MPa).

The modified input file increases the number of the points in the same ranges for both temperature (645 K–675 K) and pressure (20.9 MPa–30.0 MPa); now in new temperature set there are 184 points with 37 points covering the range, and the increment is one degree among most points; in the new pressure set there are 578 points with 468 points covering the range. To accommodate these densifications, the corresponding variable arrays are expanded accordingly.

The improvement from this modification can be illustrated in Figure 4, in which the pressure-density correlations in isotherms ($P(D, T)$) are shown. The original water table uses only two pressure points (25 MPa and 30 MPa) and three temperature points (654 K, 660 K, 675 K) to represent the region in the plot, while the new water table uses 301 pressure points and 22 using interpolation; three straight-line isotherms are used in original water table but 22 curved isotherms are used in new water table. After the modification,

TABLE 2: SCWR parameters.

Fuel Pin		Fuel assembly	
Fuel material	UO ₂	Number of fuel rods	240
Fissile enrichment	5%	Number of burnable absorber	60
UO ₂ density	10.4215 g/cm ³	Number of water rods	36
Fuel radius	0.439 cm	Number of control rods	12
Pellet to cladding gap	0.008 cm	Water rod width	3.36 cm
Cladding thickness	0.063 cm	Water rod wall thickness	0.04 cm
Fuel pitch	1.12 cm	Fuel assembly pitch	28.82 cm
P/D	1.098	Assembly wall thickness	0.3 cm
Cladding and core structure material	MA956	Interassembly gap	0.2 cm
Burnable absorber		Core	
Burnable absorber material	ZrB ₂	Thermal power	3575 MW
ZrB ₂ density	6.08 g/cm ³	Number of fuel assemblies	145
Fuel material	UO ₂	Heated fuel height	4.27 m
Fissile enrichment	5%	Total fuel pin height	4.87 m
UO ₂ density	10.4215 g/cm ³	Effective diameter	3.93 m
Fuel radius	0.439 cm	Volumetric power density	69 MW/m ³
BA cover thickness	0.0044 cm	Average linear heat rate	19.2 kW/m
Pellet to cladding gap	0.0036 cm	Fuel depletion plan	3 cycles
Cladding thickness	0.063 cm	Average burnup	0/12.5/25 GWd/MTU
Control rod		Thermal-hydraulic parameters	
Control rod material	B ₄ C	System pressure	25 MPa
B ₄ C density	2.59 g/cm ³	Coolant flow rate	1843 kg/s
Control rod radius	0.662 cm	Bypass ratio, η	10% (184 kg/s)
Control rod guide tube inner radius	0.912 cm	RPV inlet temperature	280°C
Control rod guide tube thickness	0.04 cm	RPV outlet temperature	500°C
		Thermal efficiency	44.80%

TABLE 3: Temperatures and densities of moderator and coolant.

Node number	Moderator		Coolant	
	Temperature (°C)	Density (kg/m ³)	Temperature (°C)	Density (kg/m ³)
1	353.8	612.9	354.1	611.6
2	353.7	613.1	372.8	522.6
3	352.4	617.7	381.8	419.3
4	350.1	625.1	384.8	324.8
5	347.4	633.7	387.1	255.4
6	344.3	643.1	391.5	204.8
7	340.5	653.7	399.5	168.4
8	335.9	666.2	412.6	141.6
9	329.9	680.9	431.2	121.6
10	322.0	699.1	455.2	106.5
11	311.2	721.8	481.0	95.8
12	296.8	748.9	490.4	92.7

RELAP5/Mod3.3 can calculate the water properties under pressure up to 30 MPa without large error as in original water table.

4.2. *Modification in Error Checking Routines.* Originally RDMR checks if the water density is between 1050 kg/m³ and 305 kg/m³, and this checking range is expanded to between

1050 kg/m³ and 5 kg/m³ to accommodate the water density change crossing the supercritical point.

5. Preliminary Test of the Modifications

The validation of the extended codes cannot be implemented without support of the related SCWR experiment, which

FIGURE 5: Comparison of cross sections from PARCS and HELIOS.

TABLE 4: Densities from coupled PARCS node and RELAP5 volumes.

Hydraulic volume number	From Table 3 in mapping file		Density (kg/m ³)	
	Node number	Weighting factor	RELAP5	PARCS
753030000	274	1	659.84	659.8457
753040000	475	1	660.53	660.5327
753050000	676	1	663.39	663.3935
753060000	877	1	668.55	668.5484
753070000	1078	1	675.67	675.6677
753080000	1279	1	684.22	684.2207
753090000	1480	1	693.64	693.6387
753100000	1681	1	703.33	703.3298
753110000	1882	1	714.08	714.0801
753120000	2083	1	726.54	726.5369
753130000	2284	1	739.96	739.9585
753140000	2485	1	754.07	754.0657

is not available for this concept design. The verification of the extended codes could be done with the help of other verified SCWR-capable codes, which is not accessible currently. However, some preliminary tests presented here can help to confirm the new added functions in the modified codes for SCWR analysis working properly.

5.1. Cross Section Feedback Module. Current coupled PARCS uses PMAX files to supply nuclear cross section data generated by lattice code HELIOS. And the PMAX files are produced by the GenPMAXS code, which is an interface between lattice codes and PARCS and it already has the capability to generate the cross section data based on separated moderator and coolant channels [11]. According to the assembly geometry shown in Figure 3 and parameters in Table 2, macroscopic cross sections are calculated for the

same assembly with PARCS and HELIOS, and the coolant and moderator thermal parameters in this test are shown in Table 3. A comparison of transport cross sections generated by PARCS using the modified cross section feedback module from PMAX file and transport cross sections produced directly by HELIOS in two energy groups are shown in Figure 5. The difference is acceptable considering that the interpolation of PMAX file data is used in PARCS module. The same comparisons are also accomplished successfully for absorption cross sections, fission cross sections, and capture cross sections of Xenon and Samarium.

5.2. Code Coupling Module. To confirm the coupled PARCS/RELAP5 is transporting the mapped moderator information correctly, a simple coupled SCWR calculation is carried out. A part of Table 3 of mapping file, which displays

FIGURE 6: Flow path model of RELAP5 test.

the corresponding hydrodynamics volume and nodes in two codes and the coupling weighting factor, is shown in Table 4. The comparison of the moderator densities from PARCS and RELAP5 is also shown in Table 4. It shows the coupled hydrodynamic volumes in RELAP5 and nodes in PARCS are sharing the same moderator densities. The similar comparisons are also passed for moderator temperature, coolant temperature and density, fuel temperature, and power.

5.3. RELAP5 Modification for Dealing with Supercritical Pressure. The original RELAP5 failed in the middle of the calculation because of the escalation of the fluctuation both in pressure and temperature at supercritical pressure, while the modified RELAP5 calculated successfully with no fluctuation noticed. In order to demonstrate the capability of the modified RELAP5, a simplified test model in which two connecting pipes representing moderator channel and coolant channel with counter flowing heated water passing through are shown in Figure 6, and the moderator inlet pressure is increased linearly from 26 MPa to 27.1 MPa, and coolant outlet pressure from 25.5 MPa to 26.6 MPa within 3000 seconds. The results are shown in Figure 7.

6. Discussion

The modifications in coupled codes PARCS/RELAP5 have been discussed and verified; the newly developed codes gained the capability simulating the separated moderator and coolant flow channel, simulating supercritical water beyond supercritical point and getting neutronics feedback from separated moderator. The coupled codes have been applied to analyze SCWR [12]; a moderator flow reversal has been found during burnup and transient cases, and because the separated highest power channel and highest cladding surface temperature channel, the maximum cladding temperature is lower than previous cases.

For other transients such as LOCA, in which large pressure excursion exists, the current modification is not

FIGURE 7: Pressure and temperature from test case with original and modified RELAP5.

enough to study the related system behavior. It is because the large depressurization in those transients introduces the complicated heat transfer and flow dynamics phenomena crossing pseudocritical point; sometimes a two-phase flow, further investigation to establish appropriate model based on realistic experiment data is needed, such as how to define the void fraction while crossing the pseudocritical point.

Nomenclature

- V : Volume (m^3)
- D : Density (kg/m^3)
- T : Temperature ($^{\circ}\text{C}$)
- Σ : Macroscopic cross section (m^{-1})
- η : Bypass ratio
- α : control rod insertion
- M : Moderator
- c : Coolant
- f : Fuel.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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