Development of MCATHAS System of Coupled Neutronics/Thermal-hydraulics in Supercritical Water Reactor

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Abstract

The MCATHAS system of coupled neutronics/Thermal-hydraulics in supercritical water reactor is described, which considers the mutual influence between the obvious axial and radial evolution of material temperature, water density and the relative power distribution. This system can obtain the main neutronics and thermal parameters along with burn-up.

MCATHAS system is parallel processing coupling. The MCNP code is used for neutronics analysis with the continuous cross section library at any temperature calculated by interpolation algorithm; The sub-channel code ATHAS is for thermal-hydraulics analysis and the ORIGEN Code for burn-up calculation. We validate the code with the assembly of HPLWR and analyze the assembly SCLWR-H.

Key words: Supercritical water reactor, Coupled Neutronics/Thermal-hydraulics, Relaxation Seidel method.

1. Introduction

Since the Generation IV International Forum on 2002, the Supercritical Water Cooled Reactor has been selected as one of the six Generation IV nuclear systems. Now, there have been 13 countries and 32 organizations researching the SCWR in the world ^[1]. USA, EU, Japan, South Korea and other countries have put forward different concepts for the core design successively. The operation pressure of SCWR is 25Mpa which exceeds the critical point of water (22.1Mpa, 374°C) and the water hasn't phase change. Therefore, SCWR can be design as once-through direct cycle system and the thermal efficiency exceeds light water reactors by about 30 percent with economics.

The operating pressure and core inlet/outlet temperature are 25Mpa and 280°C/500°C. In this situation, the density of coolant has sharp variation axially. It is necessary to consider the feedback of neutronics and thermal-hydraulics in core and assembly design. But the traditional codes for PWR aren't suitable disappointedly.

At present, some countries put forward their calculation programs for SCWR concept research respectively. Magnus ^[2] from Italy introduces the couple system of MCNP-MXN. YAMAJI Aki.^[3] from Japan couples the neutronics calculation system SARC with thermal-hydraulics code SPROD from Tokyo university and uses the coupled code for SCWR core design. Waata C.L. ^[4] from Germany applies the coupled code MCNP-STAFAS to the design of fuel assembly.

This thesis introduces the neutronics/thermal-hydraulics coupled system MCATHAS based on the characteristic of SCWR. In the system, the neutronics program adopts the parallel MCNP code ^[5] which can describe any complex geometry and we use interpolation algorithm to obtain the continuous cross section libraries at any temperature for the materials; ATHAS ^[6] is used as thermal-hydraulics calculation program for the sub-channels or the signal-channel, which can simulate various geometrical fuel assemblies and cores (for example PWR, BWR and HWR). The burn-up calculation program is ORIGEN code ^[7]. This coupled system can calculate the main physical and thermal parameters along with the burn-up such as: the axial and radial power distribution, the temperature distribution of the coolant, moderator, cladding surface and fuel center. It could also show us the axial density variety of the coolant and the moderator. MCATHAS system can be applied to the design of SCWR assemblies and cores with both pressure tube type and pressure vessel type, which is a measure of the future research of SCWR.

2. Description of MCATHAS system

MCATHAS system is a coupled code of three programs.

MCNP code is used as the neutron transport calculation program in this system, which is developed by the Los Alamos National Laboratory with the Monte Carlo Method. With its powerful capability of handling geometry tasks and high precision, MCNP is applied to simulating various complex geometries. But the Monte Carlo method is always inferior to the determination method in efficiency. So we use the parallel calculation MCNP in order to improve the efficiency. At the same time, the material temperature's sharp change axially. So based on the ENDF/B6 library, we use the Lagrange interpolation algorithm supplied by Tsinghua university to calculate the cross section at any temperature. F6 counter card is for calculating the axial and radical power distribution.

The sub-channel analysis code ATHAS (Advanced Thermal-Hydraulics Analysis Sub-channel), developed at Xian university of China, is used for Thermal-hydraulics calculation in MCATHAS system. ATHAS can simulate the temperature and density distribution in assemblies or cores as well as mass flux in every sub-channel. It can be used for various cores with the vertical or horizontal flow for the coolant, with the pressure tube or the clad and with the assembly box wall or not. Moreover, there are 13 optional supercritical water heat transfer correlation, 6 optional hydraulics resistance and pressure drop correlation and 13 optional mixing models in ATHAS code.

The burn-up calculation program is ORIGEN, which is developed by Oak Ridge National Laboratory and is used for calculating the burn-up of the nuclides, decay, and processing of radioactive materials. The data's transfer between MCNP and ORIGEN is realized by MCBurn code ^[8] and TCP/IP technique.

In MCATHAS system, the analytical object is divided into some axially meshes. In each mesh, the neutronics and thermal parameters are assumed to be the same. In each burn-up step, MCATHAS couples the parallel code MCNP with the sub-channel code ATHAS. Using the power distribution obtained by the MCNP code, ATHAS calculates the temperature and density distribution in the object. Then we use Lagrange three points Interpolation to update the continuous cross section library for materials which are appointed by the user. With the new cross section library, run MCNP code again and these evaluations are alternately repeated until power distribution, water density and material

temperature distributions are converged. Then run ORIGEN code to calculate the point burn-up and one burn-up step is completed. Flow chart of MCATHAS system is in Figure 1.



Fig.1 Flow chart of MCATHAS system code

The coupled code between MCNP and ATHAS uses Relaxation Seidel method. The iterative format is as follows:

$$T_{i}^{n} = (1 - \omega)T_{i}^{n-1} + \omega T_{i}^{n} \quad i = m, c, f$$
(1)

$$\rho_i^n = (1 - \omega)\rho_i^{n-1} + \omega\rho_i^n \quad i = m, c$$
⁽²⁾

The convergence criterion is:

$$\max |(P_i^n - P_i^{n-1})/P_i^n| < \varepsilon \quad i = x, y, z$$
(3)

$$\max |(T_i^n - T_i^{n-1})/T_i^n| < \varepsilon \quad i = m, c, f$$
(4)

$$\max_{i} |(\rho_i^n - \rho_i^{n-1}) / \rho_i^n| < \varepsilon \quad i = m, c$$
(5)

n means the number of iteration, n>1; ω is relaxation factor, $0 < \omega < 1$. The convergence can be accelerated by proper ω ; *x*, *y*, *z* stands for the Cartesian coordinates; Moderator, coolant and fuel are denoted by *m*, *f*, *c* respectively and temperature, density by *T*, ρ as well. ε is the maximal permissible error value.

3. Experimental calculation

Since the MCNP code is too time-consuming and the condition of the computer hardware isn't perfect, we verify the MCATHAS system on the assembly analysis elementary: High-Performance Light-Water reactor (HPLWR) and analyze High Temperature Supercritical-Pressure Light Water Reactor (SCLWR-H) assembly. The Supercritical water heat transfer correlation is Jackson^[10] in ATHAS code.

3.1 HPLWR assembly

HPLWR fuel assembly design proposed by Square ^[9] is shown in Figure 2. The fuel assembly configuration consists of a 7 fuel rod array arranged in a square lattice and a single moderator tube at the center displacing 9 fuel rods. Other geometry data in detail is listed in table 1. The feed-water enters the pressure vessel at 280°C where it is divided into 2 parts. One part flows downwards through moderate tube and assembly gap, and the other part reaches the bottom directly. Those two parts join together and flow upwards through sub-channels. The outlet temperature is 507°C.

Parameters	Value	Parameters	Value
Fuel rod radius	0.335cm	Clad outer radius	0.4cm
Fuel density	10.6g/cm ³	Clad density	7.45 g/cm^3
Fuel enrichment	Corner: 4%; others: 5%	Clad material	Alloy316
Moderator box length	2.6cm	Pitch/Diameter ratio	1.15
Gap width between fuel rod and moderator tube	0.1cm	Total power of 1/8 th fuel assembly	327.5kW
Active height	420cm	Average rod power	15.6kW/m
Inlet pressure of moderator channels	25MPa	Coolant inlet temp.	280°C
Average coolant mass flux	0.167kg/s	Coolant outlet temp	507℃

Table 1	Main Parameters of HPLWR
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We calculate the 1/8th assembly of HPLWR and compare the result with the corresponding data calculated by Waata C.L.^[4](shortening as M-S). We label the 7 fuel rods and 9 sub-channels as follows in figure 2(b).



Fig. 2 Schematic Diagram of Full and 1/8 Assembly of HPLWR

The relative error of the infinite multiplication factor k_{inf} is about 0.49% as shown in Tab.2. The axial coolant temperature distribution in the sub-channels is showed in Fig. 3. The coolant temperature in SC(9) is higher appreciably than other sub-channels and near the outlet it drops rapidly due to the heat exchange with the cold moderator entering from the top of the active height. The coolant outlet temperature in SC(2), SC(4) and SC(7) are the highest reaching 526.4°C, 528.04°C and 527.24°C respectively.

	MCATHAS	M-S
Kinf	1.17685	1.17112
Standard deviation	0.00041	0.00023



Fig. 3 Comparative Diagram of Axial Temperature Distribution in Sub-channels (MCATHAS vs. M-S)

Fig. 4 shows the coolant density distribution in sub-channels and Fig. 5 is for cladding surface temperature. The minimal coolant density value is 82.45 kg/m^3 . The results are according with M-S's. The maximum cladding surface temperature in sub-channels is 575.3° C, little lower than M-S's.



Fig. 4 Comparative Diagram of Axial Density Distribution in Sub-channels(MCATHAS vs. M-S)



Fig. 5 Comparative Diagram of Axial Temperature Distribution of Cladding surface in the subchannels (MCATHAS vs. M-S)

3.1 SCWR-H assembly

The concept of the High Temperature Supercritical-Pressure Light Water Reactor (SCLWR-H) has been developed at the University of Tokyo since 1989, and they use the system SRAC to analysis the core ^[3]. Considering its project practicability, Nuclear Power Design Institute of China improves some parameters of SCLWR-H as following in Tab. 3.



Fig. 6 Cross section of SCWR-H fuel assembly

Parameters	Value			
Fuel rod				
Fuel rod outer drameter	1.02cm			
Cladding thickness/material	0.063cm/stainless			
	steel310S ^{a)}			
Fuel pellet outer diameter	0.826cm			
Fuel density	10.266g/cm^3			
²³⁵ U fuel enrichment (average)	6.3%			
Clad density	7.98g/cm ³			
Fuel assembly				
Fuel rod lattice/pitch	Square/1.12cm			
Assembly side length	29.6cm			
Number of fuel rods per assembly	300			
Number of instrumentation rods per	1			
assembly				
Water rod wall thickness/material	0.08cm/stainless steel310S			
Assembly box wall thickness/material	0.2cm/stainless steel310S			
Assembly gap width	1.2cm			
Core				
Thermal/electric power	2740(MW)			
Active height	420cm			
Number of fuel assemblies	121			
Inlet/outlet temperature	280/500°C			
Inlet pressure of moderator channels	25MPa			
Core flow rate	1342kg/s			

Table 3 Main Parameters of SCWR-H

^{a)}stainless steel310S: (mass ratio: Mn:Cr:Ni:Si:Fe=0.02:0.25:0.2:0.01:0.52)

We calculate a simple example. The assembly is considered as a single channel in ATHAS code and the ²³⁵U fuel enrichment is 6.3% in all fuel rods with neither burnable poison nor control rods. We use MCATHAS system to calculate the infinite multiplication factor and the power peaking factors variety of the assembly with burn-up as follows in Fig.7 and Fig.8. The F_R is defined as the ratio of maximum

rod power to the average rod power with radial averaged and the F_Z is defined as the ratio of the maximum planar power to the average planar power in the assembly.



Fig.7 Burnup profile of infinite multiplication factor





Fig. 8 Burnup profile of the power peaking factors

Fig.9 Horizontal averaged axial power distribution



Fig. 10 Burnup profile of the AMCST and AMFCT

Fig.9 shows us the axial power distribution at the burn-ups of 0, 1.5, 3GWd/tU. The power distribution shifts from a center peek to a smoothness axially. Fig. 10 represents the burn-up profiles of the maximum cladding surface temperature radial averaged(AMCST) and the maximum fuel rod center temperature radial averaged(AMFCT), which satisfy the safe criteria.

4. Conclusion

The supercritical water reactor is the only reactor with water as coolant in the generation IV reactors. Due to its particular thermal-hydraulics prosperities, it is necessary to consider the relationship between the neutronics and thermal-hydraulics. MCATHAS system realizes the coupling of the neutronics and thermal-hydraulics and can calculate the burn-up for many types of core. We test the MCATHAS system on HPLWR and the result accords with the data calculated by Waata C.L.. At the same time, we use MCATHAS system to verify the SCWR-H assembly satisfies the design criteria elementarily. MCATHAS system supplies one method for SCWR assembly analysis.

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