Physical and thermal coupling calculation for accelerator driven subcritical core

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Abstract. The lead Anode (LBE) cooling ADS core is taken as the research object, and the ADS core axial one-dimensional physical thermal coupling model is established. The deterministic method is used to calculate the subcritical flux neutron flux distribution based on Monte Carlo. The method calculates the accelerator beam and the external neutron source generated by the spallation target. The ADS core thermal hydraulic analysis is carried out by a single-channel model, and the fuel elements are respectively divided into nodes in the axial direction and the radial direction, and the influence of thermal feedback on the neutronics characteristics of the subcritical core is considered. The one-dimensional physical thermal coupling model established in this paper can accurately calculate the spatial distribution of key parameters such as neutron flux density, fuel and cladding temperature in ADS core.

1. Introduction
The accelerator-driven subcritical system (ADS) benefits from its high safety, rich neutrons, and hard spectrum, and is used as a multi-purpose device for power generation, proliferation, or transmutation, and has received extensive attention in the international nuclear energy field. The ADS system is mainly composed of proton accelerator, spallation target and subcritical core. Its structural characteristics and operating principle are significantly different from traditional critical reactors, which brings new challenges to reactor safety and control.

In the process of ADS steady-state modeling, this paper uses a one-dimensional neutron diffusion model to perform subcritical core neutronics analysis, and calculates the distribution of neutron sources outside the core through the high-energy particle transport program MCNPX [1], thermal engineering. The hydraulic model includes the fuel element heat conduction model and the coolant channel heat transfer model, and the source iterative method is used to finally solve the steady state physical thermal coupling equations. In the iterative process, the subcritical core model without external source is calculated first, and the subcritical degree of the ADS core can be obtained. Then, the subcritical core model with external source is calculated to obtain the steady state physical thermal parameters of the ADS core.

2. Exogenous subcritical core neutronics model
2.1. Neutron equilibrium model
The neutron diffusion equation is based on this balance principle. When the reactor is in steady state critical operation, according to Fick's law, the one-dimensional axial single group neutron diffusion
equation is:
\[-D \nabla^2 \phi(z) + \Sigma_a \phi(z) = \nu \Sigma_f \phi(z)\]  (1)

From the theory of reactor criticality, for a given parameter \(D, \Sigma_a, \) and \(\nu \Sigma_f,\) the equation can only be established if its core size and geometry meet critical conditions. For the subcritical core with external source, the outer neutron source term \(S\) will be added to the right end of equation (1), so that the two ends of the equation can reach equilibrium, so it is not necessary to introduce the eigenvalue \(k_{eff}\) in the equation to adjust. It can be seen that the steady-state neutron diffusion equation of the external subcritical core is as follows:
\[-D \nabla^2 \phi(z) + \Sigma_a \phi(z) = \nu \Sigma_f \phi(z) + S(z)\]  (2)

The finite difference method is used to discretize the space term in the equation (2), and \(N\) nodes are divided along the core axis, as shown in figure 1, wherein each node has a length of \(\Delta_i\) (\(i = 1, ..., N\)).

![Figure 1. Core axial node division.](image)

Equation (2) is organized and written in matrix form as:

\[A \Phi = Q + S\]  (3)

Where \(A\) is the neutron disappearance term matrix which is shown in equation (4); \(\Phi\) is the neutron flux density distribution; \(Q\) is the fission neutron generation term.

\[A = \begin{bmatrix}
a_{1,1} & a_{1,2} & 0 & 0 & 0 & 0 & 0 \\
a_{2,1} & a_{2,2} & a_{2,3} & 0 & 0 & 0 & 0 \\
0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \\
0 & 0 & a_{i, i-1} & a_{i, i} & a_{i, i+1} & 0 & 0 \\
0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
0 & 0 & 0 & 0 & a_{N-1, N-2} & a_{N-1, N-1} & a_{N-1, N} \\
0 & 0 & 0 & 0 & 0 & a_{N, N-1} & a_{N, N}
\end{bmatrix}\]  (4)

It can be seen from equation (3) that \(A\) is a three-diagonal matrix, and the expressions of \(a_{i, i-1}, a_{i, i},\) and \(a_{i, i+1}\) are as follows:

\[a_{i, i-1} = -\frac{2}{\Delta_i} \frac{D_i D_{i-1}}{D_i \Delta_{i-1} + D_{i-1} \Delta_i}\]  (5)
2.2. Macro section parameter calculation

In this paper, the DRAGON program is used to generate these macroscopic cross-section parameters. The selected fuel temperature ranges from 300 to 2500 K, and the coolant temperature ranges from 400 to 1800 K. A temperature point is selected every 25 K. The parameters \( D(T_f, \rho_c), \Sigma_a(T_f, \rho_c) \) and \( \nu \Sigma_f(T_f, \rho_c) \) are obtained by the two-dimensional interpolation method as a function of fuel temperature and coolant density. In this process, a one-dimensional equivalent macroscopic section parameter is generated using the neutron flux density volume weighting method [2]:

\[
M_i(T_f, \rho_c) = \frac{\int V_i M(T_f, \rho_c, \phi) dV}{\int \phi dV}
\]

Where \( M_i \) is the macroscopic section parameter of the first node in the axial direction; \( V_i \) is the volume of the \( i \)-th node in the axial direction; \( r \) is the spatial position. The calculated cross-section parameters are substituted into the core physical thermal coupling calculation. The values of the cross-section parameters also change with the change of fuel temperature and coolant density.

2.3. External neutron source calculation

The ADS core is very different from the traditional critical reactor core in that it is driven by an external neutron source. During the operation of the ADS, the sparse neutrons generated by the interaction between the proton beam in the accelerator and the LBE target in the central region of the reactor are supplied as external sources to the subcritical core, thereby maintaining its neutron chain fission reaction process as shown in figure 2.

In the study of high-energy protons and LBE targets, the special high-energy particle transport program MCNPX is needed to calculate the spatial distribution and energy spectrum of the external neutron source generated by the analysis. Both the proton beam energy and the LBE target used in this paper refer to the European XADS concept stack [3]. The energy of the proton beam is 600 MeV, and its contact surface with the LBE target is 20 cm below the top of the core active zone, and the proton beam is irradiated with a diameter of about 8 cm. When the ADS is operating at a constant power level, the proton beam current can be calculated from the following equation [4]:

\[
a_{i,j} = \frac{2}{A} \frac{D_{i+1} D_j}{D_{i+1} A + D_i A_{i+1}} + \frac{2}{A} \frac{D_i D_{j+1}}{D_i A_{j+1} + D_{i+1} A_j} + \Sigma_{a,j}
\]

\[
a_{i,j} = -\frac{2}{A} \frac{D_{i+1} D_j}{D_{i+1} A + D_i A_{i+1}} \tag{7}
\]

Where \( \Phi, Q, \) and \( S \) are obtained by equations (8)-(10)

\[
\Phi = [\phi_1, \phi_2, \phi_3, \phi_4, \ldots, \phi_n]^T \tag{8}
\]

\[
Q = [Q_1, Q_2, Q_3, Q_4, Q_5, \ldots, Q_N]^T
\]

\[
= [\nu \Sigma_f \phi_1, \nu \Sigma_f \phi_2, \nu \Sigma_f \phi_3, \nu \Sigma_f \phi_4, \ldots, \nu \Sigma_f \phi_N]^T \tag{9}
\]

\[
S = [S_1, S_2, S_3, S_4, S_5, \ldots, S_N]^T \tag{10}
\]
Figure 2. Schematic diagram of interaction between proton beam and spallation target.

\[ I_p = \frac{P_f \nu \cdot e \cdot 1 - k_{eff}}{E_f \cdot \eta_p \cdot k_{eff}} \]  

(12)

Where \( I_p \) is the proton beam; \( P_f \) is the total power produced by fission in the core; \( E_f \) is the energy released by the core per fission; \( e \) is the amount of electron charge per unit; \( \eta_p \) is the average spallation produced by each proton Child number.

In the calculation process of the outer neutron source, the spatial distribution shape is first obtained by the MCNPX program, and its magnitude can be obtained by:

\[ S = \frac{\eta_p}{e} \cdot I_p \]  

(13)

3. Thermal hydraulic calculation model

The heat generated in the ADS core channel is mainly derived from the fission energy released instantaneously in the nuclear fuel, including the kinetic energy of the fission neutrons and fission fragments and the energy generated by the instantaneous gamma rays. It also includes the energy generated by the decay of the delayed fission products and various materials. The energy produced by the neutron absorption reaction. These energy generated by the nuclear fission reaction passes through the heat conduction of the fuel rod and the heat exchange between the cladding and the coolant, and is eventually carried out of the core by the coolant passage. In this paper, a single-channel model is used to establish a steady-state thermal hydraulic model, which neglects the mass exchange between each channel and the transfer of momentum and energy, but only calculates the heat transfer model of each fuel element and the heat transfer model of the coolant channel. For each fuel element, only the radial heat transfer of the fuel pellets is considered, ignoring the axial heat transfer. In order to couple the thermal hydraulic model to the neutronics model during calculation, the fuel element and coolant channels of the core active region are axially divided into the same number of nodes as the neutronics model.

The fuel pellet temperature distribution and coolant density distribution obtained from steady-state thermal hydraulic calculations provide the cross-sectional feedback state parameters required for neutronics calculations. On the other hand, the temperature limit and heat flux limit of the fuel element are specified in the reactor steady-state thermal design to ensure the integrity of the cladding and the safety of the core. Therefore, the established thermal hydraulic model must not only be able to Reflecting the average characteristics of the entire core, it also reflects the worst local thermal parameters in the core. In order to obtain the highest temperature point of the fuel core block and the surface of the cladding in the core average tube and the heat pipe, therefore, not only the fuel element
is divided into nodes in the axial direction, but also the nodes are divided in the radial direction. Since the coolant passages have different positions in the core due to their different positions in the core, it is assumed that the area of the coolant passage and the hydraulic circumference are averaged for the passages used in the assembly.

The radial node division of the fuel element in a single channel is shown in figure 3. The fuel core block divides the node of \( L \) radially, and the cladding is divided into three nodes in the radial direction due to the small thickness, so that the fuel core can be obtained. The temperature values of the block and the cladding at different positions in the axial and radial directions.

![Figure 3. Single channel schematic and radial node division.](image)

3.1. Fuel element heat conduction model

The differential equation of the heat conduction equation of the fuel pellet in the axial \( i \)-th node and the radial \( j \)-th node is:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r k_f^i \frac{\partial T_f^i(r)}{\partial r} \right)_{r_i} + q_r^i = \frac{1}{r_j \Delta r_f} \left[ \left( r k_f^i \frac{\partial T_f^i(r)}{\partial r} \right)_{r_{j-1/2}} - \left( r k_f^i \frac{\partial T_f^i(r)}{\partial r} \right)_{r_{j+1/2}} \right] + q_r^i
\]

\[
= \frac{1}{r_j \Delta r_f} \left[ r_{j+1/2} k_f^i (T_f^{i+1} - T_f^{i-1}) - r_{j-1/2} k_f^i (T_f^{i} - T_f^{i-1}) \right] + q_r^i = 0
\]

(14)

Ignoring the heat generated inside the cladding, the steady-state heat conduction equation and boundary conditions of the cladding in the radial direction of the \( i \)-th node are:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r k_{cl}^i \frac{\partial T_{cl}^i(r)}{\partial r} \right) = 0
\]

(15)
\[
\begin{align*}
-k_{cl}^i \frac{\partial T_{cl}^i}{\partial r} \bigg|_{r=r_{cl}} &= h'_{cl,c}^i (T^i_{cl} \big|_{r=r_{cl}} - T_{ci}^i) \\
-k_{cl}^i \frac{\partial T_{cl}^i}{\partial r} \bigg|_{r=r_{cl}} &= h'_{cl,c}^i (T^i_{cl} \big|_{r=r_{cl}} - T_{ci}^i)
\end{align*}
\]  

(16)

Where \(k_{cl}^i\) is the cladding thermal conductivity of the i-th node in the axial direction; \(h'_{cl,c}^i\) is the heat transfer coefficient between the outer surface of the cladding in the axial i-th node and the coolant; \(T_{ci}^i\) is the i-th node in the axial direction The temperature of the coolant; \(r_{cl}\) is the outer radius of the cladding.

3.2. Coolant channel heat transfer model

During the operation, the coolant always maintains a single-phase liquid state, ignoring the axial heat conduction of the coolant. The mass, energy and momentum conservation equations of the single-channel one-dimensional coolant in steady state are respectively:

\[
\frac{d}{dz} (\rho_c u_c) = 0
\]  

(17)

\[
\rho_c u_c \frac{dh}{dz} = \frac{q_i}{A_c}
\]  

(18)

\[
\rho_c u_c \frac{du_c}{dz} = -\frac{dP}{dz} - \rho_c g - \frac{f \rho_c u_c |u_c| u_c}{2D_c}
\]  

(19)

Where \(u\) is the flow rate of the coolant; \(p\) is the pressure; \(f\) is the friction factor; \(D\) is the equivalent diameter of the coolant flow path; \(h\) is the specific enthalpy of the coolant; \(q_i\) is the line power density; \(A\) is the coolant flow path area.

For the mass conservation equation (17), the differential inlet and outlet mass flow rates of the axially i-th node coolant are equal:

\[
w_c^i = A_c \rho_{c,in} u_{c,in}^i = A_c \rho_{c,out} u_{c,out}^i
\]  

(20)

Similarly, according to equations (18) and (19), the difference pattern of the coolant energy and momentum conservation equations for the first node in the axial direction can be obtained:

\[
h_{out}^i - h_{in}^i = \int_{T_{in}}^{T_{out}} C_p \left(T_c\right) dT_c = \frac{q_i^i}{A_c \rho_c u_c^i} \Delta i = \frac{q_i^i \Delta i}{w_c^i}
\]  

(21)

\[
P_{out}^i - P_{in}^i = -\frac{w_c^2}{A_c^2} \left(\frac{1}{\rho_{c,out}^i} - \frac{1}{\rho_{c,in}^i}\right) - \rho_c^i g \Delta i = -\frac{f w_c^2 \Delta i}{2D_c \rho_c A_c^2}
\]  

(22)

Where \(C_p\) is the specific heat capacity of the coolant; \(\Delta i\) is the distance between the axial nodes.

In the known core axial power distribution, coolant inlet temperature and mass flow rate, the top node is calculated one by one from the bottom node according to equation (21), and the distribution of axial coolant to enthalpy is obtained, and according to the ratio of enthalpy and temperature. The relationship can be used to determine the axial temperature and density distribution of the coolant. Substituting the coolant temperature values into equation (20) and equation (21), the temperature
distribution of the fuel pellets and cladding in the axial and radial directions can be calculated. Knowing the inlet pressure of the coolant passage, the outlet pressure of the coolant can be calculated successively by the formula (22), so that the inlet and outlet pressure drop of the core under steady state conditions can be obtained.

4. Physical thermal coupling iterative process

In the steady-state calculation of the ADS core, the heat generated by the nuclear fuel fission reaction, which transfers heat to the flowing coolant through the pellet and cladding, is carried out of the core, which in turn is due to changes in fuel pellet temperature and coolant density. It will affect the reaction cross section of neutrons and nuclear fuel, which will affect the power distribution of the core, and the change of power distribution will further affect the value of fuel pellet temperature and coolant density. Therefore, the physical thermal parameters are coupled to each other during this solution process, and iterative calculations are needed to achieve convergence conditions.

In order to consider the influence of thermal feedback on neutronics parameters, the ADS core physics thermal coupling program ARTAP is established in this paper. The macroscopic section parameters under different working conditions were generated by the DRAGON program. The MCNPX program calculated the proton beam and the LBE target spallation to generate the external neutron source. From the initial assumed core coolant density and fuel pellet temperature distribution, the initial macroscopic section parameters can be obtained, and the core neutronics model is solved according to the source iteration method to obtain the power density distribution of the core. In the case of known power density distributions, the single channel thermal hydraulic model can be used to derive the coolant density and fuel pellet temperature distribution required for the next iteration. If the calculated physical thermal parameters do not satisfy the convergence condition, the value of the section parameter is updated, and the above calculation process is repeated until the specified convergence precision is reached. The ARTAP program calculates the sub-critical core physical thermal-mechanical coupling iterative process with no external neutron source, so that the subcriticality of ADS and the steady-state physical thermal parameters of the core can be obtained.

5. Model verification

In order to verify the accuracy of the ARTAP steady-state program, this paper selects the steady-state calculated values in the OECD/NEA benchmark questions for comparison [5]. The accuracy of the program developed in this paper is verified from two perspectives: the point heap model based simulation program and the 3D neutron transport based simulation program. The axial temperature distribution of the fuel element and the coolant passage and the key parameters of the core are calculated as shown in figure 4 and table 1, respectively, and compared with the calculation results of other verification procedures.

As shown in figure 4, the axial temperature distribution of the fuel pellet, cladding and coolant calculated by the ARTAP program is located between the numerical results calculated by other research institutions in the benchmark problem, and the maximum relative deviation is less than 1.2%. The calculated values of the surface temperature of the cladding and the axial temperature distribution of the coolant channel agree well with the verification values; the calculated value deviation between the center of the fuel pellet and the surface temperature is slightly larger because of the radial heat conduction to the fuel rod. The calculation uses different physical empirical relationships, the division of nodes, and the difference in the treatment of the inner hole of the fuel pellet.

| parameters       | Reference | Result of ARTAP | Relative error/% |
|------------------|-----------|-----------------|-----------------|
| $k_{eff}$        | 0.97276   | 0.97087         | 0.19            |
| Power/MW         | 80        | 79.91           | 0.11            |
| Outlet temperature/K | 673       | 672.8           | 0.03            |
Figure 4. ADS core fuel pellet, cladding and coolant axial temperature distribution.

From the comparison results in table 1, it can be seen that the key physical thermal parameters calculated by ARTAP agree well with the reference values. Through the calculation and analysis of the ADS benchmark problem, the accuracy of the steady-state physical thermal calculation module of the ARTAP program is proved.

6. Conclusions
In this paper, a steady-state physical thermal coupling model of ADS core is established. For steady-state calculations, the neutron diffusion model is used for subcritical core neutronics analysis, the DRAGON program is used to generate macroscopic section parameters, and the high-energy particle transport program MCNPX is used to calculate the neutron source distribution outside the core. The thermal hydraulic model includes the fuel element heat transfer model and the coolant channel heat transfer model were developed and the corresponding physical properties were developed. The source iterative method is used to solve the steady-state physical thermal coupling equations. In the iterative process, the subcritical core model without external source is calculated first, and the subcriticality of the ADS core is obtained, and the subcritical core with external source is calculated. Model to obtain steady state physical thermal parameters. The accuracy of the steady state model was verified by the OECD/NEA benchmark.

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