

DAYU3D: A modern code for HTGR thermal-hydraulic design and accident analysis

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Abstract

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Full Text

Preamble

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Abstract

DAYU3D is a modern three-dimensional (3D) computer code for thermal-hydraulic design and accident analysis in high temperature gas-cooled reactors

(HTGRs), developed by the Institute of Nuclear and New Energy Technology (INET) at Tsinghua University. Compared to traditional codes like TINTE, the DAYU3D code has advantages due to its refined framework, improved models, and more efficient algorithms. It is able to simulate the continuous movement of control rods and is more rigorous in treating radiation heat transfer and break mass flow. Advanced computational methods significantly improve the computational efficiency of DAYU3D, achieving a time reduction of over 60% compared to TINTE. Extensive verification and validation with more than 100 cases demonstrate that DAYU3D is promising for HTGR 3D thermal-hydraulic design and accident analysis.

Keywords: High temperature gas-cooled reactor; Thermal-hydraulic design and accident analysis code; Three-dimensional; DAYU3D

1 Introduction

Modular pebble-bed high temperature gas-cooled reactors (HTGRs) represent an advanced reactor design due to their inherent safety features. The core of a pebble-bed HTGR is composed of a large number of fuel pebbles and utilizes TRISO-coated fuel particles to enhance reactor safety. Single-phase helium is typically employed as coolant, enabling high core outlet temperatures of 750°C. Due to the distinct thermal-hydraulic and structural features of HTGRs compared to other reactor types, specialized computer codes are required for thermal-hydraulic design and accident analysis.

Over the past few decades, several two-dimensional (2D) codes have been developed worldwide. Among these, the THERMIX [1,2] and TINTE [3] codes developed by Forschungszentrum Jülich GmbH (FZJ) in Germany are widely used in the thermal-hydraulic design and safety analyses of multiple pebble-bed HTGRs, including AVR [4,5], PBMR [6], HTR-10 [7,8], and HTR-PM [9,10].

With growing demands for higher-fidelity analysis of three-dimensional (3D) phenomena in HTGRs, various institutions have developed 3D thermal-hydraulic analysis codes. Notable developments include the MGT-3D code by Jülich (Germany) [11], the ATTICA3D code from Stuttgart University (Germany) [12,13], and the PRONGHORN code developed at Idaho National Laboratory (USA) [14].

In China, the Institute of Nuclear and New Energy Technology (INET) at Tsinghua University has conducted sustained research on pebble-bed HTGRs. Based on the framework and models of THERMIX, INET developed the two-dimensional DAYU code using Fortran. The DAYU code maintains the main functions of THERMIX while demonstrating enhanced performance in fuel temperature [15] and flow-field calculations [16]. However, the framework and algorithms employed in the DAYU code exhibit lower scalability and computational efficiency, making them unsuitable for addressing complex 3D problems. Therefore, a modern C++ code named DAYU3D has been developed, adopting a completely new code framework with good extensibility compared to the pre-

vious DAYU code. It will also serve as an excellent platform for investigating innovative methodologies in HTGR thermal hydraulics.

This paper presents the latest development status of DAYU3D. The remainder of the paper is organized as follows. Section 2 presents the mathematical models and code framework implemented in DAYU3D. Section 3 introduces the new features of DAYU3D. Section 4 presents numerical results from code verification and validation. Concluding remarks are presented in Section 5.

2.1 Thermal hydraulics models

The governing equation for solid temperature is:

$$\rho_s c_{p,s} \frac{\partial T_s}{\partial t} = \nabla \cdot (\lambda_s \nabla T_s) + q_s$$

where ρ , c_p , and λ represent density, specific heat, and thermal conductivity, respectively. t denotes time, and T is temperature. Subscripts s and g represent solid and gas, respectively. q_s is the heat source of the solid. q_{gs} is the heat transferred between gas and solid, calculated by Eq. (2) as follows:

$$q_{gs} = \frac{A_{gs} h_{gs} (T_g - T_s)}{V_{mesh}}$$

where A_{gs} and h_{gs} represent the heat transfer area and convective heat transfer coefficient between solid and gas, respectively; V_{mesh} is the mesh volume.

The DAYU3D code incorporates various empirical correlations for the thermal conductivity and specific heat of commonly used materials in HTGRs [17], such as pebble beds, matrix graphite of fuel pebbles, reflectors, carbon bricks, and concrete. In the pebble bed region, the Zehner-Schlunder formula [18], the Robold formula [19], and the Barthels formula [20] are employed to calculate the pebble-bed effective thermal conductivity.

Radiation heat transfer is also considered in DAYU3D. To simplify calculations, anisotropic effective thermal conductivity is utilized to simulate radiation heat transfer, a proven practice in the TINTE program [21]. Moreover, DAYU3D incorporates a more accurate heat radiation model based on view factor [22].

For gas flow and gas temperature calculations, the porous media model is employed. The mass, momentum, and energy conservation equations are as follows:

$$\frac{\partial(\phi \rho_g)}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}) = S$$

$$\frac{\partial(\phi \rho_g \mathbf{u})}{\partial t} + \nabla \cdot (\rho_g \mathbf{u} \mathbf{u}) = -\phi \nabla p - \mathbf{W} \mathbf{u} + \phi \rho_g \mathbf{g}$$

$$\frac{\partial(\phi\rho_g c_{p,g} T_g)}{\partial t} + \nabla \cdot (\rho_g c_{p,g} T_g \mathbf{u}) = \nabla \cdot (\phi \lambda_g \nabla T_g) + q_{gs} + q_{src}$$

where ϕ is porosity, \mathbf{u} represents superficial velocity, S is mass source, p denotes gas pressure, \mathbf{W} represents resistance coefficient, and \mathbf{g} is gravitational acceleration. Subscript g represents gas phase. q_{src} is the energy carried by the mass source, calculated by:

$$q_{src} = S c_{p,g} T_{src}$$

where subscript src represents mass source.

Helium properties are calculated using KTA formulas [23]. Flow resistance and convective heat transfer inside the pebble bed are calculated according to KTA standards [24]:

$$Nu = 1.27 \frac{1}{\phi} Pr^{1/3} + \frac{1.27}{\phi^{1.5}} Pr^{1/3} Re^{0.36}$$

where Re , Nu , and Pr represent Reynolds number, Nusselt number, and Prandtl number, respectively; d is hydraulic diameter.

In the pebble-bed region, the temperature distribution inside the fuel pebble is calculated. The governing equation for fuel pebble temperature is the one-dimensional (1D) heat conduction equation in spherical coordinates:

$$\rho_{fe} c_{p,fe} \frac{\partial T_{fe}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\lambda_{fe} r^2 \frac{\partial T_{fe}}{\partial r} \right) + q_{fe}$$

where r is radius, subscript fe represents fuel element (i.e., fuel pebble), and q_{fe} denotes nuclear power density inside the fuel pebble.

Since online refueling is used in pebble-bed HTGRs, different batches of fuel pebbles may exist in one porous media mesh, as shown in Fig. 1 [Figure 1: see original paper]. Because different batches of fuel elements have different power, they have different surface temperatures. Therefore, radiation heat transfer occurs between different batches of fuel spheres within the same mesh. The amount of radiation heat received by a single sphere of the j th batch from other batches can be calculated by [21,25]:

$$q_{rad,j} = \sum_{n=1}^{N_{batch}} \left[\frac{4\pi R^2 \varepsilon_j \varepsilon_n \sigma (T_n^4 - T_j^4)}{\varepsilon_{avg}} \right] \cdot \frac{n_p}{V_{mesh}}$$

where R is pebble radius; ε and T denote surface emissivity and surface temperature of fuel pebble, respectively; subscripts n and j represent the n th and

j th batch of fuel pebble, respectively; ε_{avg} is average surface emissivity; n_p is the fraction of the n th batch.

Fuel particle temperature is calculated using the lumped-heat-capacity method, considering the relatively small size of fuel particles. Once the temperature of each shell layer in the fuel sphere has been determined, the temperature of representative particles in each shell layer (as shown in Fig. 1) can be quickly calculated by:

$$T_{fp} = T_{fe} - f_{\alpha} q_{fe}$$

where subscript fp represents fuel particle, T_{fe} is fuel pebble temperature in one shell layer, and f_{α} represents thermal resistance between the fuel particle and matrix graphite.

2.2 Neutronics models

The neutronics kinetics calculation for HTGR is implemented in the DAYU3D code system, employing a 3D cylindrical ($r-z-\theta$) geometry to model coupled neutronic/thermal-hydraulic (N/TH) transient behavior.

The predictor-corrector quasi-static method (PCQS) is utilized to solve the space-time neutronics kinetics equation, which is written as:

$$\frac{1}{v_g(\mathbf{r}, t)} \frac{\partial \phi_g(\mathbf{r}, t)}{\partial t} = \nabla \cdot D_g(\mathbf{r}, t) \nabla \phi_g(\mathbf{r}, t) - \Sigma_{r,g}(\mathbf{r}, t) \phi_g(\mathbf{r}, t) + \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) + \chi_{p,g}(\mathbf{r}, t) \sum_{g'=1}^G (1-\beta) \nu \Sigma_{f,g'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t)$$

$$\frac{\partial C_i(\mathbf{r}, t)}{\partial t} = \beta_i \sum_{g'=1}^G \nu \Sigma_{f,g'}(\mathbf{r}, t) \phi_{g'}(\mathbf{r}, t) - \lambda_i C_i(\mathbf{r}, t), \quad i = 1, 2, \dots, 6$$

where $\phi_g(\mathbf{r}, t)$ is the g th group neutron flux (similarly hereinafter), v_g is averaged velocity, $D_g(\mathbf{r}, t)$ is diffusion coefficient, $\Sigma_{r,g}$ is removal cross section, $\Sigma_{s,g' \rightarrow g}$ is scattering cross section from the g' th group to the g th group, $\nu \Sigma_{f,g'}$ is fission production cross section, $\chi_{p,g}$ is prompt fission spectrum, $C_i(\mathbf{r}, t)$ is concentration of the i th group delayed precursor, λ_i is decay constant of the i th precursor group, and β_i is production fraction of the i th precursor group.

The equation includes six groups of delayed neutron precursor groups. The quasi-static approach decomposes the neutron flux into two components:

$$\phi_g(\mathbf{r}, t) = N(t) \psi_g(\mathbf{r}, t)$$

$$C_i(\mathbf{r}, t) = C_i(t) \chi_i(\mathbf{r}, t)$$

where $N(t)$ and $C_i(t)$ are amplitude functions representing the rapidly varying global population of flux and precursor concentration, respectively. $\psi_g(\mathbf{r}, t)$ and $\chi_i(\mathbf{r}, t)$ are shape functions describing the spatial distribution of flux and precursor concentration, which change slowly over time. To ensure uniqueness of the decomposition, a normalization condition is imposed on the shape function using the adjoint flux:

$$\int \psi_g^\dagger(\mathbf{r}) \psi_g(\mathbf{r}, t) d\mathbf{r} = 1, \quad g = 1, \dots, G$$

The adjoint flux is obtained by solving the eigenvalue adjoint diffusion equation.

PCQS consists of predictor and corrector phases, which solve shape and amplitude functions, respectively. In the predictor phase, the space-time equation is temporally discretized into large steps and solved using an implicit scheme, as shown in Eq. (16):

$$\frac{1}{v_g} \frac{\psi_g^{n+1} - \psi_g^n}{\Delta t} = \nabla \cdot D^{n+1} \nabla \psi_g^{n+1} - \Sigma_{r,g}^{n+1} \psi_g^{n+1} + \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}^{n+1} \psi_{g'}^{n+1} + \chi_{p,g}^{n+1} \sum_{g'=1}^G (1-\beta) \nu \Sigma_{f,g'}^{n+1} \psi_{g'}^{n+1} + \sum_{i=1}^6 \lambda_i C_i^{n+1}$$

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \beta_i \sum_{g'=1}^G \nu \Sigma_{f,g'}^{n+1} \psi_{g'}^{n+1} - \lambda_i C_i^{n+1}, \quad i = 1, \dots, 6$$

Then, using the normalization condition of Eq. (15), the shape function is obtained as follows:

$$\psi_g^{n+1} = \frac{\psi_g^{n+1,*}}{\int \psi_g^\dagger \psi_g^{n+1,*} d\mathbf{r}}, \quad g = 1, \dots, G$$

In the corrector phase, substituting Eq. (14) and Eq. (15) into Eq. (13) yields the point-kinetics equation for the amplitude function:

$$\begin{aligned} \frac{dN(t)}{dt} &= \frac{\rho(t) - \beta}{\Lambda} N(t) + \sum_{i=1}^6 \lambda_i C_i(t) \\ \frac{dC_i(t)}{dt} &= \frac{\beta_i}{\Lambda} N(t) - \lambda_i C_i(t), \quad i = 1, \dots, 6 \end{aligned}$$

where the point-kinetics parameters are defined by:

$$\Lambda(t) = \frac{1}{\sum_{g=1}^G \int \psi_g^\dagger(\mathbf{r}) \frac{1}{v_g} \psi_g(\mathbf{r}, t) d\mathbf{r}}$$

$$\rho(t) = \frac{\sum_{g=1}^G \int \psi_g^\dagger(\mathbf{r}) \left[\chi_{p,g}(\mathbf{r}, t) \sum_{g'=1}^G (1 - \beta) \nu \Sigma_{f,g'}(\mathbf{r}, t) - \Sigma_{r,g}(\mathbf{r}, t) + \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(\mathbf{r}, t) \right] \psi_{g'}(\mathbf{r}, t) d\mathbf{r}}{\sum_{g=1}^G \int \psi_g^\dagger(\mathbf{r}) \chi_{p,g}(\mathbf{r}, t) \sum_{g'=1}^G (1 - \beta) \nu \Sigma_{f,g'}(\mathbf{r}, t) \psi_{g'}(\mathbf{r}, t) d\mathbf{r}}$$

To precisely capture the rapid variation of the amplitude function, the point-kinetics equation is discretized and solved over minor time steps, which also requires simultaneous updating of point-kinetics parameters. Considering that the shape function appears in the expression of point-kinetics parameters as shown in Eq. (19), it is necessary to interpolate the shape functions obtained over large steps into the nested minor steps. Fig. 2 [Figure 2: see original paper] summarizes the time-step division and solution process of PCQS.

Compared with the traditional implicit method used in TINTE, PCQS enables the use of large time steps for solving high-dimensional shape equations and minor time steps for low-dimensional amplitude equations, which remarkably improves computational efficiency while maintaining accuracy.

Furthermore, the neutronics calculation module of DAYU3D employs a two-level meshing system. The coarse-level mesh characterizes the spatial distribution of macroscopic cross sections and covers some mesh grids for solid temperature computation, which are user-defined as neutronics zones. The fine-level mesh is generated by imposing refined division on the coarse-level mesh and is used to spatially discretize the space-time kinetics equation using the finite-volume method.

The multi-group macroscopic cross section corresponding to each coarse-level grid is represented by fourth-order polynomial expansions parameterized by temperatures of fuel particles and graphite moderators:

$$\Sigma(\mathbf{T}_{fuel}, \mathbf{T}_{mod}) = \Sigma_{base} + \sum_{i=1}^4 f_i \cdot (\mathbf{T}_{fuel} - \mathbf{T}_{fuel,base})^i + \sum_{j=1}^4 g_j \cdot (\mathbf{T}_{mod} - \mathbf{T}_{mod,base})^j$$

where \mathbf{T}_{fuel} and \mathbf{T}_{mod} are temperatures of fuel particle and graphite moderator, $\mathbf{T}_{fuel,base}$ and $\mathbf{T}_{mod,base}$ are basis temperatures, Σ_{base} is macroscopic cross section at basis state, and f_i, g_j are higher-order expansion coefficients. The polynomial expansions are generated by the PANGU program [27,28], developed for HTGR physics design. During coupled neutronics and thermal-hydraulics calculations, macroscopic cross sections are dynamically generated by fitting real-time temperatures into the polynomial expansions.

2.3 Code framework

The DAYU3D code employs a modular design to facilitate software development and code maintenance. The code structure and modular composition are shown in Fig. 3 [Figure 3: see original paper].

The top-level modules include the input module, calculation module, and output module. The input and output modules primarily handle XML-formatted input files, restart files, and result outputs. The calculation module manages thermal-hydraulics and neutronics calculations. The thermal-hydraulic calculation comprises several sub-modules: 3D solid temperature module, multi-batch fuel pebble and particle temperature module, 3D fluid flow module, 3D fluid temperature module, and 3D neutronics module. The calculation module also contains sub-modules for initialization, matrix solving, and material property calculations.

The computation flowchart of DAYU3D is shown in Fig. 4 [Figure 4: see original paper]. The Picard iteration framework is employed to address N/TH coupling problems. Different time steps are allowed for neutronics and thermal-hydraulics calculations to accommodate their respective time scales and numerical stability requirements. A nested Picard iteration is incorporated within the inner iteration of thermal-hydraulic fields to enhance both convergence and computational efficiency.

3 New features of DAYU3D

While ensuring high levels of user-friendliness and code maintainability, DAYU3D has implemented new capabilities and computational methods beyond traditional TINTE, THERMIX, and DAYU codes. This section summarizes some of the new features currently incorporated into DAYU3D.

3.1 Modelling of control rod' s continuous movement

In transient simulations, control rod insertion leads to drastic localized neutron flux changes, particularly near the control rod tip, known as the cusping effect. Due to mesh division limitations, the rod is often partially inserted into a coarse mesh in the axial direction, necessitating mesh grid homogenization. The difficulty lies in determining homogenized macroscopic cross sections of the mesh grid. The simple volume-weighted scheme cannot account for drastic gradients in local flux distribution. To address this issue, the TINTE code introduces the ROMO model and uses Eq. (21) to calculate the weighting factor [21]:

$$\omega = \frac{l}{L} + S \cdot \left(\frac{c_l - c}{c} \right) \cdot \left(1 - \frac{l}{L} \right)$$

However, since parameter S in Eq. (21) is empirical, users must continuously adjust its value to obtain a smooth control rod worth curve [21], where l is control rod insertion length, L is axial mesh length, c_l is absorber concentration when the rod is partially inserted, c is absorber concentration when fully inserted, and S is interpolation factor.

To overcome ROMO model limitations, an adaptive axial splitting method has been developed for DAYU3D, which fundamentally circumvents the homoge-

nization process. This method works as follows: during control rod movement, extra splitting is imposed on the axial layer of fine mesh grids where the control rod bottom is located in real-time. Once the bottom leaves this layer, adaptive axial merging restores the previously split layer, while another splitting is implemented according to the new position. Fig. 5 [Figure 5: see original paper] illustrates this process. It should be noted that the adaptive axial splitting method is imposed on the fine-level computation mesh, not the coarse-level mesh mentioned in Section 2.2, meaning the additional axial division does not impact mesh mapping between neutronics and thermal-hydraulic fields.

3.2 Rigorous radiation heat transfer model

In the initial stage of DAYU3D development, the gap radiation heat transfer model primarily referred to the TINTE code, where radiation heat transfer was treated as anisotropic heat conduction. This method equates heat transferred by radiation and conduction in each direction, thereby establishing relationships between thermal conductivities in different directions [17]. Consequently, principal components of thermal conductivity ($\lambda_1, \lambda_2, \lambda_3$) can be determined. The schematic of TINTE's heat radiation model is shown in Fig. 6 [Figure 6: see original paper]. However, this method introduces an assumption based on heat radiation between two infinite surfaces when calculating λ_1 [21], as shown in Eq. (22):

$$\lambda_1 = \lambda_{cond} + \frac{4\sigma\epsilon_s T_m^3 d}{1 + \frac{3}{4} \cdot \frac{\epsilon_s}{2-\epsilon_s} \cdot \frac{d}{\lambda_{cond}}}$$

where λ_1 is one principal component of thermal conductivity; T_1 and T_2 are temperatures of two surfaces; d indicates gap width; σ is the Stefan-Boltzmann constant; and ϵ_s is system emissivity of two surfaces. This assumption may lead to significant computational errors in wider gaps, such as the cavity at the reactor top.

To address this problem, a more accurate method based on 3D view factor and net radiation method is being developed in DAYU3D. Due to complex geometry in HTGRs, a numerical integration method is employed to compute view factors between surface elements. The calculated view factors agree well with reference results from Computational Fluid Dynamics (CFD) programs [22].

3.3 Improved break mass flow model

In the TINTE code, the mass flow model for break conditions does not account for pipe length and inlet pressure effects, leading to flow rate overestimation. To address this issue, a new set of formulas developed by Dou et al. [29] has been incorporated into DAYU3D to consider the impact of different pipe lengths and inlet pressures on critical flow. The critical mass flow rate is calculated by Eq. (23):

$$\dot{m} = A \cdot f \cdot \sqrt{\frac{p_0 \rho_0 \kappa}{2} \left(\frac{2}{\kappa + 1} \right)^{\frac{\kappa + 1}{\kappa - 1}}}$$

Numerical comparisons with CFD results indicate these formulas provide accurate calculations [29], effectively improving break flow simulation accuracy in DAYU3D. The correction factor f is calculated as follows:

If $L < 2$ m:

$$f = 1.0 - 0.1 \cdot \frac{L}{2}$$

If $2 \text{ m} \leq L \leq 10 \text{ m}$:

$$f = 0.9 - 0.05 \cdot (L - 2)$$

If $L > 10$ m:

$$f = 0.5 - 0.01 \cdot (L - 10)$$

where L is pipe length.

3.4 Efficient methods for solving flow field in HTGRs

In the traditional TINTE code, the fluid pressure equation is typically solved using TINTE matrix ordering and Gauss elimination [17]. However, this fixed solution strategy may be inefficient under complex conditions. To address this, DAYU3D introduces an efficient flow solver based on advanced matrix ordering, symbolic factorization, and block matrix techniques.

In the DAYU3D matrix ordering method, the longest path in one-dimensional (1D) flow regions is prioritized and placed at the front of the matrix. This method is termed “One-Dimensional Flow-path Priority Ordering” (ODFPO). ODFPO reduces the number of non-zero fill-ins during Gaussian elimination and makes the reordered matrix exhibit block-structured characteristics [30]. Therefore, ODFPO can be effectively combined with symbolic factorization and block matrix solving, respectively enhancing computational efficiency for 2D and 3D simulations. The computational time of DAYU3D is significantly reduced compared to TINTE [30].

3.5 Global and parallel calculation of multi-batch fuel temperature

In calculating multi-batch fuel temperature, the TINTE code adopts a batch-by-batch and grid-by-grid iteration approach, resulting in low computational efficiency. In DAYU3D, temperatures of all batches of fuel pebbles within one grid are solved simultaneously to avoid iteration between batches and improve calculation efficiency. Additionally, DAYU3D supports parallel computation of fuel pebble temperatures across all pebble-bed meshes, further enhancing efficiency.

4 Code verification and validation

Since DAYU3D is developed from scratch, all equations and models of thermal-hydraulic modules have been verified and validated through a series of constructed test cases, the SANA experiment, and HTGR cases.

4.1 Constructed cases

The verification matrix for thermal-hydraulic calculation is shown in Table 1. First, verification was carried out for individual calculation modules covering 1D, 2D, and 3D conditions, different materials, diverse flow regions, distinct boundary conditions, and both steady-state and transient conditions. After verifying individual modules, verification of coupled modules was conducted. Reference solutions include analytical solutions and calculated results from the TINTE code using identical input parameters. Verification results for DAYU3D are summarized in Table 2. The relative deviation compared to reference solutions is below 1%, and mostly below 0.2%.

A fully coupled example is presented in detail to demonstrate DAYU3D's accuracy. This simplified test case simulates steady-state conditions of a pebble-bed HTGR with 15 batches of fuel elements. Simulation results were compared against TINTE results, as shown in Fig. 7 [Figure 7: see original paper]. Solid temperature, helium temperature, and particle temperature exhibit good agreement with TINTE results.

4.2 SANA experiments

SANA experiments were conducted in Germany in the 1990s to illustrate heat transfer mechanisms in pebble beds [31]. The facility consists of a pebble bed, heating elements, insulating materials, and a pressure vessel, with thermocouples installed to measure temperature. SANA experiments tested comprehensive conditions [32,33], including both 2D and 3D heating conditions, making them highly suitable for validating 3D thermal-hydraulic codes for HTGRs. DAYU3D has performed calculations for all conditions involving helium-filled and 60 mm graphite pebbles. Example cases demonstrate DAYU3D's accuracy.

Comparison between DAYU3D calculations and experimental data for 2D SANA conditions is shown in Fig. 8 [Figure 8: see original paper]. For 2D conditions including full-length heating, upper-section heating, and lower-section heating of the central heating element, DAYU3D results accurately reflect temperature distribution within the pebble bed.

For 3D conditions, taking cases of central 0 kW with radial 3×9 kW ($0 + 3 \times 9$ kW) heating power and central 10 kW with radial 3×5 kW ($10 + 3 \times 5$ kW) heating power as examples, comparisons between DAYU3D and SANA experimental data are shown in Fig. 9 [Figure 9: see original paper] and Fig. 10 [Figure 10: see original paper]. Results illustrate that DAYU3D accurately calculates 3D temperature distribution caused by radial heating elements, showing

good agreement with experimental data.

4.3 3D HTR-PM case

Fig. 11 [Figure 11: see original paper] and Fig. 12 [Figure 12: see original paper] show the 3D calculation model of HTGR, including meshing and material settings. Helium inlet and outlet of the core are located only in the first sector. Control rod channels are assumed to be cooled by helium, whereas absorber ball channels remain uncooled. Coolant mass flow rate is 96 kg/s, with core inlet temperature set to 250°C and core outlet pressure maintained at 7 MPa. All control rods are inserted at $z = 275$ cm, while absorber balls are not dropped.

Solid temperature distribution within the pebble bed is shown in Fig. 13 [Figure 13: see original paper]. As helium flows from top to bottom of the pebble bed, temperature at the core bottom is higher while temperature at the top is lower. Additionally, due to influence from control rod and absorber ball channels, temperature at the periphery of the pebble bed is higher near $\theta = 0^\circ$, $\theta = 60^\circ$, and $\theta = 120^\circ$, while temperature in other sectors is lower. Solid temperature near 180° is generally lower than near 0° , primarily due to influence from the helium inlet in the core.

Temperature distribution on the pressure vessel sidewall is shown in Fig. 14 [Figure 14: see original paper]. The vessel temperature distribution exhibits two characteristics: first, temperature is lower in the upper region and higher in the lower region; second, temperature is higher near the helium inlet and lower farther from it. The first characteristic is mainly influenced by temperature distribution in the pebble bed region, where upper core temperature is lower and lower core temperature is higher. The second characteristic occurs because 250°C helium entering the reactor pressure vessel heats the vessel. Therefore, the helium inlet affects both pressure vessel temperature distribution and pebble bed region temperature distribution.

4.4 Performance analysis

Typical HTR-PM test cases, including steady state and depressurized loss of forced cooling accident (DLOFC), were calculated to examine DAYU3D's computational efficiency. In the DLOFC case, coolant pressure is assumed to drop instantaneously to 1 atm at accident onset. To ensure fair comparison, all codes employ identical model setups, and all cases are executed sequentially without parallel acceleration. Calculation times for TINTE, MGT-3D, and DAYU3D are compared in Table 3. DAYU3D's total calculation time is reduced by about 90% compared to TINTE in 2D cases. For 3D cases, time reduction is also remarkable compared with MGT-3D. DAYU3D's efficiency advantage stems from two main factors: first, at the algorithm level, DAYU3D employs advanced linear system solvers such as the efficient flow field solving method; second, at the implementation level, extensive optimizations have been applied to data structures and memory management, reducing overhead associated with

dynamic memory allocation and improving overall computational performance.

5 Conclusion

DAYU3D is a modern and advanced tool for HTGR thermal-hydraulic design. This paper presented mathematical models, code framework, and new features of DAYU3D, along with numerical results for code verification and validation. DAYU3D represents significant improvements over traditional THERMIX and TINTE codes, including 3D calculation capabilities, continuous control rod movement, more rigorous radiation heat transfer and break mass flow models, advanced and efficient algorithms, and improved user-friendliness and code maintainability. Additionally, DAYU3D has undergone extensive verification and validation using more than 100 cases. For most cases, relative deviation from reference solutions is within 0.2%. Calculation time for HTR-PM cases is reduced by over 60% compared to TINTE, demonstrating DAYU3D's good accuracy and significant computational efficiency advantages.

In the future, DAYU3D will be further extended to enable more refined evaluation of residual heat, non-local energy deposition, chemical corrosion, etc. It will also be coupled with the PANGU code [27,28] for 3D neutronics, thermal-hydraulics, and fuel cycle simulation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

References

- [1] J. Banaschek, Berechnungsmethoden und Analysen zum dynamischen Verhalten von Kraftwerksanlagen mit Hochtemperaturreaktor, Kernforschungsanlage Jülich GmbH, <https://juser.fz-juelich.de/record/818375>. Zentralbibliothek, Verlag, Jülich,
- [2] J.C. Cleveland, S.R. Greene, Application of THERMIX-KONVEK code to accident analyses of modular pebble bed high temperature reactors (HTRs), Oak Ridge National Lab., TN (USA), 1986.

- [3] H. Gerwin, W. Scherer, E. Teuchert, The TINTE Modular Code System for Computational Simulation of Transient Processes in the Primary Circuit of a Pebble-Bed High-Temperature Gas-Cooled Reactor, *Nuclear Science and Engineering* 103 (1989) 302–312. <https://doi.org/10.13182/NSE89-A23682>.
- [4] K. Petersen, Zur Sicherheitskonzeption des Hochtemperaturreaktors mit natürlicher Wärmeableitung aus dem Kern im Störfall, Kernforschungsanlage Jülich GmbH, Zentralbibliothek, Verlag, Jülich, 1983. <https://juser.fz-juelich.de/record/819180>.
- [5] H. Gerwin, Das zweidimensionale Reaktordynamikprogramm TINTE Teil 2: Anwendungsbeispiele, Kernforschungsanlage Jülich GmbH, Zentralbibliothek, Verlag, Jülich, 1989. <https://juser.fz-juelich.de/record/820084>.
- [6] F. Reitsma, G. Strydom, J.B.M. de Haas, K. Ivanov, B. Tyobeka, R. Mphahlele, T.J. Downar, V. Seker, H.D. Gougar, D.F. Da Cruz, U.E. Sikik, The PBMR steady-state and coupled kinetics core thermal-hydraulics benchmark test problems, *Nuclear Engineering and Design* (2006). <https://doi.org/10.1016/j.nucengdes.2005.12.007>.
- [7] Z. Gao, L. Shi, Thermal hydraulic calculation of the HTR-10 for the initial and equilibrium core, *Nuclear Engineering and Design* 218 (2002) 51–64. [https://doi.org/10.1016/S0029-5493\(02\)00198-X](https://doi.org/10.1016/S0029-5493(02)00198-X).
- [8] Z. Gao, L. Shi, Thermal hydraulic transient analysis of the HTR-10, *Nuclear Engineering and Design* 218 (2002) 65–80. [https://doi.org/10.1016/S0029-5493\(02\)00199-1](https://doi.org/10.1016/S0029-5493(02)00199-1).
- [9] Y. Zheng, L. Shi, Y. Dong, Thermohydraulic transient studies of the Chinese 200MWe HTR-PM for loss of forced cooling accidents, *Annals of Nuclear Energy* 36 (2009) 742–751. <https://doi.org/10.1016/j.anucene.2009.02.007>.
- [10] Y. Zheng, M.M. Stempniewicz, Z. Chen, L. Shi, Study on the DLOFC and PLOFC accidents of the 200 MWe pebble-bed modular high temperature gas-cooled reactor with TINTE and SPECTRA codes, *Annals of Nuclear Energy* 120 (2018) 763–777. <https://doi.org/10.1016/j.anucene.2018.06.041>.
- [11] D. Shi, Extension of the Reactor Dynamics Code MGT-3D for Pebblebed and Blocktype High-Temperature-Reactors, RWTH Aachen University, 2015. <https://juser.fz-juelich.de/record/200843>.
- [12] K. Hossain, M. Buck, W. Bernnat, G. Lohnert, Asme, TH3D, A THREE-DIMENSIONAL THERMAL HYDRAULIC TOOL, FOR DESIGN AND SAFETY ANALYSIS OF HTRS, in: Fourth International Topical Meeting on High Temperature Reactor Technology, Volume 1, American Society of Mechanical Engineers Digital Collection, 2009: pp. 709–724.
- [13] A. Seubert, A. Sureda, J. Lapins, J. Bader, E. Laurien, The Transient 3-D Transport Coupled Code TORT-TD/ATTICA3D for High-Fidelity Pebble-Bed HTGR Analyses, *Transport Theory and Statistical Physics* 41 (2012) 133–152. <https://doi.org/10.1080/00411450.2012.671212>.
- [14] A.J. Novak, R.W. Carlsen, S. Schunert, P. Balestra, D. Reger, R.N. Slaybaugh, R.C. Martineau, Pronghorn: A Multidimensional Coarse-Mesh Application for Advanced Reactor Thermal Hydraulics, *Nuclear Technology* 207 (2021) 1015–1046. <https://doi.org/10.1080/00295450.2020.1825307>.
- [15] Y. Zheng, L. Shi, F. Chen, Coated Fuel Particle Temperature Analysis of

the Pebble-bed Modular High Temperature Gas-cooled Reactor, in: Guiyang, China,

- [16] H. Dou, M. Lang, H. Zhang, D. She, Analysis and Improvement of Flow Field Calculation in Thermal Hydraulic Program for High Temperature Gas-Cooled Reactor, in: American Society of Mechanical Engineers Digital Collection, 2022. <https://doi.org/10.1115/ICONE29-92090>.
- [17] H. Gerwin, Das zweidimensionale Reaktordynamikprogramm Tinte Teil 1: Grundlagen und Lösungsverfahren, Kernforschungsanlage Jülich GmbH, Zentralbibliothek, Verlag, Jülich, 1987. <https://juser.fz-juelich.de/record/820025>.
- [18] P. Zehner, E.U. Schlünder, Einfluß der Wärmestrahlung und des Druckes auf den Wärmetransport in nicht durchströmten Schüttungen, Chemie Ingenieur Technik 44 (1972) 1303-1308. <https://doi.org/10.1002/cite.330442305>.
- [19] K. Robold, Wärmetransport in der Randzone von Kugelschüttungen, Kernforschungsanlage Jülich GmbH, Zentralbibliothek, Verlag, Jülich, 1982. <https://juser.fz-juelich.de/record/818304>.
- [20] H. Barthels, Die effektive Wärmeleitfähigkeit in Kugelschüttungen unter besonderer Berücksichtigung des inneren und äußeren Strahlungsanteils beim Hochtemperatur-Reaktors, Kernforschungsanlage Jülich GmbH, Zentralbibliothek, Verlag, Jülich, 1984. http://juser.fz-juelich.de/record/819199/files/J%C3%BCl_1893_Barthels.pdf.
- [21] H. Gerwin, W. Scherer, A. Lauer, G. Strydom, TINTE - A two-dimensional code for reactor dynamics, Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag, Jülich, 2009. <https://juser.fz-juelich.de/record/820939>.
- [22] X. Xu, H. Zhang, Y. Zheng, D. She, Three-dimensional Radiation View Factor Calculation in DAYU3D Program, in: Beijing, China, 2024.
- [23] Nuclear Safety Standards Commission (KTA), KTA 3102.1 Reactor Core Design for High-Temperature Gas-Cooled Reactor. Part 1: Calculation of the Material Properties of Helium, (1978).
- [24] Nuclear Safety Standards Commission (KTA), KTA 3102.3 Reactor Core Design of High-Temperature Gas-Cooled Reactors. Part 3: Loss of Pressure through Friction in Pebble Bed Cores, (1981).
- [25] H. Zhang, D. She, L. Shi, Progress on the Development of DAYU3D Code for HTR Thermal-Hydraulic Design and System Analysis, in: American Society of Mechanical Engineers Digital Collection, Prague, Czech Republic, 2024. <https://doi.org/10.1115/ICONE31-134375>.
- [26] H. Gerwin, W. Scherer, A. Lauer, I. Clifford, TINTE - nuclear calculation theory description report, Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag, Jülich, 2010. <https://juser.fz-juelich.de/record/820954>.
- [27] D. She, B. Xia, J. Guo, C.-L. Wei, J. Zhang, F. Li, L. Shi, Z.-Y. Zhang, Prediction calculations for the first criticality of the HTR-PM using the PANGU code, NUCL SCI TECH 32 (2021) 90. <https://doi.org/10.1007/s41365-021-00936-5>.
- [28] D. She, J. Guo, Z. Liu, L. Shi, PANGU code for pebble-bed HTGR reactor physics and fuel cycle simulations, Annals of Nuclear Energy 126 (2019) 48-58. <https://doi.org/10.1016/j.anucene.2018.11.005>.
- [29] H. Dou, M. Lang, Y. Ji, Study on the critical flow of removal pipe breakage in high-temperature gas-cooled reactor, Progress in Nuclear Energy 176 (2024)

105367. <https://doi.org/10.1016/j.pnucene.2024.105367>.

[30] H. Zhang, B. Tan, D. She, L. Shi, An efficient method for solving flow field in high temperature gas-cooled reactor, *Progress in Nuclear Energy* 180 (2025) 105599. <https://doi.org/10.1016/j.pnucene.2024.105599>.

[31] B. Stoecker, H.-F. Niessen, Data sets of the SANA experiment 1994-1996, Forschungszentrum, Jülich Institute for Safety Research and Reactor Technology, Jülich, 1997. <https://www.osti.gov/etdeweb/biblio/553720> (accessed December 25, 2023).

[32] M. Lange, Experimente zur selbsttätigen Abfuhr der Nachwärme bei Hochtemperatur-Reaktoren: Planung, Vorbereitung Ergebnisse, Forschungszentrum, Jülich Institute for Safety Research and Reactor Technology, Jülich, 1995.

[33] J. Baggemann, D. Shi, S. Kasselmann, S. Kelm, H.-J. Allelein, A. Hurtado, Use of SANA experimental data for validation and verification of MGT-3D and a CFD porous media model for VHTR application, *Nuclear Engineering and Design* 305 (2016) 678-687. <https://doi.org/10.1016/j.nucengdes.2016.05.030>.

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