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Simultaneous approach for simulation of a high-temperature gas-cooled reactor*

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Abstract: The simulation of a high-temperature gas-cooled reactor pebble-bed module (HTR-PM) plant is discussed. This lumped parameter model has the form of a set differential algebraic equations (DAEs) that include stiff equations to model point neutron kinetics. The nested approach is the most common method to solve DAE, but this approach is very expensive and time-consuming due to inner iterations. This paper deals with an alternative approach in which a simultaneous solution method is used. The DAEs are discretized over a time horizon using collocation on finite elements, and Radau collocation points are applied. The resulting nonlinear algebraic equations can be solved by existing solvers. The discrete algorithm is discussed in detail; both accuracy and stability issues are considered. Finally, the simulation results are presented to validate the efficiency and accuracy of the simultaneous approach that takes much less time than the nested one.

Key words: Differential algebraic equations (DAEs), High-temperature gas-cooled reactor (HTR), Simulation, Simultaneous approach

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1 Introduction

The modular high-temperature gas-cooled reactor (MHTGR) is attractive because of its inherent safety features and potential economic competitiveness. A high temperature gas-cooled reactor pebble-bed module (HTR-PM) project was proposed and actively supported by the Chinese government to build an MHTGR demonstration plant (Li *et al.*, 2008b). The reactor model is fundamental to the study of the overall nuclear power plant performance and the design of appropriate control systems since it explains the interactions among the input and output variables, and also explains the nature of the basic dynamic relationships (Li *et al.*, 2008c). There exist many different approaches to the dynamic modeling of processes. Although the combination of distributed and lumped parameter models has been described in the previous studies, in most cases the lumped parameters paradigm is adopted because it is less complex and sufficient to describe physical phenomena encountered in process simulation (Colonna and van Putten, 2007). Li *et al.* (2008a; 2008b; 2008c) formulated a lumped parameter dynamic model of an HTR. The model developed in that work served as the basis for control performance analysis and model-based control system design. The simulation responses to the most important variables have been presented and the trends of these responses have been shown to be correct (Li *et al.*, 2008c). However, the efficiency of the simulation was not discussed.

Simulation is an important tool in the nuclear power industry. Considerable researches have been performed regarding novel nuclear power systems based on simulations that use mathematical models of nuclear reactions and the most up-to-date nuclear data

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available (Robbins and Hoggett-Jones, 2002). A software toolbox called SimECS (Simulation Library for Energy Conversion Systems) was presented in (Colonna and van Putten, 2007). It contains only components related to gas turbine systems, though the extension to components belonging to other energy systems is planned. In the nuclear power field, many processes were simulated by SIMULINK of MATLAB software (Li *et al.*, 2008b; 2008c; Dong *et al.*, 2009; Shirazi *et al.*, 2010).

The HTR-PM model consists of many differential algebraic equations (DAEs). The DAE formulation consists of equations that describe the dynamic behavior of the system, such as mass and energy balances, and algebraic equations that ensure physical and thermodynamic relations (Biegler *et al.*, 2002). It is very difficult or even impossible to obtain an analytical solution of a dynamic mathematical model (Ni, 1996; Lv, 2002). Because of the amazing increase in computational efficiency and decrease in computational cost, one can solve the dynamic mathematical model with numerical methods.

Nuclear reactions occur in the core of the reactor. This process is described by the point neutron kinetics equations, which are stiff equations. The predictor-corrector Gear method with variable step size, the high-order generalized Lunge-Kutta method, etc., are commonly used methods to deal with stiff ordinary differential equation (ODE) (Cai, 2005). In the HTR-PM, there are many related algebraic equations beside the fundamental conservation of mass, energy, and momentum, creating a more mathematically demanding DAE than does the ODE system.

DAEs can be solved by extended ODE solvers. In a nested approach, the values of the differential variables are given at the *n*th iteration, and the algebraic equations are solved numerically. The algebraic variables can be expressed by differential variables. Then the expressions are substituted into differential equations and the DAEs system is transferred into an ODE system without algebraic equations. Thus, classical ODE solvers can be used. Eventually, the differential variables are obtained and they are the initial values of the (n+1)th iteration.

The nested approach—up to now most commonly used—requires numerical inversion of the algebraic equations: each evaluation of the vector of derivatives (called by the ODE solver) has to start an iterative procedure to solve the algebraic equation. This approach can be very expensive and time-consuming due to these inner iterations (Breitenecker and Popper, 2009), and the approach is very inefficient for stiff problems (Hangos and Cameron, 2001). This approach is appropriate when there are few algebraic equations and no algebraic loop (Lv, 2002). However, there are 58 equations in the HTR simulation model, among which, 45 equations are algebraic equations.

We have applied simultaneous approach to simulate the HTR model. Here the DAEs are discretized over a time horizon using collocation on finite elements. Radau collocation points are applied to deal with the stiff equations. Consequently, the resulting nonlinear algebraic equations can be solved by existing solvers. All the variables are solved at the same time instead of being solved in a temporal sequential mode as the nested approach does. The DAE system is solved only once. Therefore, intermediate solutions that may not exist or may require excessive computational cost can be avoided (Biegler *et al.*, 2002). The simultaneous approach already has many successful applications in dynamic optimization within the chemical process industry (Tobias *et al.*, 2003; Antonio *et al.*, 2005; Kameswaran and Biegler, 2006; Biegler, 2007).

2 Description of the HTR

A low-order dynamic model with a clear physical meaning is useful for real-time simulation, control characteristic research, and control system design. In this study, we consider the lumped parameter dynamic model of HTR. According to some general assumptions (Li *et al.*, 2008c), the reactor is nodalized to include eight sections, namely, core, reflector, lower plenum, lower header, riser, upper header, downcomer, and outlet header. Fig. 1 shows the nodalization of the reactor (Li *et al.*, 2008b).

The dynamic mathematical model of reactor is based on the fundamental conservation of mass, energy, and momentum, combined by algebraic equations. The differential equations are as follows:

$$\frac{\mathrm{d}T_\mathrm{c}}{\mathrm{d}t}=\frac{P_{100}n_\mathrm{r}-\alpha_5A_5(T_\mathrm{c}-T_5)-\alpha_\mathrm{cr}A_\mathrm{cr}(T_\mathrm{c}-T_\mathrm{r})}{\rho_\mathrm{c}C_\mathrm{c}V_5(1-\varepsilon_5)}, \quad (1)$$

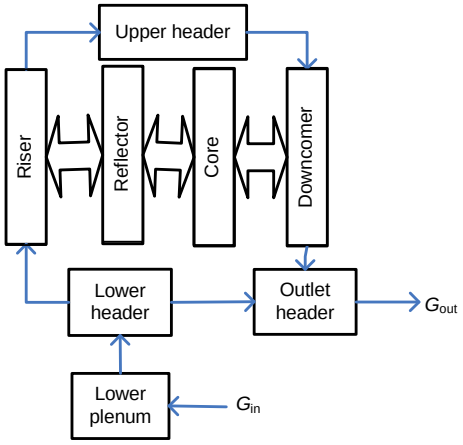

Fig. 1 Nodalization of the HTR

G_{in} and G_{out} indicate the input and output mass flow rates, respectively

$$\frac{\mathrm{d}n_r}{\mathrm{d}t}=\frac{\rho-\beta}{\Lambda}n_r+\sum_{i=1}^{6}\frac{\beta_i}{\Lambda}C_{ri}, \tag{2}$$

$$\frac{\mathrm{d}C_{ri}}{\mathrm{d}t}=\lambda_i n_r-\lambda_i C_{ri},\ i=1,2,\cdots,6, \tag{3}$$

$$\frac{\mathrm{d}T_r}{\mathrm{d}t}=\frac{\alpha_{cr}A_{cr}(T_c-T_r)-\alpha_3A_3(T_r-T_3)}{\rho_rC_rV_r}, \tag{4}$$

$$\frac{\mathrm{d}T_1}{\mathrm{d}t}=\frac{G_{in}}{\rho_1V_1}(T_{in}-T_1), \tag{5}$$

$$\frac{\mathrm{d}T_3}{\mathrm{d}t}=\frac{G_{23}C_p(T_2-T_3)+\alpha_3A_3(T_r-T_3)}{\rho_3C_pV_3}, \tag{6}$$

$$\frac{\mathrm{d}T_5}{\mathrm{d}t}=\frac{G_4C_p(T_4-T_5)+\alpha_5A_5(T_c-T_5)}{\rho_5C_p\varepsilon_5V_5}, \tag{7}$$

$$\frac{\mathrm{d}T_6}{\mathrm{d}t}=\frac{1}{\rho_6V_6}\left[G_5(T_5-T_6)+G_{26}(T_2-T_6)\right], \tag{8}$$

where V is volume (m^3), C is specific heat (J/(kg·K)), T is temperature (K), G is flow rate, P_{100} is the rated power of the reactor, C_r is the concentration of precursor, C_p is the specific heat at a constant pressure. ρ_{rod} is the control rod reactivity, α is reactivity coefficient, ε is porosity, ρ is density (kg/m^3), λ is decay constant, n_r is the relative density of neutron (power percentage), β is the delayed neutron fraction, and Λ is the neutron generation time. The subscripts c, cr, f, in, m, out, p, and r indicate core, core to reflector, fuel, input, moderator, output, pressure, and reflector, respectively. i indicates the ith delayed neutron. The numbers 0, 1, 2, 3, 4, 5, and 6 is steady-state, lower plenum, lower header, riser, upper header, downcomer, and outlet header, respectively.

These differential equations, together with the related algebraic equations, constitute the state space mathematical model of the reactor. Among the algebraic equations, some of them present the balance of the pressure, relationship of temperatures and flow rates in different parts of the reactor, and the others are physical property equations. The details of relevant parameters, correlations, and design parameters are contained in (Li *et al.*, 2008b; 2008c).

There are 13 differential equations and 45 algebraic equations. There are 58 variables, so the degree of freedom of this model is zero. Here, T_c, T_r, n_r, C_{ri}, T_1, T_3, T_5, and T_6 are differential variables.

Let $\boldsymbol{z}$ denote all of the differential variables and $\boldsymbol{y}$ denote algebraic variables. We can obtain the following DAEs:

$$\begin{aligned}\boldsymbol{z}'(t)&=\boldsymbol{f}(t,\boldsymbol{z}(t),\boldsymbol{y}(t)),\\ 0&=\boldsymbol{g}(t,\boldsymbol{z}(t),\boldsymbol{y}(t)).\end{aligned} \tag{9}$$

Eq. (9) is Hessenberg formal semi-explicit DAE, where the differential variables can be expressed explicitly by the algebraic variables $\boldsymbol{z}(t)$. For the semi-explicit DAEs, the algebraic variables $\boldsymbol{y}(t)$ can be determined uniquely by algebraic equations if $\frac{\partial g}{\partial y}$ is non-singular at any moment. Here, the DAE system is defined as index-1 (Ascher and Petzold, 1998; Betts, 2001), and the reactor model is an index-1 DAE system according to the definition.

3 Simultaneous approach

Simultaneous approach (fully discrete approach) is a direct approach that applies solvers for nonlinear algebraic equations after discretization. Thus, the DAE system is solved only once. Therefore, intermediate solutions that may require excessive computational effort or may not even exist can be avoided (Cervantes and Biegler, 1999; Kameswaran and Biegler, 2006).

The dynamic behaviors of the process systems could be described using DAEs. We consider the

general proposition in the following (Biegler *et al.*, 2002; Kameswaran and Biegler, 2006; Biegler, 2007).

Problem 1:

$$\begin{aligned}
&\boldsymbol{z}'(t) = \boldsymbol{f}(\boldsymbol{z}(t), \boldsymbol{y}(t), \boldsymbol{u}(t), \boldsymbol{p}), \boldsymbol{z}(t_0) = \boldsymbol{z}_0,\\
&\boldsymbol{g}(\boldsymbol{z}(t), \boldsymbol{y}(t), \boldsymbol{u}(t), \boldsymbol{p}) = 0,\\
&\boldsymbol{g}_{\mathrm{f}}(\boldsymbol{z}(t_{\mathrm{f}})) = 0,\\
&\boldsymbol{z}_{\mathrm{L}} \le \boldsymbol{z}(t) \le \boldsymbol{z}_{\mathrm{U}}, \boldsymbol{u}_{\mathrm{L}} \le \boldsymbol{u}(t) \le \boldsymbol{u}_{\mathrm{U}}, \boldsymbol{y}_{\mathrm{L}} \le \boldsymbol{y}(t) \le \boldsymbol{y}_{\mathrm{U}},
\end{aligned}$$

where the subscripts L and U indicate the lower bound and upper bound, respectively.

The unknowns are differential state variables $\boldsymbol{z}(t)\in\mathbb{R}^n$, algebraic variables $\boldsymbol{y}(t)\in\mathbb{R}^m$, control variables $\boldsymbol{u}(t)\in\mathbb{R}^\pi$, and time independent variables $\boldsymbol{p}\in\mathbb{R}^q$, $t\in[t_0,t_{\mathrm{f}}]$. In addition, f_i (i=1,2,…,n), g_i (i=1,2,…,m), and $g_{\mathrm{f},i}$ (i=1,2,…,r) are components of vectors $\boldsymbol{f}$, $\boldsymbol{g}$, and $\boldsymbol{g}_{\mathrm{f}}$, respectively.

Fully discrete approaches are often currently applied to solve DAEs (Betts, 2001), and they are equivalent to the projected implicit Runge-Kutta integration (Feehery *et al.*, 1995). For DAEs in semi-explicit Hessenberg form, results based on the implicit Runge-Kutta methods are shown to be valid for linear constant coefficient systems of arbitrary index, along with nonlinear index-1 and index-2 systems (Feehery *et al.*, 1995).

The simultaneous approach requires efficient and precise discrete techniques. The orthogonal collocation on finite element method (OCFE) is a well-known method with high-order accuracy and excellent stability properties, and it is a less expensive way to obtain accurate solutions compared with other methods (Biegler, 2007). According to OCFE, the computational domain is divided into finite non-overlapped and connective elements. Some proper points are chosen as collocation points and then the values of the variables and their derivatives at these points are obtained. The differential variables are rewritten as the linear expression of the values and an interpolative function. The Lagrange polynomial is the most commonly used interpolation polynomial function, and internal residuals on collocation points should be zero in the collocation method.

The whole integral region is divided into several elements $t_0<t_1<\ldots<t_{\mathrm{NE}}=t_{\mathrm{f}}$ (NE is the number of the elements), and the integral step size is $h_i=t_i-t_{i-1}$, (i=1,2,…,NE). There are K collocation points on each element. The state variables and control variables are approximated by piecewise polynomials, which are expressed by the collocation points and Lagrange interpolation function. Thus, the state variable at an arbitrary point $t=t_{i-1}+h_i\tau$ ($\tau\in[0,1]$) in the element $[t_{i-1},t_i]$ is expressed as (Kameswaran and Biegler, 2006)

$$z(t) = \sum_{j=0}^{K} l_j(\tau) z_{ij}, \tag{10}$$

where the Lagrange interpolation polynomial is

$$l_j = \prod_{k=0,k\neq j}^{K} \frac{(\tau-\tau_k)}{(\tau_j-\tau_k)}. \tag{11}$$

Similarly, the control and algebraic variables can be expressed as

$$\begin{cases}
u(t) = \sum_{j=1}^{K} \bar{l}_j(\tau) u_{ij}, \quad y(t) = \sum_{j=1}^{K} \bar{l}_j(\tau) y_{ij},\\
\bar{l}_j = \prod_{k=1,k\neq j}^{K} \frac{(\tau-\tau_k)}{(\tau_j-\tau_k)}.
\end{cases} \tag{12}$$

The differential variables need to be continuous along the time horizon while the control and algebraic variables are allowed to be discontinuous at the boundaries of the elements. In addition, the collocation conditions must be satisfied at the collocation points:

$$\begin{cases}
\sum_{k=0}^{K} \dot{l}_k(\tau_j) z_{ik} - h_i f(z_{ij}, y_{ij}, u_{ij}, p) = 0,\\
g(z_{ij}, y_{ij}, u_{ij}, p) = 0,\\
i = 1,2,\ldots,\mathrm{NE}, \quad j = 1,2,\ldots,K,
\end{cases} \tag{13}$$

where $\dot{l}(\tau) = \dfrac{\mathrm{d}l(\tau)}{\mathrm{d}\tau}$.

Dynamic systems are transformed into large-scale nonlinear algebraic equations after discretization. The discrete approach affects not only the accuracy of solution, but also the convergence of the solution process. Generally, more collocation points lead to better approximation and higher accuracy.

However, there is no benefit to apply equal interval collocation points because Runge's phenomenon may occur: oscillations arise at both ends of the interpolation curve along with increasing number of discrete points, and worsen the approximation to the original function (Shen and Tang, 2006). Thus, choosing the appropriate discrete method is an important precondition when it comes to determining a successful solution.

The highest algebraic accuracy can be reached with the orthogonal collocation points (Shen and Tang, 2006). There are three kinds of widely used orthogonal collocation points: Gauss points, Gauss-Radau points, and Gauss-Lobatto points. All of these collocation points are distributed more densely towards the edges of the interval, and can avoid Runge's phenomenon effectively (Shen and Tang, 2006). Problem 1 is transformed into the following formulation after discretization, and the Gauss collocation points are applied in the discrete process (Kameswaran and Biegler, 2006):

Collocation equations:

$$\begin{cases} \sum_{k=0}^{K} \dot{l}_k(\tau_j) z_{ik} - h_i f(z_{ij}, y_{ij}, u_{ij}, p) = 0, \\ g(z_{ij}, y_{ij}, u_{ij}, p) = 0. \end{cases} \tag{14}$$

Linking conditions:

$$z_{i+1,0} = \sum_{j=0}^{K} l_j(1) z_{ij}, \quad i = 1, 2, ..., \mathrm{NE} - 1. \tag{15}$$

Initial conditions:

$$z_{1,0} = z(t_0). \tag{16}$$

Final conditions:

$$g_{\mathrm{f}}(z_{\mathrm{f}}) = 0, \quad z_{\mathrm{f}} = \sum_{j=0}^{K} l_j(1) z_{\mathrm{NE},j}. \tag{17}$$

Since the first point in the next finite element is the last point in the previous finite element with Gauss-Radau points, the connecting equation can be simplified according to the property of Lagrange interpolation

$$z_{i+1,0} = z_{i,k}, \quad i = 1, 2, ..., \mathrm{NE} - 1. \tag{18}$$

The final condition is reduced to

$$g_{\mathrm{f}}(z_{\mathrm{NE},K}) = 0. \tag{19}$$

Generally speaking, if more elements and collocation points are used in a fixed time span, the OCFE has better accuracy. The accuracy also depends, however, on the smoothness of the problem (Chen *et al.*, 2010). Discrete methods based on different orthogonal collocation points have different levels of algebraic precision. In the case of K collocation points, Gauss points are the roots of orthogonal collocation polynomials with order K and the algebraic precision of the corresponding quadrature formula is of degree $2K-1$ (Haire and Wanner, 2006). The accuracy of Gauss-Radau points is one order lower than that of Gauss points. However, Gauss-Radau points have an attractive property called stiff decay (Ascher and Petzold, 1998). This property is stricter than that of absolute stability. The advantage of methods with stiff decay lies in their ability to skip fine level solution details and converge to the solution even in very stiff cases.

4 HTR-PM case studies

The point kinetics equations are a stiff problem because all the real parts of eigenvalues of its Jacobian matrix are negative and the absolute value of the real part of the ratio of maximum and minimum is very large (Cai, 2005). This stiff problem includes some terms that can lead to rapid variation in the solution. It is essential to choose a proper step size to solve stiff problems.

The step size should be kept within the region of stability. Commonly used ODE algorithms, such as the Euler method, Runge-Kutta method, and Adams method, must use a very small step size to satisfy the stability and accuracy of the rapid variables. However, the small step size is not appropriate for slow variables (Cai, 2005), requiring expensive computation and memory costs to solve the problem. On the other hand, the accumulated error will significantly increase with the total number of steps. In order to avoid these defects, implicit algorithms are recommended. In our simultaneous approach, we can take a larger step size since the approach based on Radau collocation points is implicit. Of course, the step size should satisfy the precision requirement.

All numerical results are obtained on the machine running Windows XP and with 1.66 GHz CPU and 1.49 GB of RAM. After discretization with the

OCFE method, the resulting problem is solved by a nonlinear algebraic equation solver. There are many efficient solvers. Here interior point optimizer (IPOPT) (Biegler and Zavala, 2009) is applied. Five hundred elements are applied with three Radau collocation points in each of them. The length of element or the step size is 1 s. After discretization, the total number of variables and equality constraints are 43 500. To compare the simultaneous approach with the nested approach, the model is also implemented on the same computer with the nested approach using an explicit ODE solver. The variable step ODE method is adopted here and the step size is from $1\times e^{-7}$ to 10 s.

The system is in steady state at 100% full power and the reactivity is zero. The Helium input pressure P_{in}, Helium input flow rate G_{in}, Helium input temperature T_{in}, and control rod reactivity ρ_{rod} are selected as the four input variables. The Helium output pressure P_6, Helium output flow rate G_6, Helium output temperature T_6, reflector temperature T_r, relative density of neutron (relative power) n_r, and core temperature T_c are selected as the six output variables.

Figs. 2 and 3 show the transient responses of six different output variables according to changes in one of the four input variables in the rated power level.

As shown in Fig. 2, all the variables are in steady state for 100 s and the Helium inlet flow rate is allowed to increase 5 kg/s with the other three input variables remaining constant. The curves obtained by the two approaches overlap each other.

In Fig. 3, the control rod reactivity input is kept constant for 100 s and allowed to increase 5% with the other three input variables remaining constant.

The numerical simulation of the model shows that the transient results are properly predicted and the steady state results agree with the design data. The step size of the nested approach should be small to obtain a stable solution. The lines, according to the two approaches, are very close to each other, indicating that error accumulation due to the small step size of the nested approach does not lead to divergence from the solution of the problem. The simulation takes approximately 10 s in the nested approach and only takes 3 s in the simultaneous approach because there are inner iterations in each step of the

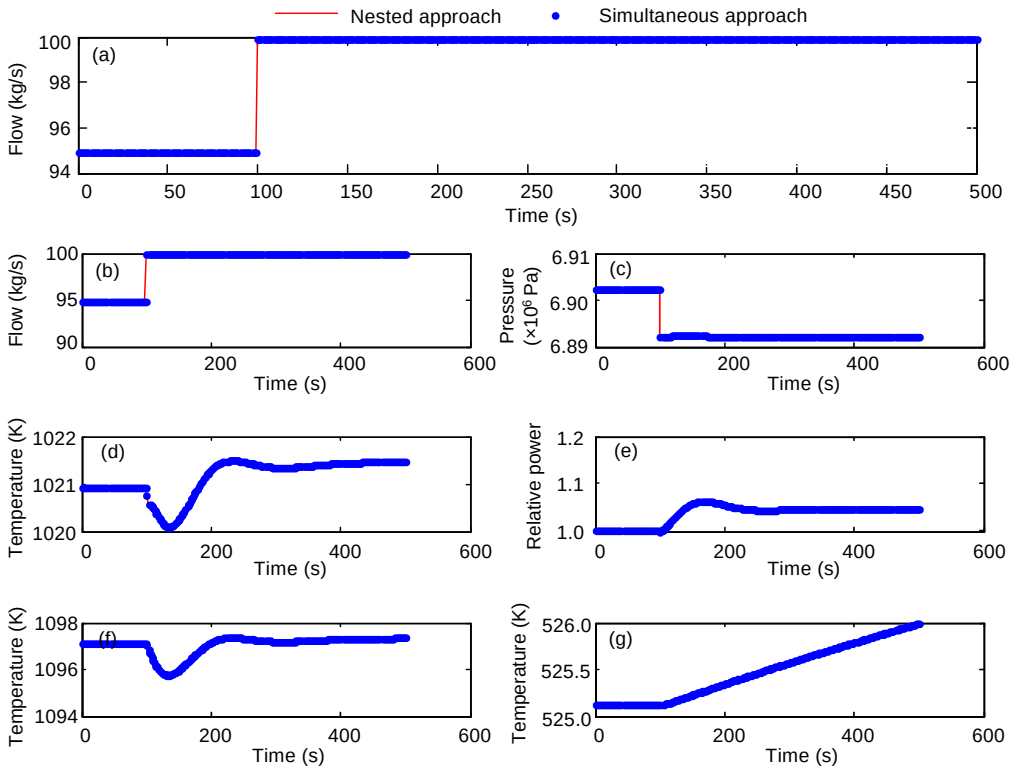

Fig. 2 Transients due to 5 kg/s step increase in the Helium inlet flow

(a) Helium input flow rate; (b) Helium outlet flow rate; (c) Helium outlet pressure; (d) Helium outlet temperature; (e) Relative power; (f) Core temperature; (g) Reflector temperature

nested approach which can be avoided in the simultaneous approach. An alternative way to implement the nested approach is to call an implicit ODE solver, which will not suffer from the small step size limitation. However, that is very time-consuming for large-scale problems because of the way the approach reaches convergence. In consequence, the implicit ODE solver may require much more time to solve large-scale problems than explicit ODE solvers.

Relative error can be defined to give an indication of how good the terminal value of the simultaneous approach is relative to that of the nested approach. Fig. 4 shows the relationship among the error, step size, and the computational effort in solving the resulting nonlinear algebraic equations after discretization in the simultaneous approach. If the step size becomes smaller, the error will be smaller and the resulting equations will become larger. Then the computational time will also become longer. We can increase the step size to reduce the computational time in solving the nonlinear algebraic equations. We take the appropriate step size as a trade-off between the accuracy and the efficiency. However, we can hardly increase the step size in the nested approach because of instability.

5 Conclusions

The simulation of HTR-PM is presented. The lumped parameter dynamic HTR-PM model is a DAE system and the core fission reactor described by point kinetics equations represents a stiff problem. The index of DAE affects the solution to the problem. Since the index of the HTR-PM is 1, we simulated the model with the simultaneous approach, which solves all the variables simultaneously. The nonlinear algebraic equation solver was called after full discretization by the OCFE. The collocation method based on

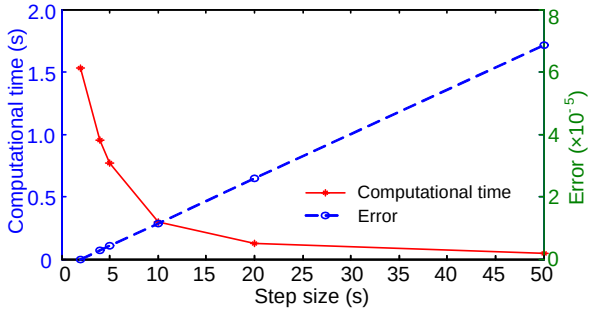

Fig. 4 Relationship among the calculation error, step size, and computational time in the simultaneous approach

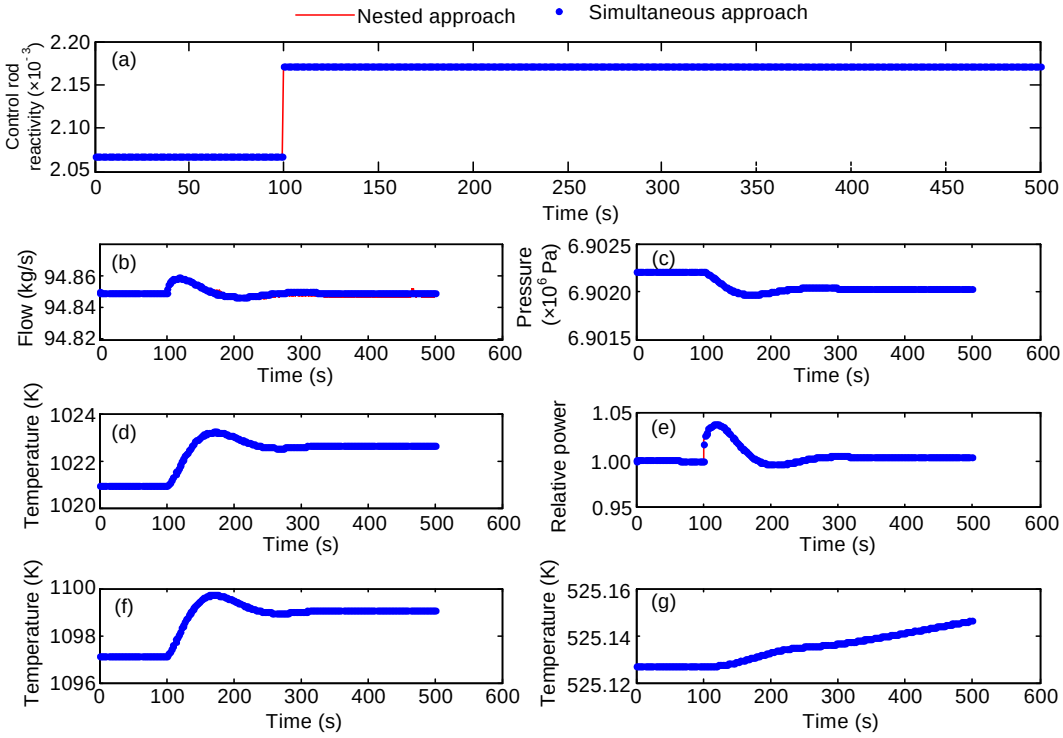

Fig. 3 Transients of 5% step increase in the control rod reactivity input

(a) Control rod reactivity; (b) Helium outlet flow rate; (c) Helium outlet pressure; (d) Helium outlet temperature; (e) Relative power; (f) Core temperature; (g) Reflector temperature

Gauss-Radau points, not only has high accuracy in terms of discretization, but also is good at solving the stiff problem.

Though there are stiff equations in the HTR-PM model, according to the previous analysis, we can take a large step size that meets the accuracy demand in the discretization and will not lose stability. The results show the efficiency and validity of this approach. The results in the simulations of the simultaneous approach and the nested approach are very similar, but the former takes much less computational time. The efficiency of the simultaneous approach is essential to the real time control and simulation of the HTR plant.

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