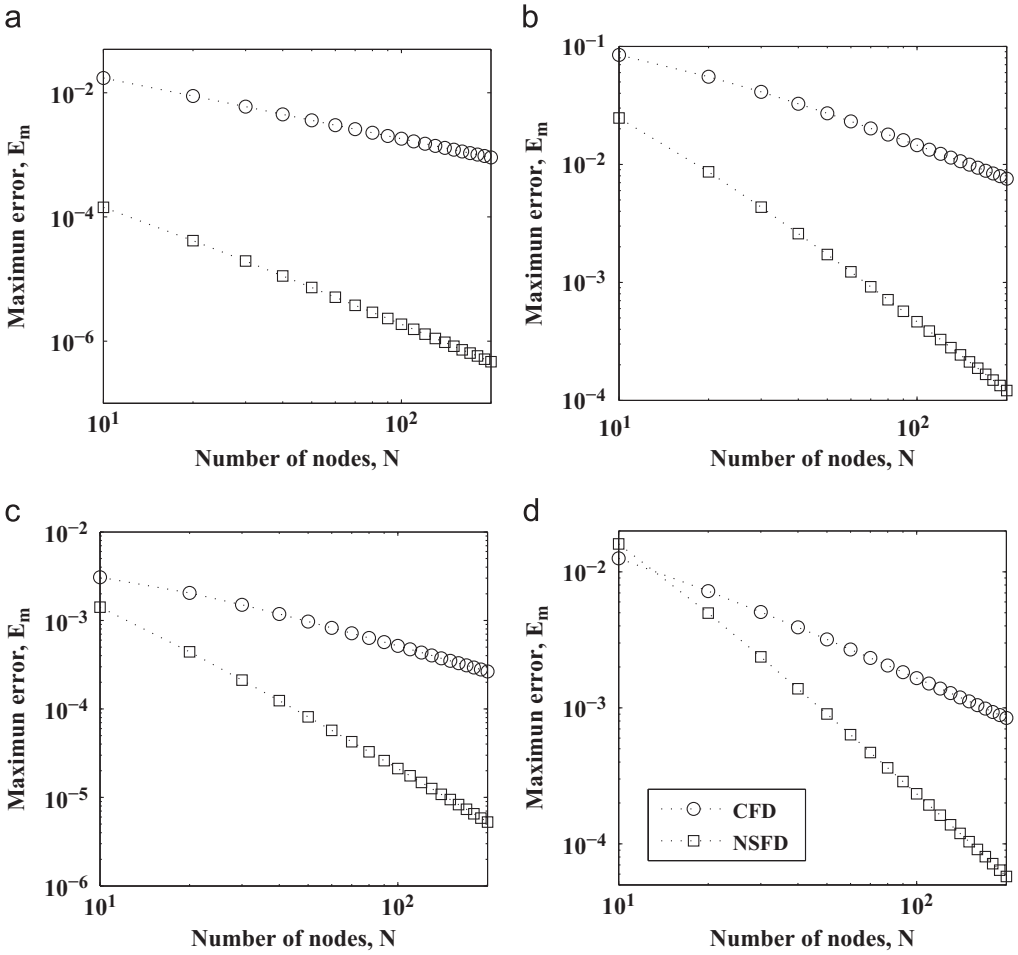

Fig. 6. Steady-state profiles of the tubular chemical reactor. Maximum error vs number of nodes for (a) $Pe=0.1$ and $Da=0.875$, (b) $Pe=10$ and $Da=0.875$; (c) $Pe=5.0$ and $Da=0.5$; (d) $Pe=5.0$ and $Da=5.0$.

Table 2
CPU-time (sec) for the steady-state solution of the tubular reactor model, (a) $Da=0.875$ and (b) $Pe=1.0$.

(a)			(b)		
Pe	NSFD	CFD	*Da*	NSFD	CFD
0.01	14.352	12.729	0.01	8.408	7.347
0.05	14.008	11.746	0.05	7.051	7.815
0.1	13.603	11.715	0.1	10.795	7.971
0.5	13.854	11.512	0.5	12.495	10.436
1.0	14.118	11.965	1.0	16.146	12.963
5.0	15.865	13.135	5.0	56.846	48.235
10.0	15.631	12.745	10.0	23.150	19.681
50.0	16.161	12.776	50.0	155.002	140.68
100.0	17.113	13.228	100.0	121.896	107.749

4.2.1. NSFD scheme based on Green's function

Unlike Eq. (1) where the Péclet number is multiplying the convection operator, in the tubular reactor model the inverse of Péclet numbers are multiplying to the diffusion and convection operators. For simplicity in the development, we consider $Pe_y = Pe_z = Pe$. Then, the self-adjoint operator is $L = \frac{\partial}{\partial x}[(\exp(-Pex)/Pe)(\partial/\partial x)]$. Therefore, the integral formulation and Green's function are

$$u(x,t) = \frac{\exp(-Pea)}{Pe}\frac{\partial G(a,x)}{\partial z}\frac{\gamma_a}{\beta_a} - \frac{\exp(-Peb)}{Pe}\frac{\partial G(b,x)}{\partial z}\frac{\gamma_b}{\beta_b} + \int_a^b \frac{G(z,x)}{\exp(Pez)}\Psi(z,t)\,dz \tag{29}$$

$$G(z,x) = \frac{1}{G^*}\begin{cases} [\exp(Pez)-\exp(Pea)k_a][\exp(Pex)-\exp(Peb)k_b] & \text{if } z<x \\ [\exp(Pez)-\exp(Peb)k_b][\exp(Pex)-\exp(Pea)k_a] & \text{if } z\geq x \end{cases} \tag{30}$$

where $G^* = [\exp(Peb)k_b - \exp(Pea)k_a]$. Following the procedure presented in Eqs. (14)–(19), it is not hard to show that the NSFD scheme is given by

$$\begin{aligned} \frac{du_1(t)}{dt} &= \frac{a_1\frac{\gamma_a}{\beta_a} - b_1u_1(t) + c_1u_2(t)}{Pe} - R(u_1(t)) \\ \frac{du_i(t)}{dt} &= \frac{a_iu_{i-1}(t) - b_iu_i(t) + c_iu_{i+1}(t)}{Pe} - R(u_i(t)) \\ \frac{du_N(t)}{dt} &= \frac{a_Nu_{N-1}(t) - b_Nu_N(t) + c_N\frac{\gamma_b}{\beta_b}}{Pe} - R(u_N(t)) \end{aligned} \tag{31}$$

where the parameters a_i, b_i and c_i are described in Eqs. (20).

4.2.2. Steady-state case

Consider Eqs. (27) and (28) under steady-state conditions, i.e. $\partial y/\partial t = 0$ and $\partial z/\partial t = 0$. The maximum error is calculated by Eq. (25). In order to appreciate the effect of the physical phenomena (i.e., transport phenomena and reaction rate) in the numerical predictions, we show the maximum errors for different values of *Pe* and *Da*.