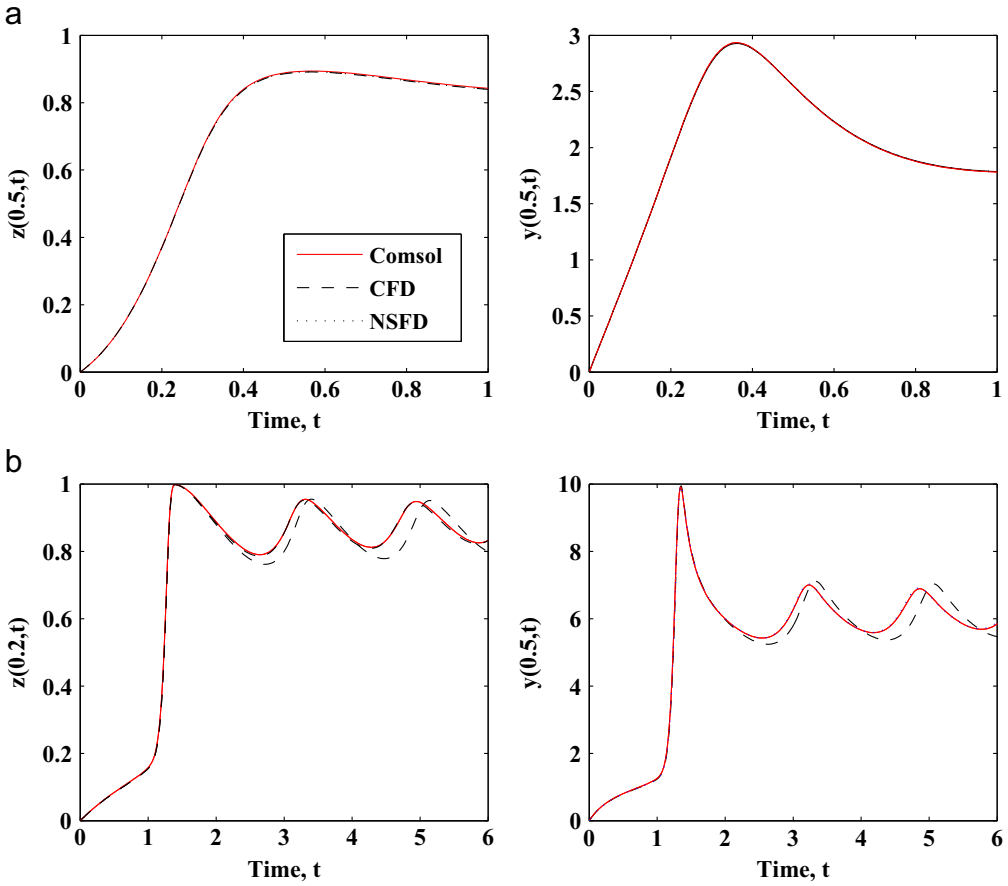

Fig. 7. Dynamic profiles of the tubular chemical reactor, (a) temperature profiles with hot spot and (b) temperature and concentration profiles with periodic oscillations.

Table 3
CPU-time (sec) for the dynamical 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	4.867	5.569	0.01	8.985	9.937
0.05	4.098	4.149	0.05	9.212	10.077
0.1	4.823	4.960	0.1	9.469	9.656
0.5	7.597	7.488	0.5	9.204	9.764
1.0	9.219	9.734	1.0	9.110	9.845
5.0	10.670	13.946	5.0	9.469	9.672
10.0	6.271	6.286	10.0	9.500	9.687
50.0	6.011	6.443	50.0	9.342	9.078
100.0	5.112	5.148	100.0	9.893	10.322

Consider the set of parameters corresponding to hot spot behavior (Table 1). Fig. 6 shows that NSFD scheme performs better numerical approximations than CFD scheme. Given the mathematical structure of tubular reactor model ($1/Pe$ multiplying the diffusive operator), the best performance of NSFD is observed when the global process is dominated by diffusion phenomena. Although the numerical approximation of NSFD is diminished for high Pe values, $O(h^2)$ in the numerical approximations is maintained, while the classical FD schemes the usage of first order approximations in the derivative of boundary conditions leads to numerical approximations of $O(h)$.

On the other hand, the CPU-time required for the numerical solution of the tubular reactor model to different conditions is shown in Table 2. The CPU-time is calculated as the average time needed to obtain the profile $u(x)$ for 10–200 nodes with a spacing of 10 nodes. To observe the effects of both the reactive and transport phenomena on the CPU-time, we proposed to vary the Damköhler and Péclet numbers. In general, Table 2 indicates that the traditional central FD scheme exhibits slightly better computation times than NSFD. That is, since the α, β and γ parameters are functions of exponential functions, these functions require more time to calculate. Nevertheless, NSFD exhibits acceptable CPU-time and the approximation order is maintained in $O(h^2)$.

4.2.3. Dynamical case

In this case, the numerical solution with 2000 nodes obtained from the COMSOL package is considered as reference solution. For the numerical simulations, we used the MOL method with a 4/5-order Runge-Kutta method (ode45 from Matlab Package) and $\delta t=0.01$ for the integration of the differential equations. The tubular reactor with periodic oscillations and hot spot dynamics are considered. In order to compare the performance of NSFD based on Green's function, Fig. 7 shows the temperature and concentration profiles using $N=100$, where it is possible to observe that for hot spot dynamic, both methods present an adequate agreement with the reference solution. However, for periodic oscillations behavior, NSFD scheme shows better correspondence with the COMSOL solution than CFD. This result suggests that NSFD based on integral formulations is a good alternative for the numerical solution of models with complex spatio-temporal patterns. To evaluate the CPU-time, we consider $N=200$ and $t=50$ for different Da and Pe values. For this case, the NSFD scheme exhibits less CPU-time than CFD (Table 3). This suggests that the proposed methodology is a good alternative to solving RDC systems.