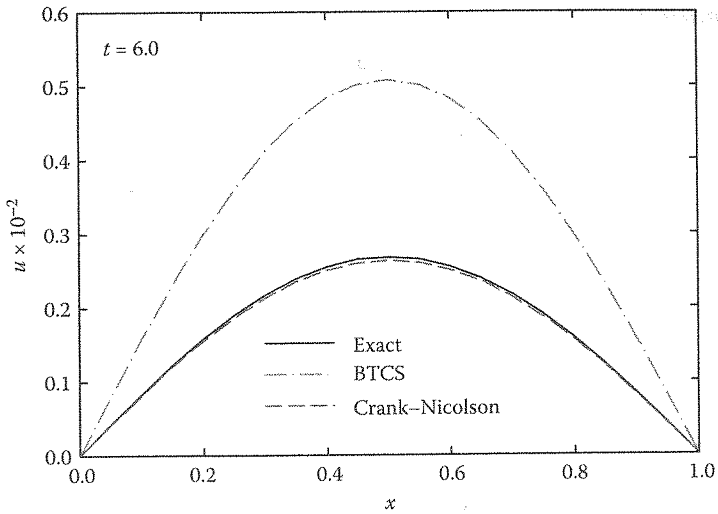

FIGURE 13.10 Numerical solutions of the diffusion problem 13.51–13.53 obtained for $t = 6.0$ by the implicit and the Crank–Nicolson methods using the spatial spacing $h_x = 0.05$ and the time step size $h_t = 0.25$.

The calculations employ the same, spatial step size, $h_x = 0.05$, as with the explicit FTCS method, while for the time step, we use $h_t = 0.25$, which is 20 times larger than the limiting value still ensuring the stability of the FTCS scheme (see Figure 13.8). As can be seen from Figure 13.10, showing profiles for $t = 6.0$, unlike the solution provided by the BTCS method, which substantially departs from the exact result, the solution yielded by the Crank–Nicolson method agrees fairly, in spite of the very large time step. The example points to the fact that the stability of a difference method (absence of spurious oscillations) does not also entail a reasonable degree of precision.

13.3.5 Spatially Variable Diffusion Coefficient

In many applications of practical importance, involving, for instance, the permeation of substances through membrane stacks, the diffusion coefficient cannot be considered by any means constant, but rather piecewise constant under the most simplifying assumptions. In such problems, the 1D diffusion equation needs to be formulated as

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right). \tag{13.78}$$

Aiming to consistently maintain the second order of the discretization methods, we approximate the spatial derivative at the space–time point (x_i, t_n) by the central-difference scheme:

$$\begin{aligned}\left[\frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)\right]_{i,n} &\cong \frac{1}{h_x}\left[\left(D\frac{\partial u}{\partial x}\right)_{i+1/2,n} - \left(D\frac{\partial u}{\partial x}\right)_{i-1/2,n}\right] \\ &\cong \frac{1}{h_x}\left[D_{i+1/2}\frac{u_{i+1}^n - u_i^n}{h_x} - D_{i-1/2}\frac{u_i^n - u_{i-1}^n}{h_x}\right],\end{aligned} \tag{13.79}$$

where the midpoints $x_{i\pm 1/2} = (x_i + x_{i\pm 1})/2$ ensure, on the one hand, the proper centering of the involved quantities about the reference point x_i and lead, on the other, to an $O(h_x^2)$ scheme. The median values of the diffusion coefficients, $D_{i\pm 1/2}$, can be conveniently approximated assuming a linear dependence