

Example – Reaction with Axial Dispersion

For the next example, we consider nonisothermal flow through a chemical reactor with axial conduction and dispersion. The governing equations for this problem are:

$$\begin{aligned} \frac{1}{Pe_m} \frac{d^2 y}{dx^2} - \frac{dy}{dx} - r_m(y, T) &= 0 \quad \text{and} \\ \frac{1}{Pe_t} \frac{d^2 T}{dx^2} - \frac{dT}{dx} - \alpha T - r_t(y, T) &= 0 \end{aligned} \quad (54)$$

with:

$$\begin{aligned} \frac{dy}{dx} = Pe_m y \quad \text{and} \quad \frac{dT}{dx} = (Pe_t + \alpha)T \quad \text{at } x = 0 \quad \text{and} \\ \frac{dy}{dx} = 0 \quad \text{and} \quad \frac{dT}{dx} + \alpha T = 0 \quad \text{at } x = 1 \end{aligned}$$

The model allows for cooling at the wall using a lumped parameter model with an overall heat transfer coefficient, parameter α . These problems are convection dominated, since the Peclet numbers, Pe_m and Pe_t , are normally large. The solution is nonsymmetric and all the boundary conditions are of the second or third kind. The boundary conditions for the energy equation are an accurate approximation of those described by Young and Finlayson (1973).

In an industrial reactor model several component balances could be required to represent a system of reactions, so Eq. (54) is formulated as the following system of coupled equations:

$$\frac{1}{Pe_k} \frac{d^2 y_k}{dx^2} - \frac{dy_k}{dx} - \alpha_k y_k - r_k(\mathbf{y}) = 0 \quad (55)$$

with:

$$\frac{dy_k}{dx} = (Pe_k + \alpha_k) y_k \quad \text{at } x = 0, \quad \text{and} \quad \frac{dy_k}{dx} + \alpha_k y_k = 0 \quad \text{at } x = 1$$

The energy balance corresponds to $k=1$ and the total number of equations will normally be determined by the complexity of the reacting system.

As an example, we will only consider the energy balance and one mass balance. A first order exothermic reaction is used:

$$r_k = \beta_k (1 - y) \exp\left(20 - \frac{20}{T + 1}\right) \quad (56)$$

The parameter values considered in the example are: $Pe_t = 100$, $Pe_m = 200$, $\alpha = 3$, $\beta_t = 0.2$, $\beta_m = 0.5$.

After the application of conventional orthogonal collocation Eq. (55) is approximated by:

$$\sum_{i=0}^{n+1} \left(\frac{1}{Pe_k} B_{ji} - A_{ji} - \alpha_k \delta_{ji} \right) y_{ik} - r_k(\mathbf{y}_j) = 0 \quad (57)$$

for $j = 1, \dots, n$ and

$$\sum_{i=0}^{n+1} [A_{0,i} - (Pe_k + \alpha_k) \delta_{0,i}] y_{ik} = 0 \quad \text{and}$$

$$\sum_{i=0}^{n+1} [A_{n+1,i} + \alpha_k \delta_{n+1,i}] y_{ik} = 0$$

As discussed previously, Eq. (57) produces a good approximation to the moments method when Gaussian quadrature base points are used. Eq. (57) produces poor results with Lobatto points because of the flux boundary conditions.

To solve the problem accurately with Lobatto quadrature base points, the problem is formulated with the Galerkin method and a weak treatment of the boundary conditions:

$$\delta_{0,j} \left(1 + \frac{\alpha_k}{Pe_k} \right) + \delta_{n+1,j} \frac{\alpha_k}{Pe_k} + \sum_{i=0}^{n+1} \left(\frac{1}{Pe_k} C_{ji} + W_j A_{ji} - \alpha_k \delta_{ji} W_j \right) y_{ik} - W_j r_k(\mathbf{y}_j) = 0 \quad (58)$$

As discussed previously, the use of Eq. (24) shows that Eq. (58) is equivalent to Eq. (57) at the interior points, while at the boundaries Eq. (58) applies modifications which are proportional to the residual evaluated at the boundaries. Compared to a Galerkin method with the reaction terms interpolated by the trial functions, see Eq. (19), the dispersion and convection terms are integrated exactly, while the heat transfer term and reaction terms miss exact integration by one degree. Eq. (58) can also be used for Gauss points if the \mathbf{C} matrix is calculated using Eq. (24) (see discussion above and in the appendix).

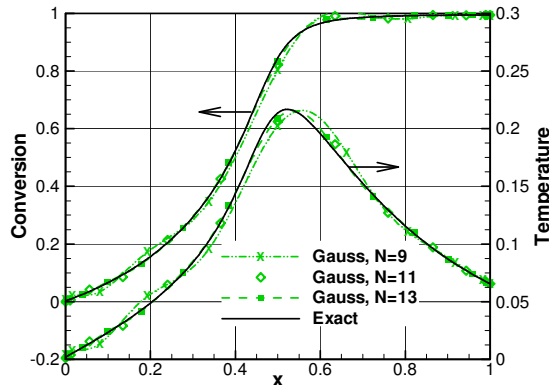


Fig. 14 Reactor with axial dispersion, conversion and temperature

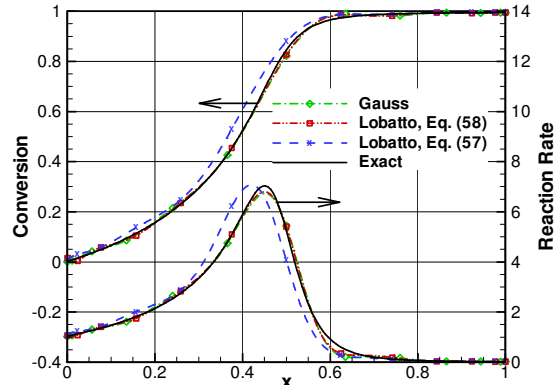


Fig. 15 Reactor with axial dispersion with $n = 11$

Fig. 14 shows a sample of the solutions using Gauss points. With $n = 9$ the polynomial cannot match the sharp profiles, so the approximate solution oscillates about the exact one. With $n = 11$ or 13 the results are noticeably better. Fig. 15 shows a plot of conversion, y , and reaction rate, r , for three approximate solutions all with $n = 11$. The sharp changes in conversion and temperature are due to the strong nonlinearity of the reaction rate. The results with Lobatto points and Eq. (57) are clearly poor and support our claim that Eq. (58) must be used.

Fig. 16 shows the average absolute error or L_1 error norm for the conversion, y . Due to the sharp gradients, a large number of points are required to obtain acceptable solutions. The errors are similar with either Gauss or Lobatto points. With $n = 11$, the average conversion errors and the error in outlet conversion are less than 0.001 with both methods, while the errors in conversion at the center average 0.0025. To reduce the errors at the center to 0.001 requires $n = 15$, and then the outlet errors are less than 0.0001. The temperature errors follow the same trends as the conversion errors, but are about 3 times larger, so the errors would be about the same if they were normalized by the maximum value of temperature. For this problem, the errors with an even number of points are much larger than with an odd number, possibly because most of the activity occurs near the center and an even number of points has no point at $x = 0.5$. Also, the error using Lobatto points and Eq. (57) are very erratic and some were an order of magnitude larger than errors with the other two methods.

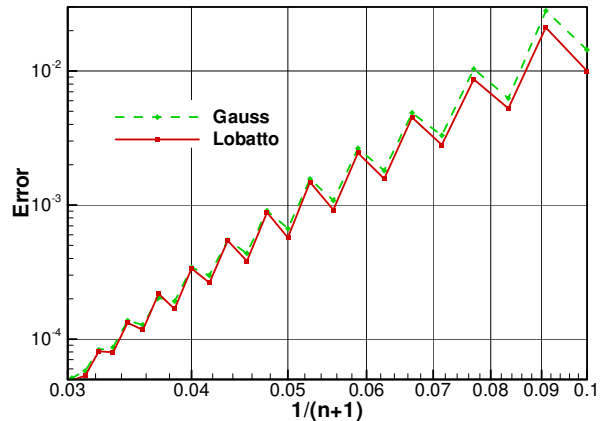


Fig. 16 Reactor with axial dispersion, L_1 error norm

These problems were solved by the Newton Raphson method, with the results iterated until roundoff was reached, i.e. typically when the change became about 10^{-15} . For the error calculations, the results with $n = 51$ were assumed to be exact. To confirm the accuracy of the results they were checked with up to $n = 65$ and computations in quad-precision.

We should briefly discuss the solution of these equations. The set of equations, Eq. (57) or (58), are coupled only through the reaction term. For our simple case with an energy balance and only one mass balance, it would be possible to combine the equations to eliminate the reaction term. This would produce a set of $n + 2$ linear equations in conversion and temperature and one of the original balances, say the mass balance. Temperature could be eliminated from this set of equation by LU decomposition. This decomposition would not change from one Newton iteration to the next and could be reused each time to eliminate temperature from the linearization of the mass balance. The conversion could then be calculated by normal forward elimination and back substitution, followed by back substitution to update the temperature. This approach would be more efficient than solving the entire set of $2(n+2)$ equations each iteration. If more than one mass balance is needed, it should still be possible to eliminate temperature in a similar fashion. Alternatively, a simplified Newton iteration could be used. We have done some experimentation with methods of this sort, but have found that simplified methods sometimes break down for tough problems.