The following problem accompanies the book, Method of Weighted Residuals and Variational Principles, by Bruce A. Finlayson, a SIAM Classic reprinted in 2014. The original version was printed by Academic Press in 1972. See www.ChemEComp.com/MWR. Order the book from the Society of Industrial and Applied Mathematics, www.SIAM.org. The problems and solutions refer to equations and references in that book.

Problem 7, part a. Solve by trying $u = e^{kx}$ and finding that $k^2 = \phi^2$. The solution is then

$$u = A\sinh(\phi x) + B\cosh(\phi x)$$

The first derivative is then

$$\frac{du}{dx} = A\phi\cosh(\phi x) + B\phi\sinh(\phi x)$$

To fit the boundary condition at x = 0 requires A = 0. To fit the boundary condition at x = 1 requires $B = 1/\cosh(\phi)$. Thus, the solution is

$$u = \frac{\cosh(\phi x)}{\cosh(\phi)}$$

The effectiveness factor is the average rate of reaction divided by the rate of reaction at x = 1.

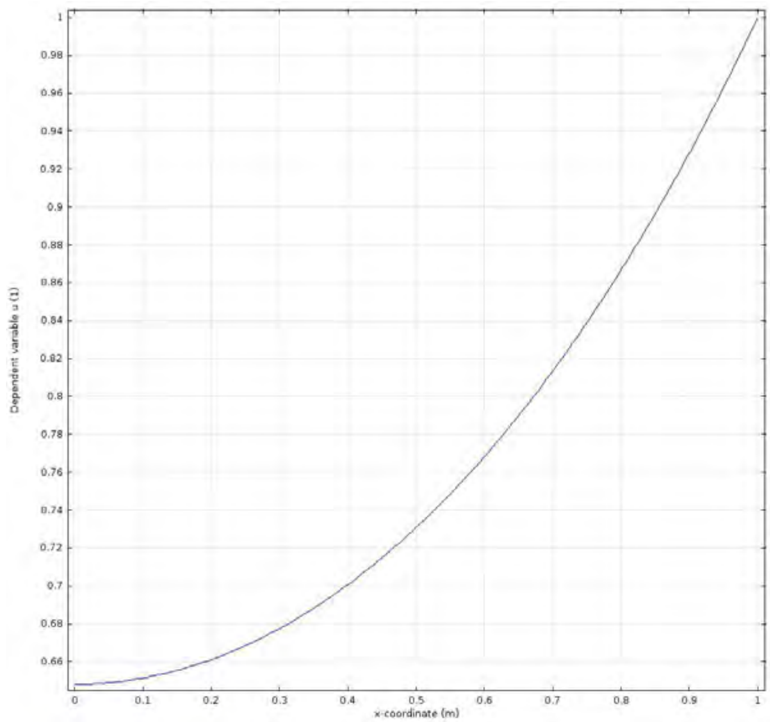
$$\eta = \frac{1}{\phi^2}\int_0^1 \phi^2 u(x)dx = \frac{1}{\phi^2}\int_0^1 \frac{d^2u}{dx^2}dx = \frac{1}{\phi^2}\left.\frac{du}{dx}\right|_{x=1} = \frac{\tanh(\phi)}{\phi}$$

For ϕ = 1, this is η = 0.7615941559557649.

Part b. The problem was solved in Comsol Multiphysics using the coefficient form of an ODE with c = 1 and $f = -\phi^2$ u, zero flux at x = 0 and the Dirichlet condition u = 1 at x = 1. The results were evaluated to give the following quantities:

$$\int_0^1 u\,dx, \quad \frac{1}{\phi^2}\left.\frac{du}{dx}\right|_{x=1}, \quad \int_0^1 R^2\,dx = \int_0^1\left[\frac{d^2u}{dx^2} - \phi^2 u\right]^2 dx$$

The residual was evaluated using $R = uxx - \phi^2 u$ in Comsol. A typical solution is shown in the next figure. As can be seen, the concentration drops from its boundary value, thus lowering the reaction rate in the interior of the catalyst pellet and making the effectiveness factor less than 1.0.



Numerical results are in the Table for Hermite cubic polynomial finite elements. The total number of points is given, but with n = 4, there are two degrees of freedom at each node, hence the number of degrees of freedom is 8. As can be seen, the mean-square residual decreases as more elements are used, and the point-wise error decreases as well. For this problem only the extremely coarse mesh need be used, since even with four points the approximate solution is accurate within 0.0041. The upper bound for the error in effectiveness factor is essentially the point-wise error bound, since here

$$\left|\eta-\eta_n\right| \le \frac{K\left\|u-u_n\right\|_\infty}{\left|f(u)\right|_{x=1}\right|} = \left\|u-u_n\right\|_\infty$$

Thus the actual error is from 4 to 8 orders of magnitude smaller than the estimated error.

Hermite, total nodes, n	η using integral	η using slope at x = 1	Mean square residual^2	Point-wise error bound	Actual error in η
4, extremely coarse	0.761594174	0.761217508	1.242e-05	4.069e-03	1.757e-08
6, extra coarse	0.761594157	0.761508034	1.510e-06	1.419e-03	9.797e-10
9, coarser	0.761594156	0.761572451	2.201e-07	5.417e-04	6.413e-11
11, coarse	0.761594156	0.761582918	8.864e-08	3.438e-04	1.734e-11
28, fine	0.761594156	0.761593568	1.592e-09	4.608e-05	2.909e-14