Numerical solution of the advection diffusion equation

Derek W. Harrison

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Introduction

The steady state advection diffusion equation is solved using the finite volume method. Central differencing is applied to the diffusion terms and the upwind differencing scheme is applied to the convection terms. The resulting linear system is solved using the Gauss-Seidel method.

Model equations

From a component balance at an arbitrary location in the domain it follows that the advection diffusion equation is given by:

$$\frac{D_a}{U}\frac{d^2C_a}{dz^2} - \frac{dC_a}{dz} + \frac{r_a}{U} = 0 \tag{1}$$

Where D_a is the diffusion coefficient, U is the fluid velocity, C_a the concentration of component a, z the axial coordinate and r_a the reaction rate law of component a.

Verification

When Danckwerts boundary conditions for a closed-closed system apply and the reaction rate law is first order an analytical solution to (1) can be obtained:

$$\frac{C_{al}}{C_{a0}} = \frac{4q\exp\left(Pe/2\right)}{(1+q)^2\exp\left(Pe\cdot q/2\right) - (1-q)^2\exp\left(-Pe\cdot q/2\right)} \tag{2}$$

Where C_{al} is the concentration of component a at the reactor outlet, C_{a0} is the concentration of component a at the reactor inlet, Pe is the Peclet number $Pe = UL/D_a$ with L the length of the reactor and q is a quantity that depends on the Peclet and Damkohler numbers:

$$q = \sqrt{1 + 4Da/Pe} \tag{3}$$

Where Da is the Damkohler number $Da = kL/U$ with k the reaction rate constant.

Numerical solutions to equation (1) are compared with (2). Results are given in table 1. Results show that analytical and numerical solutions agree well and that discrepancies are within 1 %.

Table 1: Exit concentration vs Peclet number

Pe	Concentration analytical	Concentration numerical
0.1	0.909	0.907
0.2	0.832	0.832
0.4	0.709	0.709
0.8	0.534	0.534
1.6	0.319	0.320
3.2	0.118	0.120