Numerical solution of the coupled convection diffusion equation

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Introduction

A set of coupled convection diffusion equations 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 balance for component a at an arbitrary location in the domain it follows that the advection diffusion equation is given by:

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

Where D 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. Similarly, it follows that a balance for component b gives:

$$\frac{D}{U}\frac{d^2C_b}{dz^2} - \frac{dC_b}{dz} + \frac{r_b}{U} = 0 \tag{2}$$

Where C_b is the concentration of component b and r_b the reaction rate law of component b. Danckwerts boundary conditions apply to equations (1) and (2).

Discretization

The discrete form of equation (1) for 'central' nodes is:

$$-D\frac{C_{a,i} - C_{a,i-1}}{\delta z} + D\frac{C_{a,i+1} - C_{a,i}}{\delta z} + UC_{a,i-1} - UC_{a,i} + r_{a,i}\delta z = 0 \tag{3}$$

Where $C_{a,i}$ is the concentration of component a at node i and δz is the discrete axial coordinate. For the left most node in the domain the discrete form of equation (1) is given by:

$$-D\frac{C_{a,0} - C_{a,in}}{1/2 \cdot \delta z} + D\frac{C_{a,1} - C_{a,0}}{\delta z} + UC_{a,in} - UC_{a,0} + r_{a,0}\delta z = 0 \tag{4}$$

For the right most node the discrete form of equation (1) becomes:

$$-D\frac{C_{a,n-1} - C_{a,n-2}}{\delta z} + UC_{a,n-2} - UC_{a,n-1} + r_{a,n-1}\delta z = 0 \tag{5}$$

Where n is the number of nodes in the domain. Since Danckwerts boundary conditions apply an equation is required for the 'inlet' node:

$$(1 + \frac{D}{1/2 \cdot U\delta z})C_{a,in} = C_{a0} + \frac{D}{1/2 \cdot U\delta z}C_{a,0} \tag{6}$$

Where C_{a0} is the concentration of component a just before the reactor inlet. Note that C_{a0} and $C_{a,0}$ are different quantities ($C_{a,0}$ is the concentration at node 0, which lies within the reactor domain). The reaction rate laws depend on the concentrations of both component a and b. Therefore the reaction rate laws need to be linearized:

$$r_{a,i} = r^*_{a,i} + \frac{\partial r^*_{a,i}}{\partial C_{a,i}}(C_{a,i} - C^*_{a,i}) + \frac{\partial r^*_{a,i}}{\partial C_{b,i}}(C_{b,i} - C^*_{b,i}) \tag{7}$$

The asterisk denotes values from the previous iteration. The linear system represented by equations (3) to (7) is solved using the Gauss-Seidel method. Equations for component b are obtained by simply replacing the subscript a with b in equations (3) to (7), except in equation (7) where only the subscripts for $r_{a,i}$ are changed.

Verification

To verify that the computation of concentration distributions is performed correctly it is checked that equations (3) to (6) are satisfied. Analysis shows that equations (3) to (6) are satisfied to a high degree of accuracy (error = 3.6e-13).