Numerical solution of the coupled convection diffusion and energy equations

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Introduction

A set of coupled 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. An energy balance results in:

$$\frac{\lambda}{U\rho C_p}\frac{d^2T}{dz^2} - \frac{dT}{dz} + \frac{r_a\Delta H_a}{U\rho C_p} = 0 \tag{3}$$

Where λ is the heat conduction coefficient, ρ the density, C_p the heat capacity and ΔH_a the reaction enthalpy. Danckwerts boundary conditions apply to equations (1), (2) and (3).

Discretization

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

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

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:

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

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

$$-D\frac{C_{a,n-1} - C_{a,n-2}}{\delta z} + UC_{a,n-2} - UC_{a,n-1} + r_{a,n-1}\delta z = 0 \tag{6}$$

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

$$(1 + \frac{D}{1/2 \cdot U\delta z})C_{a,in} = C_{a0} + \frac{D}{1/2 \cdot U\delta z}C_{a,0} \tag{7}$$

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 and temperature. Therefore the reaction rate laws need to be linearized:

$$r_{a,i} = r^*_{a,i} + \frac{\partial r^*_{a,i}}{\partial C_{a,i}}(C_{a,i} - C^*_{a,i}) + \frac{\partial r^*_{a,i}}{\partial C_{b,i}}(C_{b,i} - C^*_{b,i}) + \frac{\partial r^*_{a,i}}{\partial T_i}(T_i - T^*_i) \tag{8}$$

The asterisk denotes values from the previous iteration. The linear system represented by equations (4) to (8) is solved using the Gauss-Seidel method. Equations for component b are obtained by simply replacing the subscript a with b in equations (4) to (8), except in equation (8) where only the subscripts of $r_{a,i}$ are changed. Equations for temperature are obtained by discretizing the energy equation (3) in a similar manner.

Verification

To verify that the computation of concentration and temperature distributions is performed correctly it is checked that equations (4) to (7), and corresponding equations for component b and temperature, are satisfied. Analysis shows that equations (4) to (7), and equations for b and temperature, are satisfied with an error in the order of 1e-13.