Two phase mass transfer and reaction

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Introduction

The equations describing a gas-liquid reactor are solved numerically using the finite volume method. Plug flow applies to the gas phase and the liquid phase is ideally mixed.

Model equations

The mass balance for component A in the gas phase is:

$$\frac{\partial C_{Ag}}{\partial t} = -U_g \frac{\partial C_{Ag}}{\partial x} - \frac{k_g}{H}(C_{Ag} - C_{Ag}^i) \tag{1}$$

Where C_{Ag} is the concentration of component A in the gas phase, U_g is the gas phase velocity, k_g the gas phase mass transfer coefficient, H is the height of the gas phase above the liquid surface, C_{Ag}^i the gas phase interface concentration, x the axial coordinate and t time. The mass balance for component A in the liquid phase is:

$$HL\frac{dC_{Al}}{dt} = U_l H \cdot C_{Al0} - U_l H \cdot C_{Al} + \int_0^L k_l(C_{Al}^i - C_{Al})dx + r_A HL \tag{2}$$

Where C_{Al} is the concentration of component A in the liquid phase, C_{Al0} is the liquid phase inlet concentration, U_l is inlet velocity of the liquid phase, k_l the liquid phase mass transfer coefficient, H is the height of the liquid phase (note: the height of the gas phase and liquid phase are both H), L is the length of the reactor, C_{Al}^i is the liquid phase interface concentration and r_A the reaction rate law. From a mass balance over the gas-liquid interface it follows that the gas phase interface concentration is:

$$C_{Ag}^i = \frac{k_g C_{Ag} + k_l C_{Al}}{k_g + \frac{k_l}{K}} \tag{3}$$

The ratio of the gas phase interface concentration to the liquid phase interface concentration is equal to the equilibrium coefficient K:

$$K = \frac{C_{Ag}^i}{C_{Al}^i} \tag{4}$$

Discretization

A one dimensional grid is used to represent the gas phase and a single node is used to represent the liquid phase. The upwind differencing scheme is applied to the convection terms. Time discretization is fully implicit. The resulting linear system is solved using the Gauss-Seidel method.

Discretization of equations for the gas phase

The discrete form of equation (1) for the first, or left-most, node of the gas phase is:

$$H\Delta x \frac{(C^p_{Ag,0} - C^{p-1}_{Ag,0})}{\Delta t} = U_g H \cdot C_{Ag0} - U_g H \cdot C^p_{Ag,0} - k_g \Delta x C^p_{Ag,0} + k_g \Delta x \cdot C^{p,i}_{Ag,0} \tag{5}$$

Where $C^p_{Ag,0}$ is the concentration of component A at node 0 in the gas phase, $C^{p-1}_{Ag,0}$ is the concentration of component A of the previous timestep $p-1$, C_{Ag0} is the inlet gas phase concentration and $C^{p,i}_{Ag,0}$ is the gas phase interface concentration at node 0. The discrete form of equation (1) for the remaining nodes (second node until the last node) of the gas phase is:

$$H\Delta x \frac{(C^p_{Ag,j} - C^{p-1}_{Ag,j})}{\Delta t} = U_g H \cdot C^p_{Ag,j-1} - U_g H \cdot C^p_{Ag,j} - k_g \Delta x C^p_{Ag,j} + k_g \Delta x \cdot C^{p,i}_{Ag,j} \tag{6}$$

The subscript j denotes values at node j.

Discretization of equations for the liquid phase

The discrete form of (2) for the node representing the liquid phase is:

$$HL\frac{(C^p_{Al} - C^{p-1}_{Al})}{\Delta t} = U_l H \cdot C_{Al0} - U_l H \cdot C^p_{Al} + \sum_{j=0}^{n-1} k_l (C^{p,i}_{Al,j} - C^p_{Al})\Delta x + r_A HL \tag{7}$$

The term in equation (7) containing the reaction rate law needs to be linearized:

$$r_A = r_A^* + \frac{dr_A^*}{dC_{Al}}(C_{Al} - C_{Al}^*) \tag{8}$$

The asterisk denotes values from the previous iteration.

Verification

In order to verify that the computation proceeds correctly it is verified that equations (5) to (7) are satisfied. Analysis shows that the equations are satisfied with an error in the order of 1e-15.