Kinetics & Reactor Design 2: Liquid Reactors

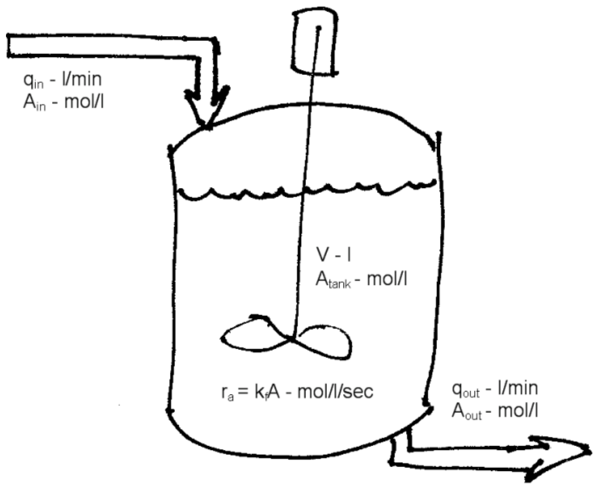
Continuing Ed workshop by Richard Skeirik,PE

CSTR Balance Exercise

Consider a stirred tank, with constant level. A liquid mixture is fed (the mixture is made just before the inlet). It consists of solvent and a single reactant A. In the solvent, A isomerizes to form B. B is very stable in the solvent so there is no reverse reaction. Since we are feeding/withdrawing continuously, it is well mixed, and a reaction takes place, this is CSTR – continuous stirred tank reactor.

Steady state, first order kinetics

The reaction rate is $r_a = k_f A$. the units of k_f are sec^{-1}



Write an expression for the rate of disappearance of A by reaction. Be clear about which A you are using. Show the units. Remember, rates are intrinsic (don't depend on how much you have)

[rate of reaction of A]

Now, adding a parameter given in the drawing, write an expression to compute how many mols are disappeared/lost in the whole reactor, by reaction, per unit time. This is extrinsic. Use your knowledge from the last exercise to get rid of A_{tank} and just use A_{out}.

[Mols A lost in whole reactor per unit time]

What are the units?

Remember, for reactors, the molar component material balance is

Flow of A in – flow of A out – rate of loss of A by reaction = Rate of accumulation of A

Now, using the parameters from the drawing, and what you've done above, write the steady state molar balance of A. (reminder: steady state means accumulation = 0)

[flow in] – [flow out] - [rate of loss by reaction] = [accumulation]

Compute the units of each term in your balance and be sure they are consistent. Adjust your material balance if you need to.

[flow in units] [flow out units] - [rate of loss by reaction units] = [accumulation units]

You've just written a steady state CSTR balance for first order irreversible kinetics.

Dynamic, first order

Just like the last exercise, write an expression that allows you to compute the total mols of A in the reactor. Please get rid of A_{tank} in favor A_{out}

[total mols of A in reactor]

Using derivative notation, write an expression for the rate of change of total mols of A in the reactor.

[rate of change of total mols A in reactor wrt time]

Remember, for reactors, the molar component material balance is

Flow of A in – flow of A out – rate of loss of A by reaction = Rate of accumulation of A

The derivative you just wrote is the rate of change of mols of A: that is, the rate of accumulation of A. Now extend your steady state balance by adding the accumulation term:

[flow in] – [flow out] - [rate of loss by reaction] = [accumulation]

Check the units on each term to make sure they match.
[flow in units]   [flow out units] - [rate of loss by reaction units] = [accumulation units]

You've just written a dynamic CSTR balance for first order irreversible kinetics.

If the level is always well controlled, one of the terms in your derivative will be constant. Bring it outside the derivative. This is easier to solve, which we'll do later.

Second order kinetics

Everything is the same, except the reaction rate is $r_a = k_f A^2$. the units of k_f are l $mol^{-1} sec^{-1}$
Modify your dynamic balance by substituting these kinetics.
[flow in] – [flow out] - [rate of loss by reaction] = [accumulation]

Check the units on each term to make sure they match.
[flow in units]   [flow out units] - [rate of loss by reaction units] = [accumulation units]

You've just written a dynamic CSTR balance for second order irreversible kinetics.

Now if I handed you some arbitrary kinetic expression, do you think you could write a CSTR balance for those kinetics?