ABSTRACT FOR CONTINUOUS CRYSTALLIZER

Description:

This code is for continuous crystallizer, taking in account the case as follows:
1) Isothermal Continuous crystallizer operating at steady state

The transient state crystallizer is given by equation:

$$\frac{dC^*}{dt^*} = 1 - C^* - 2\,Si\,Op^4\,C^{*4}\left(1 - \left(\frac{t^{*2}}{2} + t^* + 1\right)\exp\{-t^*\}\right)$$

Where,

$$n^* \equiv \frac{n}{n_{in}}$$

$$L^* \equiv \frac{LQ}{VK(C_{in} - C_s)} \qquad Si \equiv \Phi L_{ref}^3 \frac{\rho\, n_{in}\, L_{ref}}{C_{in} - C_s}$$

$$t^* \equiv \frac{tQ}{V}$$

$$C^* \equiv \frac{C - C_s}{C_{in} - C_s} \qquad Op \equiv \frac{KV(C_{in} - C_s)}{QL_{ref}}$$

Where, n denotes population density
L denotes size of crystal in length units
Q is volumetric flow rate of feed
K is growth rate constant
C denotes concentration, subscript s denotes saturation
V denotes volume of crystallizer
Φ denotes area factor
ρ denotes crystal density
Si, Op are dimensionless constants.
L_{ref} is any quantity in length dimension which is assumed to be 1.

(The derivation of above equations can be seen in the given reference)

At time t tending to infinity, concentration is given by the following equation:

$$2\,Si\,Op^4\,C_{ss}^{*4} + C_{ss}^{*} - 1 = 0$$

This bi-quadratic equation is solved using Newton Raphson iterative method. The final equation using newton Raphson is:

$$C_{ss}^*(i+1) = C_{ss}^*(i) - \frac{(2SiOp^4C_{ss}^{*4}(i) + C_{ss}^*(i) - 1)}{(8SiOp^4C_{ss}^{*3}(i) + 1)}$$

Where, i is the iteration number.

Using this steady state concentration, the amount of mass of solute entering crystal phase is calculated. The final size of crystal is then calculated using the following formula:

$$L_{final} = (\frac{(volume\ change)}{Volume\ factor} + L_{initial}^3)^{1/3}$$

Reference:
https://repositorio.ucp.pt/bitstream/10400.14/6707/1/Mathematical%20design%20of%20continuous%2C%20isothermal.pdf

Examples:

1) A solution with 0.7 mole fraction water and 0.3 mole fraction carbon, flowing at rate 186mole/s enters a crystallizer. Initial size of crystal is 0.02m. Area and volume factor can be assumed to be 1. Assume crystal density to be 5000 kg/m3. Assume Growth rate constant to be 0.1 m^4/mol-s. Assume density of mother liqour to be 1000 Kg/m^3. Assume Volume of reactor to be 1m^3. The volumetric flow rate is 3.14 m^3/s.
Thermodynamic Package used: Peng-Robinson
Flash Method: SVLLE

Ans)

Si from above equation can be calculated as: $Si = \frac{1\times5000\times(186\times\frac{0.3}{3.14}/0.02)}{186\times\frac{0.3}{3.14}-2} = 281704$

Op from above equation is calculated as: $Op = \frac{0.1\times1\times(186\times\frac{0.3}{3.14}-2)}{3.14} = 0.502$

The bi-quadratic equation to be solved is: $35780C_{ss}^{*4} + C_{ss}^{*} - 1 = 0$
On solving the equation in graphical calculator, we get the answer: C^*_{ss} = 0.0714.
This corresponds to concentration of: C=0.0714*(186*0.3/3.14 – 2) + 2 = 3.126 mol/m^3
Flow of carbon in product stream can be calculated as (assuming constant volumetric flow since removed compound is solid): F_0 = 3.126 * 3.14 = 9.82 mol/s.

The molar flowrate of water is the same as molar flowrate in feed stream i.e. 130.2 mol/s

The flow calculated in DWSIM code is 9.81 mol/s which is very close to theoritical calculation.

Compound	Flowrate in product Stream (in mol/s)	
	Analytical Calculation	DWSIM
Water	130.2	130.34
Carbon	9.82	9.81