Biomaterials HW 6

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1. Initially, the instantaneous copolymer compositions can be calculated using the formula

$$F_A = \frac{r_A f_A^2 + f_A f_B}{r_A f_A^2 + 2 f_A f_B + r_B f_B^2}$$

At 10% conversion,

$$f_A = \frac{60}{40 + 60} = 0.6, f_B = 0.4, F_A = 0.2308$$

Assuming there are a total of 10 mol of starting material, we can calculate the mols of A consumed as

$$0.2308 * 10mol * 10 = 0.2308mol$$

Thus, the new monomer composition is

$$f_1 = \frac{6 - 0.2308}{10 - 1} = 0.641$$

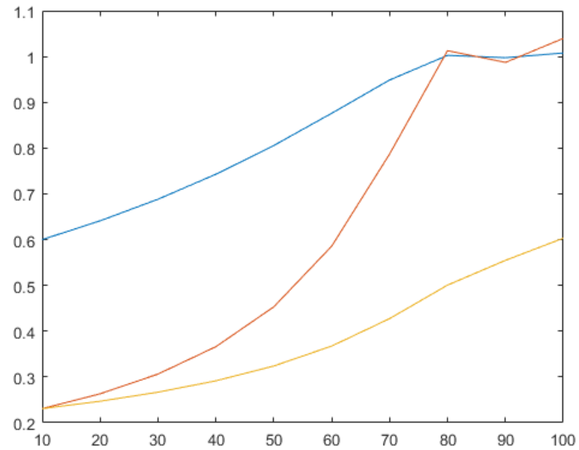
The new copolymer composition can be calculated from this number, and the average copolymer composition is

$$\frac{0.2308mol}{1mol} = 0.2308$$

The remaining numbers can be calculated in a similar way and are shown below.

% Conversion	*Monomer Composition*	*Copolymer Composition*	*Cumulative Copolymer Composition*
10%	0.6	0.2308	0.2308
20%	0.6410	0.2632	0.2470
30%	0.6883	0.3063	0.2667
40%	0.7428	0.3662	0.2916
50%	0.8056	0.4532	0.3239
60%	0.8761	0.5857	0.3676
70%	0.9487	0.7871	0.4275
80%	1	1	0.5007
90%	1	1	0.5547
100%	1	1	0.6032

Below, blue represent monomer composition, red represents copolymer composition, and yellow represents cumulative copolymer composition



2A. Vinyl Chloride

a. At equimolar concentrations, $f_a = f_b = 0.5, r_A = 0.23, r_B = 1.68$. Therefore,

$$F_A = \frac{r_A f_A^2 + f_A f_B}{r_A f_A^2 + 2 f_A f_B + r_B f_B^2} = 0.31$$

b. If $F_A = 0.5$, we can reverse-solve for f_A using the formula above after substituting $f_B = 1 - f_A$ to get

$$0.5 = \frac{r_A f_A^2 + f_A(1 - f_A)}{r_A f_A^2 + 2 f_A(1 - f_A) + r_B(1 - f_A)^2} = \frac{(r_A - 1) f_A^2 + f_A}{(r_A + r_B - 2) f_A^2 + (2 - 2r_B) f_A + r_B}$$

Therefore,

$$f_A = 0.73, \frac{[A]}{[B]} = \frac{f_A}{1 - f_A} = 2.70$$

2B. Acrylonitrile

a. At equimolar concentrations, $f_a = f_b = 0.5, r_A = 0.06, r_B = 4.05$. Therefore,

$$F_A = \frac{r_A f_A^2 + f_A f_B}{r_A f_A^2 + 2 f_A f_B + r_B f_B^2} = 0.17$$

b. Using the same method above, we get that

$$f_A = 0.89, \frac{[A]}{[B]} = 8.09$$

2C. Styrene

a. At equimolar concentrations, $f_a = f_b = 0.5, r_A = 0.01, r_B = 55$. Therefore,

$$F_A = \frac{r_A f_A^2 + f_A f_B}{r_A f_A^2 + 2 f_A f_B + r_B f_B^2} = 0.018$$

b. Using the same method above, we get that

$$f_A = 0.98, \frac{[A]}{[B]} = 49$$