

EXERCISES TO THE LECTURE POLYMER REACTION & COLLOID ENGINEERING

SERIES 6

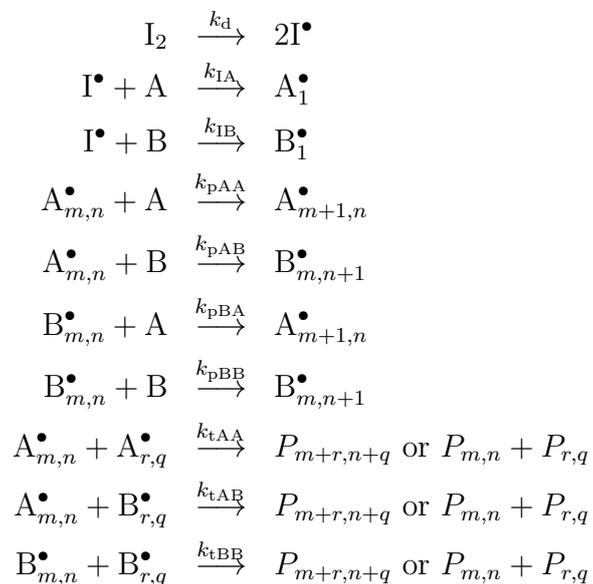
issue date: 21.12.2016

due date: 11.01.2017

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Copolymerization

The styrene(A)/MMA(B)-copolymerization is to be carried out in a 15-L batch reactor under bulk conditions at 65°C. In order to be prepared for the planned experiments you decide to make a few calculations first. In the literature you found values for the reactivity ratios which are $r_A = 0.52$ and $r_B = 0.46$, respectively. You decide to consider the following typical reaction steps of a free-radical copolymerization:



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Making good experience in the past you decide to use again the Buback-expression to describe glass and gel effect:

$$k_p = \frac{1}{\frac{1}{k_p^0} + \frac{\exp(C_\eta w_p)}{k_{p,D}^0}}$$

$$k_t = \frac{1}{\frac{1}{k_t^0} + \frac{\exp(C_\eta w_p)}{k_{t,D}^0}} + C_{RD} k_p (1 - w_p)$$

where w_p is the weight fraction of the polymer in the reaction mixture. Finally, you elect to carry out the following pre-calculation:

- The determination of the instantaneous as well as the cumulative composition of the produced polymer chains as a function of the overall conversion. In addition, the computation of the instantaneous composition of the produced polymer chains as a function of monomer mixture composition. (**Hint:** To solve this part you only need the initial composition and the reactivity ratios.)
- The evaluation of the evolution of the monomer concentrations versus time as well as the overall conversion versus time.
- The calculation of the cumulative number average, \bar{n}_N^c and weight average \bar{n}_W^c of the CLD as well as the cumulative polydispersity index σ^c as a function of the overall conversion for the above described copolymerization system assuming that disproportionation is the dominating termination step.

Additional information:

$c_A^0 =$	3.5	mol/L	$w_I^0 =$	0.01	
$\rho_A =$	0.90	kg/L	$\rho_B =$	0.94	kg/L
$M_{m,A} =$	104	g/mol	$M_{m,B} =$	100	g/mol
$M_{m,I} =$	164	g/mol	$k_{tAB} =$	$\sqrt{k_{tAA} k_{tBB}}$	L/mol/s
$k_d =$	6.77e-6	1/s	$f =$	0.5	
$k_{pAA}^0 =$	4.1e2	L/mol/s	$k_{tAA}^0 =$	2.4e7	L/mol/s
$k_{pA,D}^0 =$	2e11	L/mol/s	$k_{tA,D}^0 =$	5e8	L/mol/s
$C_{\eta,A} =$	25		$C_{RD,A} =$	180	
$k_{pBB}^0 =$	9.3e2	L/mol/s	$k_{tBB}^0 =$	9.2e6	L/mol/s
$k_{pB,D}^0 =$	2e11	L/mol/s	$k_{tB,D}^0 =$	5e8	L/mol/s
$C_{\eta,B} =$	25		$C_{RD,B} =$	180	

