Equations

$$\Delta S = -R\left(N_1 \ln v_1 + N_2 \ln v_2\right)$$

$$\Delta H = \chi_1 RTN_1 v_2$$

$$\Delta G = \Delta H - T\Delta S$$

$$\Delta G_m = \chi_1 RTN_1 v_2 + RT\left(N_1 \ln v_1 + N_2 \ln v_2\right)$$

$$\Delta G_m = RT\left(\chi_1 N_1 v_2 + N_1 \ln v_1 + N_2 \ln v_2\right)$$

Put into two phase system with monomer droplets

$$\Delta G_S = RT\left(\ln\left(\frac{v_{s2}}{v_{s1}}\right) + \left(1 - \frac{N_1}{N_2}\right)\left(v_{p2} - v_{p1}\right) + \left(v_{p2}^2 + v_{p1}^2\right)\chi_{12}\right)$$

no polymer in droplets, sub in 1/x for N1/N2

$$\Delta G_S = RT\left(\ln(v_{s2}) + \left(1 - \frac{1}{x}\right)v_{p2} + v_{p2}^2\chi_{12}\right)$$

similarly for the polymer phase...

$$\Delta G_p = RT\left(\ln\left(v_{p2}\right) + (x-1)\left(1 - v_{p2}\right) + \left(1 - v_{p2}\right)^2 x\chi_{12}\right)$$

Convert to activity cof form (dG = RTln(a))

$$a_1 = v_1 e^{1 - v_1 - \frac{v_2 x_1}{x_2} - \frac{v_3 x_1}{x_3} + (\chi_{12} v_2 + \chi_{13} v_3)(v_2 + v_3) - \chi_{23}\frac{x_1}{x_2} v_2 v_3}$$

$$a_2 = v_2 e^{1 - v_2 - \frac{v_1 x_2}{x_1} - \frac{v_3 x_2}{x_3} + (\chi_{21} v_1 + \chi_{23} v_3)(v_1 + v_3) - \chi_{13}\frac{x_2}{x_1} v_1 v_3}$$

$$a_3 = v_3 e^{1 - v_3 - \frac{v_2 x_3}{x_2} - \frac{v_1 x_3}{x_1} + (\chi_{31} v_1 + \chi_{32} v_2)(v_2 + v_1) - \chi_{12}\frac{x_3}{x_1} v_2 v_1}$$

Surface tension terms

$$a_1 = a_1^{\circ} e^{\frac{2\sigma_{I,water} v_1}{r_{drop} RT}} \approx a_1^{\circ}$$

$$a_2 = a_2^{\circ} e^{\frac{2\sigma_{II,water} v_2}{r_{particle} RT}}$$

$$a_3 = a_3^{\circ} e^{\frac{2\sigma_{III,water} v_3}{r_{particle} RT}} e^{\frac{2\sigma_{II,III} v_3}{r_{core} RT}} \approx a_3^{\circ} e^{\frac{2\sigma_{III,water} v_3}{r_{particle} RT}}$$

Nomenclature

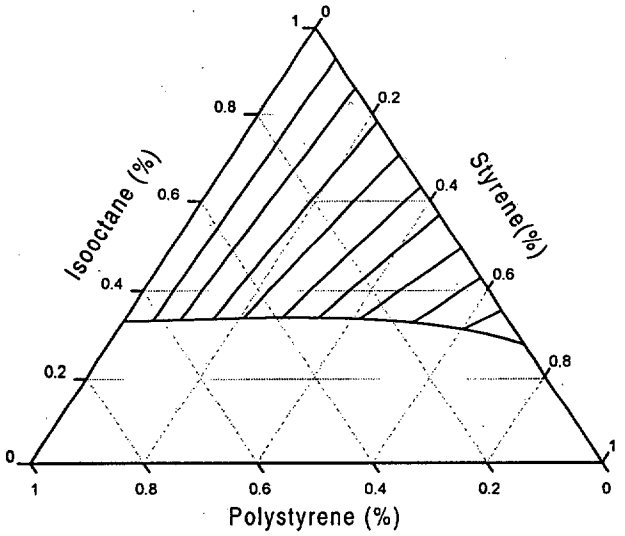
v_1 = Volume Fraction of solvent
v_2 = Volume Fraction of polymer
v_{p1} = Bolume Fraction of polymer in solvent
v_{s1} = Volume Fraction of solvent in solvent
v_{p2} = Volume Fraction of polymer in polymer
v_{s2} = Volume Fraction of solvent in polymer

ΔS_m = Entropy of Mixing
ΔH_m = Heat of Mixing
ΔG_m = Free Energy of Mixing
T = Temperature
χ = Interaction Parameter
k = Boltzmann Constant
N = Number of molecules
x = Number of segments in chain

Subscripts

1 = Solvent
2 = Polymer
3 = Nonsolvent

Ternary diagram for equilibrium within a growing polymer particle (MW = infinite)



Ternary diagram for equilibrium between hydrocarbon droplets and swollen gel (MW = infinite)