

Free Energy of the Binary XPFC Model

The free energy of the binary xpfc model can be written as,

$$\frac{\beta\mathcal{F}[n, c]}{\rho_0} = \int dr \frac{n^2}{2} - \chi \frac{n^3}{6} + \eta \frac{n^4}{12} + \frac{W_c}{2} |\nabla c|^2 + (1+n) \Delta f_{mix}(c) - \frac{1}{2} n \int dr' C_{eff}^n(r-r'; c) n(r'). \quad (1)$$

Where the free energy of mixing is,

$$\Delta f_{mix}(c) = \omega \left(c \ln \left(\frac{c}{c_0} \right) + (1-c) \ln \left(\frac{1-c}{1-c_0} \right) + \frac{\epsilon(T)}{2} (c - c_0)^2 \right). \quad (2)$$

We assume that both the total density, n , and the concentration, c , follow conservative, diffusive dynamics to relax to equilibrium.

$$\frac{\partial c}{\partial t} = M_c \nabla^2 () \quad (3)$$