

<u>UNIQUAC formulation</u>	
$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$	Expression for activity coefficient
$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_j x_j l_j$	Combinatorial part
$\ln \gamma_i^R = q_i \left[1 - \ln \left(\sum_j \theta_j \tau_{ji} \right) - \sum_j \frac{\theta_j \tau_{ij}}{\sum_k \theta_k \tau_{kj}} \right]$	Residual part
$l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1)$	z = coordination number = 10
$\phi_i = \frac{x_i r_i}{\sum_j x_j r_j}$	Φ_i is volume fraction r_i is volume parameter
$\theta_i = \frac{x_i q_i}{\sum_j x_j q_j}$	θ_i is area fraction q_i is area parameter
$\tau_{ji} = \exp \left[-\frac{(u_{ji} - u_{ii})}{RT} \right]$	τ_{ji} is interaction parameter u_{ji} is average interaction

Calculate the activity coefficient:

1) Estimate the activity coefficients of ternary mixture at 345 K and 1 bar pressure by UNIQUAC model. The mole fraction, area, volume parameters, interaction parameters are given below. Calculate the azeotropic compositions at the same condition.

$$u = \begin{pmatrix} 1.0 & 1.216 & 0.203 \\ 0.617 & 1.0 & 0.048 \\ 0.838 & 0.612 & 1.0 \end{pmatrix}$$

parameter	Benzene	Toluene	water
x	0.2	0.3	0.5
r	2.5755	3.1878	2.7694
q	2.588	2.634	2.400