

# Non - Random Two Liquid (NRTL)

Proposed by Scott.

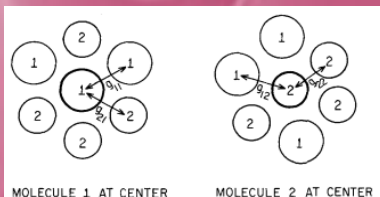
**Basis:** Semi-empirical, considers  $\alpha_{12}$  as an empirical constant independent of temperature and specific for a particular pair of species.

The NRTL model include the concept of binary interaction parameters and require to be fitted with experimental data.

## Molecules & intermolecular forces

Molecular thermodynamics of liquid solution behavior are often based on the concept of local composition, presumed to account for the short-range order and nonrandom molecular orientations resulting from differences in molecular size and intermolecular forces.

A mixture of molecules with strongly non-ideal interactions, the molecules are grouped in a non-random in which due to the physical properties of the molecules are formed localized compositions, different from the overall composition



## Mathematical Equation

$$\frac{g^E}{RT} = x_1 x_2 \left( \frac{\tau_{21} G_{21}}{x_1 + x_2 G_{21}} + \frac{\tau_{12} G_{12}}{x_2 + x_1 G_{12}} \right)$$

$$\tau_{12} = \frac{\Delta g_{12}}{RT} \quad \tau_{21} = \frac{\Delta g_{21}}{RT}$$

$$\ln G_{12} = -\alpha_{12} \tau_{12} \quad \ln G_{21} = -\alpha_{12} \tau_{21}$$

$$\ln \gamma_1 = x_2^2 \left[ \tau_{21} \left( \frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right]$$

$$\ln \gamma_2 = x_1^2 \left[ \tau_{12} \left( \frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right]$$

Parameters:  $\alpha_{12}$ ,  $\Delta g_{12}$ ,  $\Delta g_{21}$

There are 2 types of molecules according to Scott's two-liquid theory of binary mixtures: type 1 and type 2

The residual Gibbs energy,  $g_{i-j}$ , is the sum of all residual Gibbs energies of the interactions experienced by the molecule 1 that is in the center.

## APPLICATIONS

Binary systems

Multicomponent systems

Azeotropic systems

Liquid-Liquid equilibria

Limitations → Moderately nonideal systems

For strongly non ideal systems and especially for partially immiscible systems, the equations of this model represent a good representation of experimental data and its possible to obtain adjustable parameters.