

Four descriptions of vapour-liquid equilibrium, and what each one costs

more physics → more parameters, more data, more computation ↑

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ϕ - ϕ formulation

$$y_i \hat{\phi}_i^V P = x_i \hat{\phi}_i^L P$$

costs: one EOS for both phases, k_{ij} , and a root/stability test



+ one EOS for both phases: no P^{sat} , valid above T_c

3

γ - ϕ formulation

$$y_i \hat{\phi}_i P = x_i \gamma_i P_i^{\text{sat}} \phi_i^{\text{sat}} \mathcal{F}_i$$

costs: a vapour EOS, virial coefficients, and an inner iteration



+ vapour non-ideality: $\hat{\phi}_i$, ϕ_i^{sat} and the Poynting factor

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Modified Raoult's law

$$y_i P = x_i \gamma_i P_i^{\text{sat}}$$

costs: a G^E model and 2 parameters fitted to binary VLE data



+ liquid non-ideality: $\gamma_i(x, T)$ from an excess Gibbs energy

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Raoult's law

$$y_i P = x_i P_i^{\text{sat}}$$

costs: nothing but $P_i^{\text{sat}}(T)$ — no binary parameter, no data

Every rung is exact given its own assumptions. Choosing a rung is choosing which assumption to defend.