Problem Statement

Solve BUBL-P for the binary ETHANOL / WATER system at T = 343.15 K using the Modified Raoult formulation (target: Bubble).

Knowns (Given)

Quantity	Symbol	Value	Source
Temperature	T	$343.15\,\mathrm{K}$	Configured
Liquid mole fraction, ETHANOL	$x_{ETHANOL}$	0.5	Configured
Liquid mole fraction, WATER	x_{WATER}	0.5	Configured
Activity model	γ_i	NRTL	Configured
NRTL τ12 coefficients	$a_{12}, b_{12}, e_{12}, f_{12}$	$a_{12} = -0.9223,\ b_{12} = 284.2856\,\mathrm{K},\ e_{12} = 0,\ f_{12} = 0\,\mathrm{K}^{-1}$	Library
NRTL τ21 coefficients	$a_{21}, b_{21}, e_{21}, f_{21}$	$a_{21} = 3.622,\ b_{21} = -636.726\,\mathrm{K},\ e_{21} = 0,\ f_{21} = 0\,\mathrm{K}^{-1}$	Library
NRTL α coefficients	c, d	$c = 0.3,\ d = 0\,\mathrm{K}^{-1}$	Library
Valid T range	—	298.14–408.65 K	Library

Unknowns (Find)

- Bubble pressure P
- Incipient vapor composition y
- Equilibrium ratios K_i

Assumptions

- The vapor phase is an ideal gas.
- Liquid-phase non-ideality is described by the NRTL activity model.

Step 1: Model Equations

BUBL-P at known T and liquid composition x: find the bubble pressure P and the incipient vapor composition y using the Modified-Raoult equilibrium ratio K_i.

The Antoine coefficients expect T in °C and P in mmHg: $T[^\circ\mathrm{C}] = T[\mathrm{K}] - 273.15$, and P^{sat} is converted to bar with $1\ \mathrm{bar} = 750.062\ \mathrm{mmHg}$.

Relation	Equation
Phase-equilibrium condition (Modified Raoult's law)	$$y_i P = x_i \gamma_i(x,T) P_i^{sat}(T)$$
Equilibrium ratio	$$K_i = \frac{\gamma_i(x,T)\, P_i^{sat}(T)}{P}$$

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Relation	Equation
Saturation pressure (imported)	$\log_{10} P_i^{sat}[\text{mmHg}] = A_i - \dfrac{B_i}{T[^\circ\text{C}] + C_i}$
Activity coefficient (imported)	$\ln \gamma_i = x_j^2 \left[\tau_{ji} \left(\dfrac{G_{ji}}{x_i + x_j G_{ji}} \right)^2 + \dfrac{\tau_{ij} G_{ij}}{(x_j + x_i G_{ij})^2} \right]$
τ12 correlation	$\tau_{12} = a_{12} + \dfrac{b_{12}}{T} + e_{12} \ln T + f_{12} T$
τ21 correlation	$\tau_{21} = a_{21} + \dfrac{b_{21}}{T} + e_{21} \ln T + f_{21} T$
α correlation	$\alpha = c + d\,(T - 273.15)$
Bubble-point pressure	$P = \sum_i x_i \gamma_i(x, T) P_i^{sat}(T)$
Incipient vapor composition	$y_i = x_i K_i$
Bubble closure	$R_B = \sum_i x_i K_i - 1$

Step 2: Upstream property values

Saturation pressures at $T = 343.15$ K from Pure Properties (Antoine):

$$P^{sat}_{ETHANOL} = 0.7229 \text{ bar}$$
$$P^{sat}_{WATER} = 0.3109 \text{ bar}$$

Activity coefficients from Solution Thermodynamics (NRTL, parameters listed in Knowns); x and T are known, so no iteration is needed:

$$\gamma_{ETHANOL} = 1.245$$
$$\gamma_{WATER} = 1.474$$

Step 3: Calculate the bubble pressure

$$P = \sum_i x_i \gamma_i(x, T) P_i^{sat}(T)$$

$$P = 0.5 \times 1.245 \times 0.7229 + 0.5 \times 1.474 \times 0.3109 \approx 0.6791 \text{ bar}$$

Step 4: Calculate the equilibrium ratios Kᵢ

$$K_i = \frac{\gamma_i(x, T)\, P_i^{sat}(T)}{P}$$

$$K_{ETHANOL} = \frac{1.245 \times 0.7229}{0.6791} \approx 1.325$$

$$K_{WATER} = \frac{1.474 \times 0.3109}{0.6791} \approx 0.6748$$

Step 5: Calculate the incipient vapor composition y

$$y_i = x_i K_i$$

$$y_{ETHANOL} = 0.5 \times 1.3252 \approx 0.6626$$

$$y_{WATER} = 0.5 \times 0.6748 \approx 0.3374$$

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Step 6: Final result

$$\boxed{P = 0.6791 \text{ bar}}$$

At the fixed $T = 343.15$ K, the bubble point lies at $P = 0.6791$ bar. The liquid composition x is known; the incipient vapor y is calculated.

$K_{ETHANOL} = 1.325 > 1$, so ETHANOL is the more volatile component at this state: the vapor is enriched in it ($y_{ETHANOL} = 0.6626$ exceeds $x_{ETHANOL} = 0.5$).

Component	x	y	K
ETHANOL	0.5	0.6626	1.325
WATER	0.5	0.3374	0.6748

> ***Check:*** $\sum_i x_i K_i = 1$ at the solved state; both phase compositions are normalized and lie between 0 and 1.

Discussion

- Because $\gamma_i \neq 1$, each K_i differs from the ideal Raoult value $P_i^{sat}(T)/P$ by the factor γ_i; that factor is the whole liquid-phase non-ideality effect at this state.

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