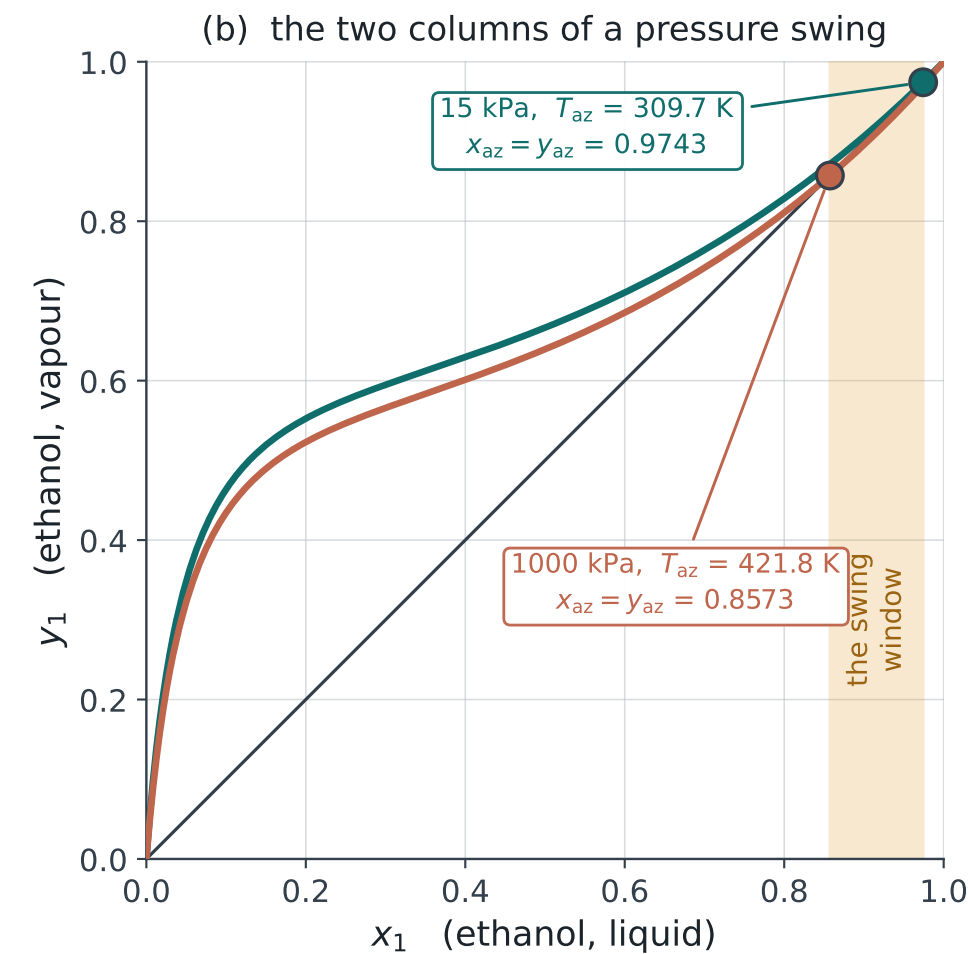
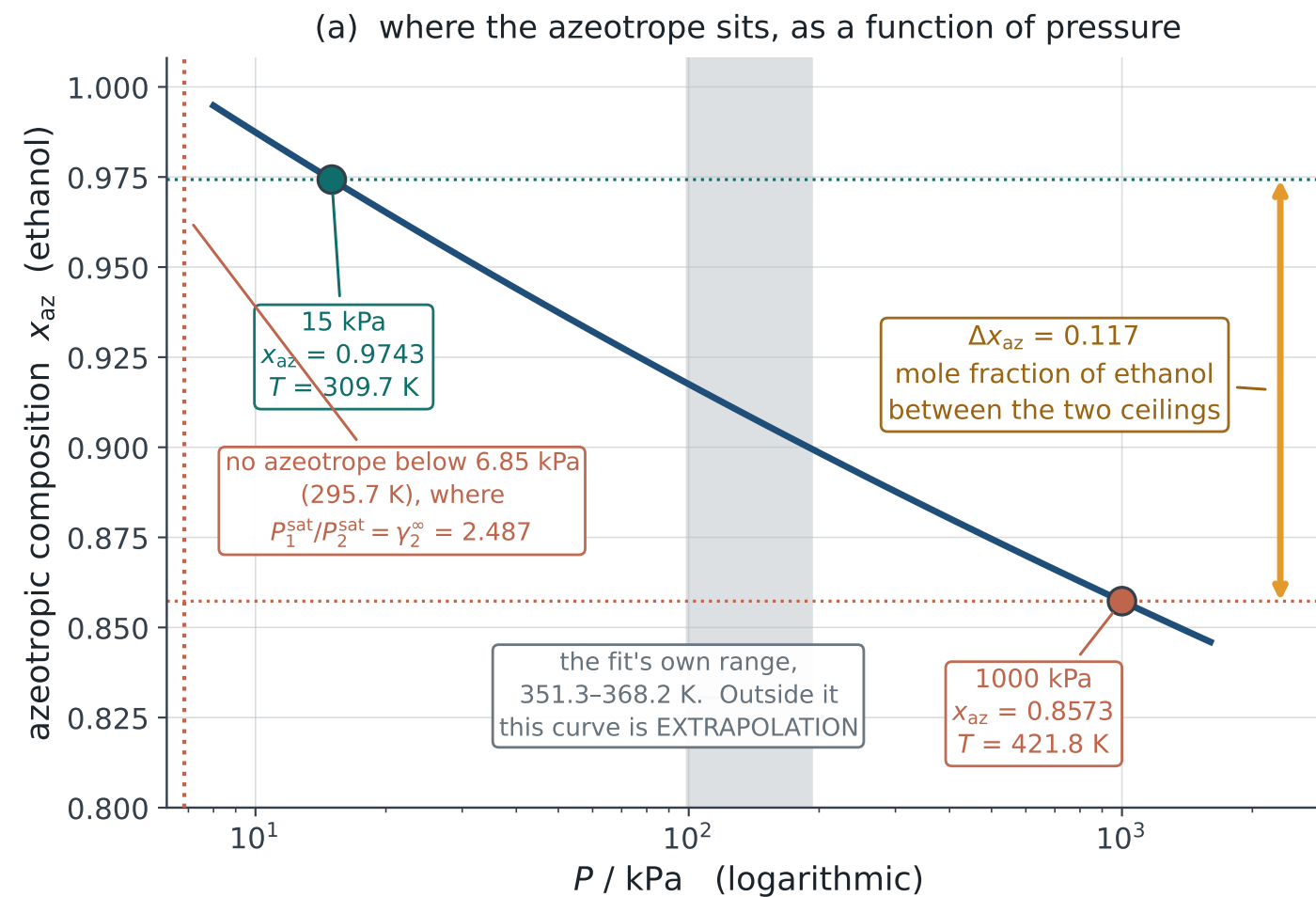


Pressure-swing distillation of ethanol + water: the azeotrope is a property of the pressure, not of the mixture



MODEL: NRTL ($\alpha = 0.3$, $\tau_{12} = -0.1712$, $\tau_{21} = +1.9330$) fitted by Barker's method to Kamihama et al. 2012, doi:10.1021/je2008704 — 21 points, 101.3 kPa, 351.3–368.2 K, rms $\delta T = 0.059 \text{ K}$. P_i^{sat} from vlekkit.data.LIBRARY.

THE PARAMETERS ARE HELD FIXED AS P IS VARIED. τ_{ij} carries no temperature dependence of its own, so in this calculation the whole shift comes from $P_1^{\text{sat}}/P_2^{\text{sat}}(T)$; the real G^E also changes with T , and a fit at one pressure cannot know how.

For scale: at 101.3 kPa this model puts the azeotrope at $x_1 = 0.9172$ where the published table gives 0.8946, a difference of 0.0226 in mole fraction.