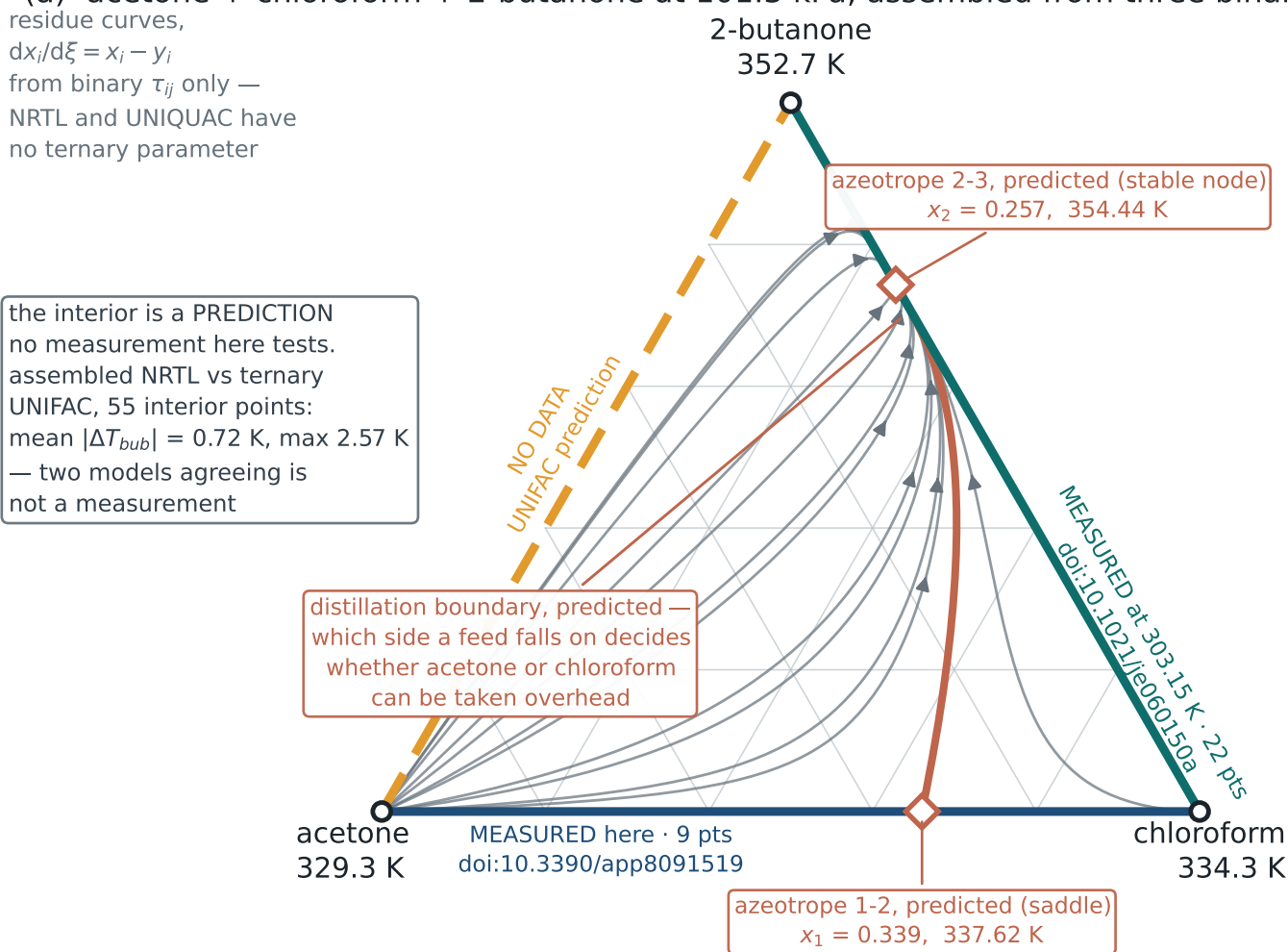
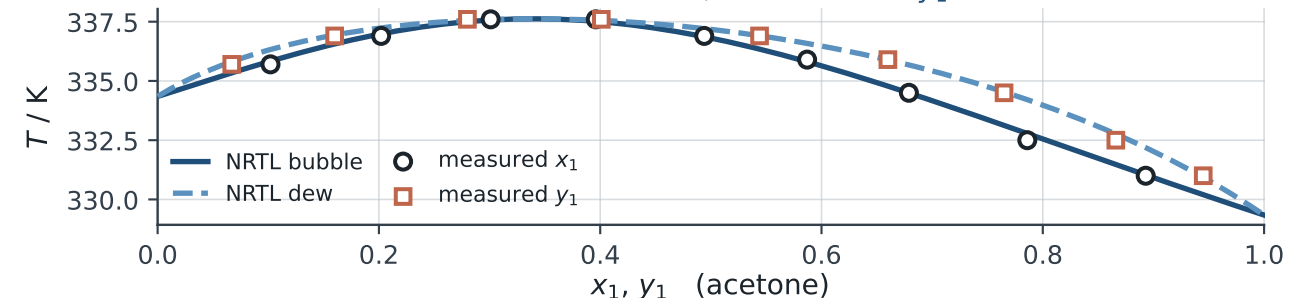


The reason NRTL and UNIQUAC replaced Margules and van Laar: a ternary needs no ternary parameter — but a prediction still needs a measurement

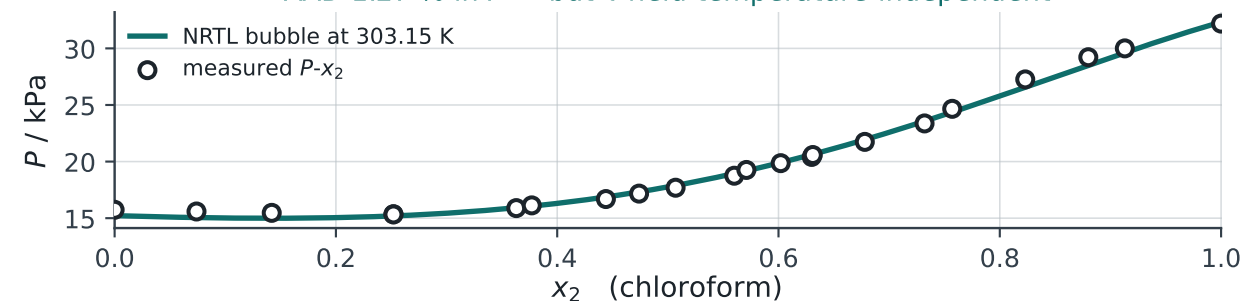
(a) acetone + chloroform + 2-butanone at 101.3 kPa, assembled from three binary parameter sets



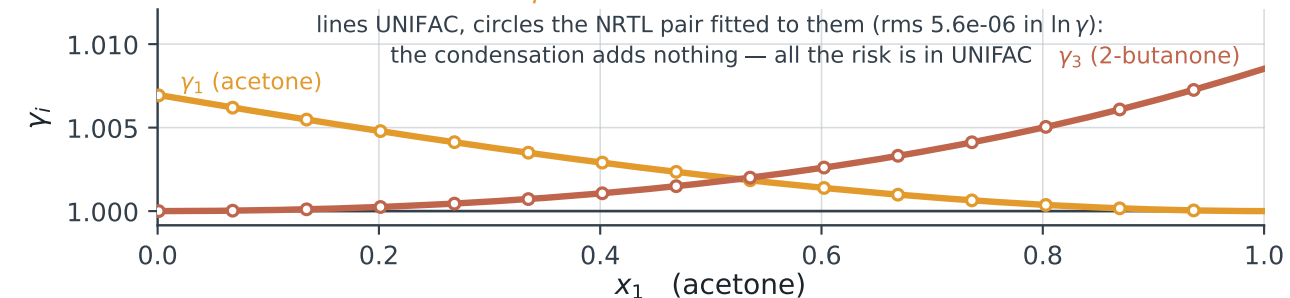
(b) edge 1-2 FITTED — and it reproduces its own data
 AAD 0.087 K in T , rms 0.0072 in y_1



(c) edge 2-3 FITTED at 303.15 K, used 50 K higher
 AAD 1.27 % in P — but τ held temperature-independent



(d) edge 1-3 PREDICTED — there is no data to fit
 UNIFAC: $\gamma^\infty = 1.0070$ and 1.0085 at 341.0 K



acetone (1) + chloroform (2) + 2-butanone (3) at 101.3 kPa. NRTL ($\alpha = 0.3$) on every pair; the ternary uses the three fitted pairs unchanged and adds NO parameter of its own. Edge 1-2: Barker on T , doi:10.3390/app8091519 (9 points, 101.3 kPa). Edge 2-3: Barker on P , doi:10.1021/je060150a (22 points, 303.15 K). Edge 1-3 has no measurement in this module and is predicted by original VLE UNIFAC (Fredenslund-Jones-Prausnitz form, Hansen et al. VLE table, the subset embedded in vlekkit.unifac), then condensed to an NRTL pair at 341.0 K. ASSUMPTIONS, stated because none of them is tested here: τ is taken temperature-independent, so edge 2-3 is used 50 K above its data; the vapour is ideal and $\Phi_i = 1$; $\alpha = 0.3$ is assumed, not fitted; and the residue curves, the azeotropes, the boundary and the whole interior are PREDICTIONS. There is no measured ternary datum on this figure. WHAT WOULD TEST IT: measured ternary P - x - y or T - x - y for this system at 101.3 kPa, a ternary azeotrope search, or a measured residue curve. Absent those, the only handle is a second independent prediction: ternary UNIFAC on the same grid (55 points, every $x_i \geq 0.05$) sits within 0.72 K on average and 2.57 K at worst of the assembled NRTL — a consistency check between two models, NOT a validation. On edge 1-2, where measurements do exist, that same UNIFAC is off by 0.25 K (F4.20).