

VLE data and model checks

Week 2 follow-up · A guided Lab 08 review

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A clearer route through Lab 08

Your feedback asked for clearer unit conventions, a guided demonstration and more explanation of the results.

Open: [Lab 08](#) and the [three-page Lab guide](#).

We will use one synthetic dataset throughout this review. Follow along for **15 minutes at the start of Session 3**. The last three slides are optional reference material.

Keep your original worksheet. Add corrections beside it. This review adds no attendance submission.

What the activity coefficient describes

At the same measured temperature, modified Raoult's law gives

$$y_i P = x_i \gamma_i P_i^{sat}, \quad \gamma_i = \frac{y_i P}{x_i P_i^{sat}}.$$

- x_i : liquid mole fraction. y_i : vapor mole fraction.
- P : total pressure. P_i^{sat} : pure-component saturation pressure.
- γ_i : departure from the ideal-liquid reference. It is dimensionless.

Assumptions here: ideal vapor and negligible Poynting correction. Use the same pressure unit in numerator and denominator.

Your action: Locate these quantities on guide page 1 before opening any fit.

The worksheet and Lab use different examples

	Worksheet page 2, Section C	Lab 08 synthetic example
Equilibrium temperature	50 °C = 323.15 K	350 K = 76.85 °C
Temperature in Antoine equation	°C	K
Constants	A = 4, B = 1000, C = 200	Supplied separately for each component
Purpose	Practice equation conventions	Work with a complete VLE dataset

Your action: Select **Load synthetic example** in Lab 08. Use its own constants. Keep the Section C constants in that paper exercise.

Both examples are synthetic teaching data.

Three temperature labels

Setting or display	Meaning	Lab example
Measured-data temperature unit	Unit of the numbers in the input file	350 with K selected
Temperature inside Antoine equation	Convention attached to A, B and C	Insert 350 in this K correlation
Valid temperature limits	Range fields always use K	300–390 K

The calculated observation table always displays **K and kPa**.

Your action: Check all three locations on guide page 2. An equivalent measured input is **76.85 with °C selected**. Merely relabeling 350 as °C changes the temperature.

One observation and its calculated properties

Your action: After validation, locate $x_1 = 0.5$ in Imported observations. Use guide page 1.

Input observation	Value	Calculated property at 350 K	Value
T	350 K	P_1^{sat}	150 kPa
P	158.707198 kPa	P_2^{sat}	60 kPa
x_1	0.500000	$\ln \gamma_1$	0.399813
y_1	0.704857	$\ln \gamma_2$	0.445568

P_1^{sat} and P_2^{sat} come from the two Antoine correlations. They are not the total mixture pressure P .

A hand calculation beside the Lab result

$$\gamma_1 = \frac{0.704857144627 (158.707198211)}{0.5 (150)} \approx 1.491545$$

$$\gamma_2 = \frac{(1 - 0.704857144627) (158.707198211)}{(1 - 0.5) (60)} \approx 1.561377$$

All pressures are in kPa. Both results are dimensionless.

Your action: Calculate γ_1 and compare it with $\exp(0.399813)$, allowing for display rounding. The table reports **ln γ** , so comparing 1.491545 directly with 0.399813 compares different quantities.

Agreement checks the calculation with the chosen inputs. Real property accuracy needs an independent reference.

The demonstrated workflow

Your action: Follow guide page 2 and repeat these steps in the open Lab.

1. **Load synthetic example.** Inspect the measured units and both Antoine definitions.
2. **Validate & inspect data.** Keep endpoint handling at **No extrapolation**. Inspect the $x_1 = 0.5$ row.
3. **Export complete study JSON.** Save a baseline before changing models.
4. Choose **Margules • 1 parameter**, then **Fit selected model**. Save JSON and residuals CSV. Repeat with **NRTL • fixed α** , $\alpha = 0.3$ and temperature dependence off.

Select **Pressure and vapor residuals** in View. Guide page 2 explains Excel/CSV preparation and reopening saved studies.

A comparison using the same observations

Default synthetic dataset: 19 observations at 350 K. Same property inputs and fitting objective.

Fitted model	Mean absolute pressure error (%)	Mean absolute y_1 error (percentage points)
Margules, one parameter	1.14098	0.675676
NRTL, $\alpha = 0.3$	About 1.14×10^{-6}	About 3.83×10^{-7}

Small final digits may vary. The data generator uses NRTL, so near-exact recovery is expected.

Your action: Name each metric and its unit in worksheet E2. A mole-fraction error of **0.01** equals **1 percentage point**. Near-zero training error alone does not establish consistency or prediction.

What each check can establish

Check	Evidence it supplies
Hand calculation versus Lab	Agreement for this calculation with the chosen equation and inputs
P^{sat} versus independent measurements or a trusted reference	External support for the property inputs at the same T
Applicable thermodynamic diagnostic	Agreement with a constraint, under stated assumptions
Data excluded from fitting	Evidence about prediction on those held-out observations

Your action: On guide page 3, identify which check you have actually performed. Describe any remaining checks as future work.

The synthetic example has no real-fluid measurements against which to validate its property constants.

Why consistency needs more than a fit

For a binary liquid at fixed T and P, Gibbs–Duhem requires

$$x_1 d \ln \gamma_1 + x_2 d \ln \gamma_2 = 0.$$

The two activity coefficients are linked. A fitted model can obey this relation while only approximating inconsistent measurements.

Lab 08 assumes negligible excess-volume pressure effects for its isothermal diagnostics. Isobaric diagnostics need their temperature correction and, for the differential test, independent H^E data.

Your action: Read the diagnostic's applicability message. With incomplete composition coverage and **No extrapolation**, a full-area verdict is unavailable. **Not assessed** is not a pass or a failure.

A one-minute self-check

Your action: Answer these on paper before the next slide. No form submission is required.

1. The CSV contains **350**. Which measured temperature unit matches the synthetic example?
2. The table shows **$\ln \gamma_1 = 0.399813$** . What value should you compare with your hand-calculated γ_1 ?
3. NRTL gives a smaller training residual. Which further checks are needed to support consistency and prediction?

Use guide pages 1–2 for units and page 3 for the types of evidence. Then check the answers on the next slide.

Answers and the next question

1. **K.** The equivalent Celsius input is 76.85. The example Antoine equation also uses K.
2. **$\exp(0.399813) \approx 1.49155$** , dimensionless.
3. An **applicable thermodynamic diagnostic** for consistency, and **observations excluded from fitting** for prediction. Separately validate real-fluid property inputs against an independent reference.

Your action: Add one correction to your worksheet if needed. Return to [Session 3: liquid stability](#).

Next we ask whether an equilibrium calculation gives the **lowest admissible Gibbs energy**. A good VLE fit alone does not settle that question.

Reference: Excel to CSV

Optional: Use guide page 2 when preparing your own dataset.

1. Create four columns with exact headers **T, P, x1, y1**. Each row is one equilibrium observation. Keep units out of the header and record them separately.
2. Use mole fractions between 0 and 1, dot decimals and numeric cells. Remove titles, blank rows and extra calculated columns.
3. Save as **CSV UTF-8**. In Lab 08, load the CSV or paste the table, then set its measured units and supply both Antoine definitions and sources.

The supplied template uses **350 K and kPa**. A CSV contains observations only. It does not set or restore the Lab's units or constants. Excel workbooks (.xlsx) must first be saved as CSV.

Reference: saved files and troubleshooting

File	What it contains	How to use it
Observation CSV	Raw T, P, x1, y1	Import as data, then set units and properties
Complete study JSON	Controls, sources and recorded results	Study workspace, load JSON, Restore, then validate/refit
Fitted residuals CSV	Calculated residual table	Open in a spreadsheet to inspect/export results

If results differ: compare the raw data, units, component order, equation form, sources and model settings first. Then check convergence and parameter-bound warnings.

Keep the JSON and a screenshot of any error. Guide page 2 gives the exact restore steps. You do not need to edit JSON by hand.

Reference: an evidence-based explanation

Finding: On the same 350 K synthetic dataset, NRTL reproduces the training observations more closely than one-parameter Margules.

Evidence: Mean absolute pressure error decreases from about **1.14098%** to **0.00000114%**, with the same property inputs and fitting objective.

Limit: The generator uses NRTL. This comparison establishes model recovery on these observations. Thermodynamic consistency, real-fluid property accuracy and prediction each require their own applicable evidence.

Your action: Use this structure for worksheet F, with your own saved results. Include the metric, units, controlled inputs and a limitation.

[Lab guide PDF](#) · [Original worksheet](#) · [Learning path](#)