

One row, one property check

Use this guide beside **Lab 08: Your measurements. Inspect, test, fit.** Start with the built-in synthetic example. You do not need to write JSON or code.

Companions: [Week 2 clarification slides](#) · [Week 2 worksheet, Sections C-F](#). This is a review aid, not a new attendance task.

1. Understand what gamma means

x_i and y_i are liquid and vapor mole fractions. For the liquid reference used here, $a_i = \gamma_i x_i$. The activity coefficient γ_i represents departure from ideal-solution behavior; $\gamma_i = 1$ is the ideal limit. Mole fractions, activities and activity coefficients are dimensionless.

At equilibrium, with ideal vapor and negligible Poynting correction:

$$y_i P \approx x_i \gamma_i P_i^{\text{sat}}, \text{ so } \gamma_i \approx y_i P / (x_i P_i^{\text{sat}}).$$

Use P and P^{sat} in the same pressure unit. Do not apply this division to an absent component at a pure endpoint.

2. Keep the two teaching examples separate

Worksheet Section C: standalone exercise	Lab 08: built-in synthetic dataset
At 50 °C (323.15 K): $\log_{10}(P^{\text{sat}}/\text{kPa}) = 4 - 1000/(T_K + 200)$ Equation temperature is °C . Valid at 20-80 °C; result: 1 kPa .	At 350 K (76.85 °C): $\log_{10}(P^{\text{sat}}/\text{kPa}) = A - B/(T_K + C)$ Equation temperature is K . Declared range: 300-390 K; C = 0.

Do not copy Section C constants into Lab 08. Both are synthetic examples, not real-compound correlations. Changing the selected equation form does not convert its constants.

3. Load and inspect the baseline

1. Select **Load synthetic example**, then **Validate & inspect data** →. Expect **19 interior points**, with measured $T = \text{K}$ and measured $P = \text{kPa}$.
2. For both components, verify the displayed equation is **$\log_{10}(P_{\text{sat}}) = A - B/(T + C)$** ; equation T unit = **K**; P_{sat} unit = **kPa**; valid range = **300 to 390 K**.
3. Open **Imported observations**. Find $x_1 = 0.5$ (input row 11, including the header).

Synthetic component	A	B	C
1	6.653258697961224	1567.0086036169398	0
2	7.00151326244011	1828.176704219763	0

$$P_1^{\text{sat}} = 10^{[6.653258697961224 - 1567.0086036169398/350]} = \mathbf{150 \text{ kPa}}.$$

$$\text{Using component 2's own constants gives } P_2^{\text{sat}} = \mathbf{60 \text{ kPa}}.$$

For the chosen row: $P = 158.707198211 \text{ kPa}$, $x_1 = 0.5$, $y_1 = 0.704857144627$.

$$\gamma_1 = (0.704857144627 \times 158.707198211) / (0.5 \times 150) = \mathbf{1.491545}$$

$$\gamma_2 = [(1 - 0.704857144627) \times 158.707198211] / [(1 - 0.5) \times 60] = \mathbf{1.561377}$$

The table shows **$\ln \gamma_1 \approx 0.399813$** and **$\ln \gamma_2 \approx 0.445568$** . Compare your γ with **$\exp(\text{table } \ln \gamma)$** , not directly with $\ln \gamma$.

A hand calculation checks implementation and conventions. Agreement with the same supplied correlation does not independently establish that the property source is physically accurate.

Prepare, compare and save

4. Move a table from Excel into the Lab

Use four numeric columns. Here is the exact header and **one preview row**:

```
T,P,x1,y1
350,158.707198211,0.5,0.704857144627
```

1. Select **Download synthetic CSV template (K, kPa)**. Keep all **19 rows** for this comparison. Import requires at least five distinct interior points.
2. Save Excel data as **CSV**, not .xlsx. Alternatively, copy the four columns with headers into **Or paste the table, including headers**.
3. Use dot decimals, mole fractions (0-1), and sufficient precision. Scientific notation such as $1.58707198211\text{E}+2$ is valid. No units in cells, thousands separators, blank cells or Psat columns.
4. Use **Load CSV or tab-separated text**. Check component order, sources, experimental path, units and both Antoine definitions. Select **Validate & inspect data** →.

Loading CSV does not restore units or constants. Only **Load synthetic example** fills the synthetic table and its complete property setup together.

Unit setting	Meaning
Measured-data T / measured P	Units of CSV numbers: baseline K / kPa .
Antoine equation T / Psat	Units required by the constants' source: baseline K / kPa .
Minimum / maximum valid T	Always K . Thus 20-80 °C becomes 293.15-353.15 K.

The Lab converts measured T to each equation's unit. Do not convert twice. Revalidate after changing inputs; temperatures outside either correlation's range block import.

5. Fit two models to the same observations

1. Choose **Margules · 1 parameter** → **Fit selected model**. Wait for convergence. Select **View** → **Pressure and vapor residuals**.
2. Record both errors and bound warnings. Select **Export complete study JSON** and **Export fitted residuals CSV**; rename files “Margules”.
3. Choose **NRTL · fixed α** ; set **Fixed NRTL $\alpha = 0.3$** . Leave **Fit $\tau_{ij} = c_{ij} + d_{ij}(350/T - 1)$** unchecked. Fit and export again as “NRTL”.

19-point baseline	Mean absolute pressure error / %	Mean absolute vapor error / percentage points
Margules, 1 parameter	≈ 1.14098	≈ 0.675676
NRTL, $\alpha = 0.3$	$\approx 1.14 \times 10^{-6}$	$\approx 3.83 \times 10^{-7}$

Keep data, properties and objective unchanged. NRTL generated these synthetic data, so near-zero training error is expected, not experimental validation.

Residual CSV: $y_error = y_{calc} - y_1$ in mole fraction; multiply by 100 for percentage points. `pressure_error_percent` is already percent.

6. Reopen a saved study

Near the top, expand **Study workspace · reopen and compare cases**. Select **Load studies or a comparison JSON** → **Restore [case label]**, then **Validate & inspect data** → **Fit selected model**. JSON preserves the setup and recorded results; restoring requires fresh validation and fitting. A residuals CSV is output, not an input dataset.

Explain what the result establishes

7. Separate four questions

Question	Evidence and limits
Did the model fit?	Inspect training residuals, error units and warnings. Low error does not establish correct properties, consistency or prediction.
Are properties credible?	Check equation, log base, signs, units and range. Compare real-fluid P_{sat} with an independent reliable source at the same T. Hand/Lab agreement checks implementation only.
Are data consistent?	Use an applicable Gibbs-Duhem-based diagnostic; report assumptions and coverage. A pass does not prove experimental accuracy. Missing endpoints and noisy derivatives limit conclusions.
Will it predict?	Test observations excluded from fitting within a justified range. A single-temperature fit does not validate temperature extrapolation.

Keep **Unmeasured endpoint intervals** → **No extrapolation** · **no full-area verdict**. A withheld verdict reflects limited evidence; do not assume endpoints merely to obtain a verdict.

At fixed T and P, Gibbs-Duhem links the activity coefficients. Lab 08 isothermal diagnostics neglect excess-volume pressure effects. An isobaric differential verdict needs independent H^E data for the temperature correction.

8. Give a claim, a number and a limitation

“For 19 synthetic points at 350 K, NRTL reduced mean absolute pressure error from 1.141% to approximately $1.14 \times 10^{-6}\%$. This improves training-data reproduction. Because NRTL generated the data, it does not demonstrate experimental consistency or new-temperature prediction.”

Always identify the dataset, model, settings, quantity, value and unit.

9. If results differ, check in this order

- Table:** 19 baseline rows; correct component order; mole fractions, precision, missing cells and repeated x_1 .
- Properties:** measured units, equation forms, constants, equation units and validity limits in K. Revalidate.
- Fit:** correct model; NRTL $\alpha = 0.3$; temperature dependence off; completed fit and warnings.
- Evidence:** correct error metric and units. Save study JSON when asking for help so the setup can be inspected.

10. Self-check, then read the answers

- CSV 350 means 350 K, but measured T is set to °C. What temperature is interpreted?
- Table $\ln \gamma_1 = 0.399813$. What do you compare with hand-calculated γ_1 ?
- Why is synthetic NRTL error near zero? What remains unproven?
- Which file reopens the setup, and what do you do after restoring?

Answers

- 623.15 K, outside the baseline range. Select K for this CSV.
- $\exp(0.399813) \approx 1.49155$, dimensionless; differences from page 1 are rounding.
- NRTL generated the data. Reproduction does not prove experimental consistency or new-condition prediction.
- Export complete study JSON.** Load and Restore in the Study workspace, then validate and refit.