

Your questions before Week 4

Week 4 · Questions from Week 3

Consistency scores: what does a pass mean?

Gibbs graphs: which state has lower energy?

Equilibrium compositions and phase amounts

Keep a calculator and notebook ready. Write R1–R3 at the pause.

This opening replaces the separate reading. H1–H4 is optional.

Match the question to the evidence

Identify the question first

Question	Evidence
Thermodynamic relationship?	Gibbs–Duhem diagnostics
Model reproduces VLE?	Calculated versus observed P and y
Phase state is stable?	Lowest admissible total Gibbs energy

A fit, a consistency score and a stability test answer different questions.

What Gibbs-Duhem requires

Binary liquid · stated path and assumptions

$$g_E = x \ln \gamma_1 + (1 - x) \ln \gamma_2$$

$$dg_E/dx = \ln(\gamma_1/\gamma_2) + x d\ln\gamma_1/dx + (1 - x) d\ln\gamma_2/dx$$

$$\text{At fixed } T, P: x d\ln\gamma_1/dx + (1 - x) d\ln\gamma_2/dx = 0$$

The simplified isothermal example neglects the pressure contribution.

Changing temperature at constant pressure requires an excess-enthalpy correction.

D measures net area imbalance

Area diagnostic

$$f(x) = \ln(\gamma_1/\gamma_2)$$

$$D = 100 |A_+ - A_-| / (A_+ + A_-)$$

Lab criterion: $D < 5\%$

A_- is the positive magnitude below zero.

Small net imbalance can hide cancellation.

The full-range test needs full composition coverage.

D is not a percentage error for every point.

Local residual and average score

Local evidence versus a summary score

$$r(x) = dg_E/dx - \ln(\gamma_1/\gamma_2)$$

Displayed score = 100 mean $|r|$

Teaching threshold: score < 5

$r(x)$ shows where departures occur.

The average can hide a narrow peak.

Numerical differentiation and noise affect r .

The score is dimensionless, not a percentage error.

More points do not remove a defect

Lab 03 · synthetic localized defect

At 81 points: $r(0.35) \approx -0.250$

Points	D (%)	100 mean r
41	2.013463	1.671839
81	1.956058	1.590767
161	1.941724	1.565607

Both summaries pass, while a local departure remains.

350 K; amplitude 0.25. Denser samples of the same function.

What the Van Ness-type fit tests

Modeling capability within consistency testing

$$\Delta p = \text{mean} [100 |P_{\text{calc}} - P_{\text{obs}}| / P_{\text{obs}}]$$

$$\Delta y = \text{mean} [100 |y_{\text{calc}} - y_{\text{obs}}|]$$

$$\Delta p < 1\% \quad \Delta y < 1 \text{ percentage point}$$

Consistent NRTL model fitted jointly to P and y.

A successful fit is evidence of reproduction.

It does not certify every observation.

Lab 03 uses a Van Ness-type teaching variant, not the full NIST TDE implementation.

Read what the Gibbs curve represents

Fixed T, P and conserved overall composition

$$g(x) = \Delta_{\text{mix}} G / (nRT)$$

$$g(x) = x \ln x + (1 - x) \ln(1 - x) + A x(1 - x)$$

$$A = 3; \text{ overall feed } z = 0.12$$

x: composition of a possible homogeneous liquid

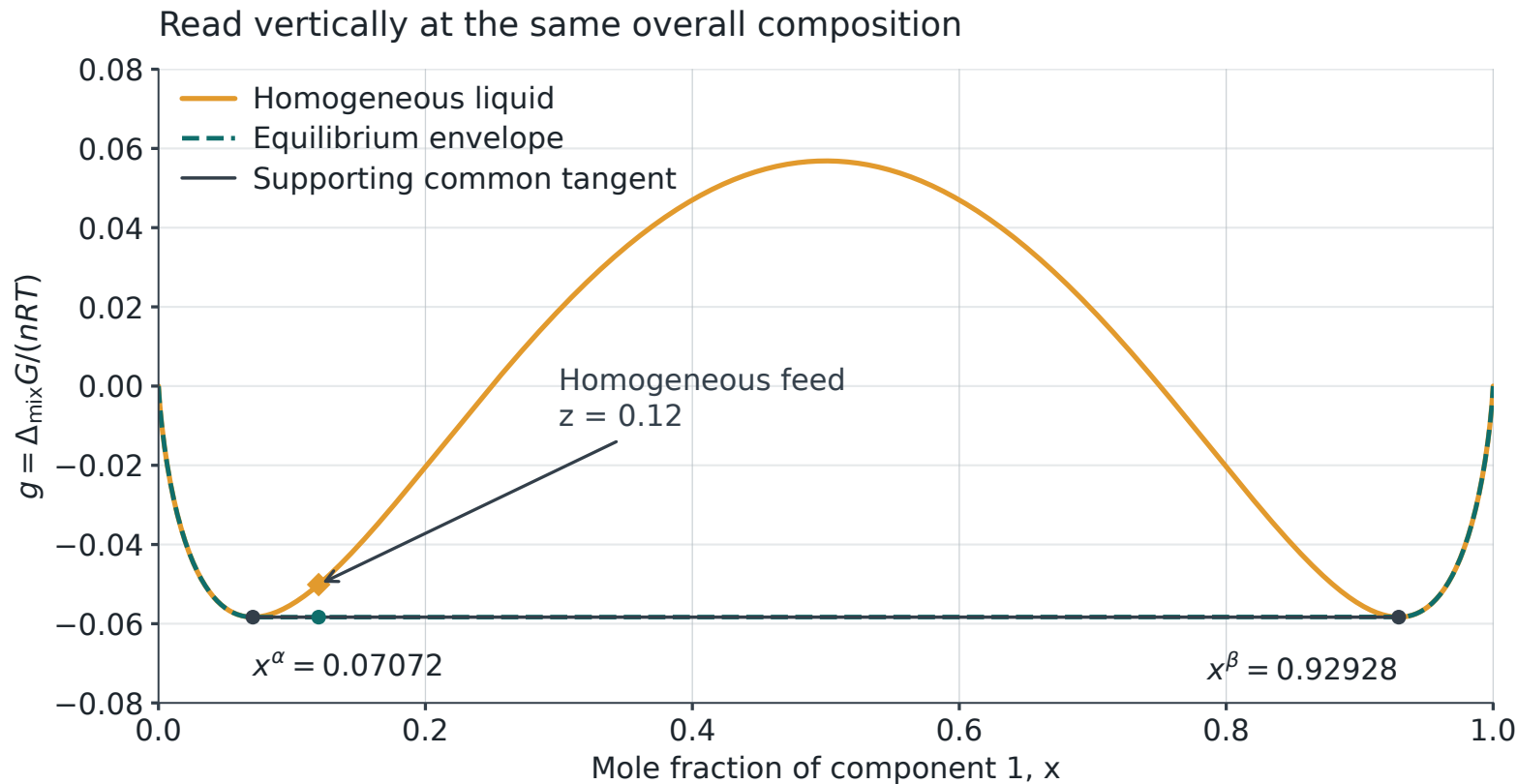
z: overall composition of our material

Total mixing g includes ideal and excess terms.

The horizontal axis is composition, not time.

Identify the curve, contacts and markers

Read vertically at $z = 0.12$



Amber curve and diamond:
homogeneous liquid and feed

Graphite line: supporting common
tangent

Dashed teal line and circle:
equilibrium envelope and split feed

Contact compositions $x^\alpha =$
 0.07072018 and $x^\beta = 0.92927982$
are not phase fractions.

Positive curvature is only a local check

Step 1 · local curvature

$$g''(x) = 1/x + 1/(1 - x) - 2A$$

$$g''(0.12) = 1/0.12 + 1/0.88 - 6$$

$$= +3.469697$$

Positive: resists infinitesimal composition fluctuations.

Negative: locally unstable homogeneous state.

Zero: requires further examination.

Positive curvature does not establish global stability.

Use the lever rule, then compare energies

Step 2 · conserve composition and compare energy

$$f^{\beta} = (0.12 - 0.07072018)/(0.92927982 - 0.07072018)$$

$$f^{\beta} = 0.057398; f^{\alpha} = 0.942602$$

$$f^{\alpha}x^{\alpha} + f^{\beta}x^{\beta} = 0.120000$$

$$g_{\text{one}} = -0.05012499; g_{\text{split}} = -0.05834135$$

$$g_{\text{one}} - g_{\text{split}} = +0.00821636$$

The homogeneous feed is metastable: locally resistant, but not the global minimum.

Global support and the Lab checks

Step 3 · global support and conserved amounts

$g(x) - \ell(x) \geq 0$ for every admissible x

Change only z : $0.12 \rightarrow 0.35$

x^α and x^β unchanged; $f^\beta \rightarrow 0.325289$

Common-tangent residual: coexistence equations

Feed TPD: negative somewhere rejects feed stability

Full supporting line: global test within the liquid model

Equilibrium compositions stay fixed; the relative amounts change.

Pause and write R1-R3

Four-minute notebook pause

$$x^{\alpha} = 0.07072018; x^{\beta} = 0.92927982$$

R1. D and the mean residual score pass, but $r(x)$ has a narrow peak. Can you certify every point? What should you inspect?

R2. $A = 3$, $z = 0.12$: positive curvature, lower supported split. Is the homogeneous feed globally stable, metastable or locally unstable? Why?

R3. Move z to 0.35 on the same tie line. What stays fixed? Calculate f^{β} . Why will Week 4 still need material balances?

Write first. Then continue to the check. No extra form or export.

Check your answers, then continue

Notebook check and transition

R1: No. Inspect the local curve, assumptions, coverage and numerical sensitivity.

R2: Metastable. Positive curvature, but a lower supported split.

R3: x^α and x^β stay fixed. $f^\beta = 0.325289$; $f^\alpha = 0.674711$.

Continue with worksheet A-G and I. H1-H4 is optional.

Equilibrium conditions plus inventory balances determine the state and amounts.

Solid equilibria and adsorption

Session 4: Independent study during the ECS meeting · about 3 hours

Soorathep Kheawhom

Your independent lesson

Keep your first answers, then add corrections after each check.

[Practice worksheet · 6 pages](#)

Complete A–G and I. H1–H4 is optional.

[Lab guide · 4 pages](#)

Use the named settings, controls and interpretation checks.

[Worked solutions](#)

Open the relevant answer only after your own attempt.

Predict before the Lab 10 and Lab 11 demonstrations. Then repeat independently and retain your calculations and study JSON.

The study route

Opening review completed: keep your R1-R3 answers.

Next action	Worksheet
Processes, solubility and finite inventory	pp. 1-2, A-C
Predict, watch and investigate Lab 10	p. 3, D
Take a 10-minute break	
Adsorption calculations and Lab 11	pp. 4-5, E-G
Submit exit ticket and feedback once	p. 6, I

Required: full recording + 104 min of work + 10 min break.
H1-H4 is optional (+20 min). No second required reading.

Process predictions

Your action: Pause for about **8 minutes**. Complete **A1–A3, worksheet p. 1**, before viewing the next slide.

A1. Classify dissolution of a crystal, sublimation into a vessel, and adsorption on a porous solid. Identify whether the process transfers material between bulk phases or changes surface uptake.

A2. Week 3 used Gibbs energy at fixed T , P . Which thermodynamic potential is minimized for a closed, rigid vessel at fixed T , V ?

A3. In an ideal gas mixture, distinguish the partial pressure of the subliming species from total pressure. Predict how an inert gas contributes.

For each answer, name the **process**, the **constraints**, and one quantity that a material balance must determine.

Process check

Your action: Check **A1–A3**. Keep your first answers and record the reason for any change.

PROCESS	EQUILIBRIUM DESCRIPTION	AMOUNT INFORMATION
Crystal and liquid	Solid–liquid equilibrium, SLE	Dissolved and remaining solid
Solid and vapor	Gas–solid equilibrium, GSE	Gas and remaining solid
Surface uptake	Adsorption equilibrium	Gas and adsorbed material

At fixed T, P , equilibrium minimizes Gibbs energy. At fixed T, V , it minimizes Helmholtz energy, subject to conserved inventories.

For ideal gases, $P_{tot} = p_A + p_{inert}$. Lab 10 treats nonreacting bulk equilibria. Lab 11 treats adsorption. A gas–solid chemical reaction would require species and reaction constraints beyond these demonstrations.

Pure-solid standard state

Your action: Read the two phase descriptions. Use them to set up **B1, worksheet p. 1**.

For component i in a liquid and its **present pure solid**:

$$\mu_i^L = \mu_i^S, \quad \mu_i^L = \mu_i^{L,*} + RT \ln(x_i \gamma_i)$$

The liquid reference $\mu_i^{L,*}$ is the **subcooled pure liquid** at the same temperature and pressure.

The present pure solid has **unit activity on its pure-solid standard state**. Unit activity does not mean zero chemical potential or a zero amount of solid.

$x_i \gamma_i$ specifies a liquid activity. A material balance is still needed to determine phase amounts.

Solubility equation

Your action: Identify the units and assumptions before substituting into **B1**.

For a present pure solid, with constant fusion enthalpy and negligible fusion heat-capacity correction:

$$\ln(x_i \gamma_i) = -\frac{\Delta H_{fus,i}}{R} \left(\frac{1}{T} - \frac{1}{T_{m,i}} \right)$$

Use **kelvin**, ΔH_{fus} in **J mol⁻¹**, and $R = 8.314462618 \text{ J mol}^{-1} \text{ K}^{-1}$.

For $T < T_m$ and positive ΔH_{fus} , the right side is negative. With an ideal liquid, $\gamma_i = 1$ and the result gives $x_i^{sat} < 1$.

This model excludes solid solutions, chemical reactions and heat-capacity corrections. Other solid forms or transitions require additional data.

Solubility attempt

Your action: Pause for about **6 minutes**. Complete **B1–B2, worksheet p. 1**. Calculate before advancing.

Synthetic inputs:

$$T_m = 350 \text{ K}, \quad \Delta H_{fus} = 10000 \text{ J mol}^{-1}, \quad T = 300 \text{ K}$$

B1. Assume an ideal liquid. Calculate the saturated liquid mole fraction x^{sat} using the equation on slide 7.

B2. Does this number give the moles of solid remaining? State what additional information you would need.

Before calculating, predict whether the saturated mole fraction is above or below 1.

Solubility check

Your action: Check **B1–B2**. Correct units and distinguish composition from phase amount.

$$x^{sat} = \exp \left[-\frac{10000}{8.314462618} \left(\frac{1}{300} - \frac{1}{350} \right) \right] = 0.563986$$

The result is a **liquid mole fraction**, not moles of dissolved solute or remaining solid.

With a nonideal liquid, the equation constrains $x\gamma(x, T)$. The composition must satisfy that relation and the admitted phase model.

Phase amounts require total composition and inventory balances. A binary eutectic adds a second solid branch; it is optional background for this lesson.

Sublimation equilibrium

Your action: Read the condition on solid presence. Begin **C1, worksheet p. 2** by identifying the gas species.

For a present pure bulk solid A in equilibrium with its vapor:

$$\mu_A^S = \mu_A^g$$

With an ideal gas, negligible solid pressure correction, and the stated sublimation-pressure model:

$$p_A = P_{sub}(T) \quad \text{while solid remains}$$

p_A is the **partial pressure of the subliming species**. An inert gas contributes to total pressure.

If all solid disappears, there is no remaining bulk-solid phase to enforce this equality. The finite inventory may give $p_A < P_{sub}$.

Finite-vessel inventory

Your action: Use this decision sequence for **C1–C3**. Write the capacity before deciding which phases are present.

For a closed, rigid vessel at fixed T , V_g with ideal gases:

$$n_g^{sat} = \frac{P_{sub} V_g}{RT}, \quad n_A^g = \min(n_A^{tot}, n_g^{sat}), \quad n_A^s = n_A^{tot} - n_A^g$$

$$p_A = \frac{n_A^g RT}{V_g}, \quad P_{tot} = p_A + \frac{n_{inert} RT}{V_g}$$

Use $R = 8.314462618 \text{ kPa L mol}^{-1} \text{ K}^{-1}$ with pressure in kPa and gas volume in L.

For C3, $(\mu_A^g - \mu_A^s)/(RT) = \ln(p_A/P_{sub})$. A present solid requires zero. An exhausted-solid state may have a **negative** value.

Inventory worked example

Your action: Follow the arithmetic, then cover these results before attempting worksheet **C**.

Synthetic case: $T = 300\text{ K}$, $V_g = 1\text{ L}$, $P_{sub} = 10\text{ kPa}$.

$$n_g^{sat} = \frac{10(1)}{8.314462618(300)} = 0.00400908\text{ mol}$$

$n_A^{tot}\text{ (MOL)}$	$n_A^g\text{ (MOL)}$	$n_A^s\text{ (MOL)}$	$p_A\text{ (KPA)}$
0.010	0.00400908	0.00599092	10.0000
0.002	0.00200000	0	4.98868

Adding **0.002 mol inert gas** at the same T , V_g adds **4.98868 kPa** to total pressure in either case. It leaves p_A and the inventory threshold unchanged in this model.

Inventory attempt

Your action: Pause for about **10 minutes**. Complete **C1–C3, worksheet p. 2**, before viewing slide 14.

Use a new synthetic vessel: $T = 300$ K, $V_g = 2$ L and $P_{sub} = 8$ kPa.

C1. Calculate n_g^{sat} . Find gas moles, solid moles and p_A for $n_A^{tot} = 0.010$ mol and **0.004 mol**.

C2. Add $n_{inert} = 0.001$ mol to each case at the same T , V_g . Calculate P_{tot} and identify which results change.

C3. Calculate $\ln(p_A/P_{sub})$ for both cases. Explain why zero is required when solid remains, while a negative value can be a valid exhausted-solid boundary state.

Use $R = 8.314462618$ kPa L mol⁻¹ K⁻¹. Show substitutions and units.

Inventory check

Your action: Check **C1–C3**. Keep enough digits in the capacity before subtracting the remaining solid.

$$n_g^{sat} = 0.00641453 \text{ mol}, \qquad p_{inert} = 1.24717 \text{ kPa}$$

n_A^{tot} (MOL)	n_A^g (MOL)	n_A^s (MOL)	p_A (KPA)	P_{tot} (KPA)
0.010	0.00641453	0.00358547	8.00000	9.24717
0.004	0.00400000	0	4.98868	6.23585

The first case retains solid and has $\ln(p_A/P_{sub}) = 0$. The second exhausts it and has $\ln(p_A/P_{sub}) \approx -0.472271$.

In each row, $n_A^g + n_A^s = n_A^{tot}$. The inert changes total pressure, while p_A is unchanged at fixed T, V_g in this model.

Lab 10 predictions

Your action: Pause for about **5 minutes**. Complete **D1, worksheet p. 3**. Read **Lab guide pp. 1–2**, but predict before running the Lab.

Lab 10: Solid equilibria

Select **GSE • sublimation in a rigid vessel** at $T = 300\text{ K}$ and $V_g = 1\text{ L}$. Set the sublimation reference pressure to **10 kPa at 300 K**.

CASE	SUBLIMING-SPECIES INVENTORY (MOL)	INERT GAS (MOL)
10A	0.010	0
10B	0.002	0
10C	0.002	0.002

Predict solid presence, p_A and total pressure. Identify the single input changed between successive cases.

Lab 10 demonstration

Your action: Watch the actual Lab 10 demonstration. Follow the controls using **Lab guide pp. 1–2**. Keep D1 predictions visible.

The demonstration follows this route:

1. Select the gas–solid vessel mode and enter the reference state.
2. Compare inventories above and below the solid-depletion threshold.
3. Add inert gas and compare partial pressure with total pressure.
4. Read the plots and check the species inventory balance.
5. Save study JSON, reopen it, verify inputs, and calculate again.

Record results during your **independent rerun at slide 18**. Verify restored controls and calculate again before trusting a displayed result.

Lab 10 evidence

Your action: Use **Lab guide pp. 1–2** to identify the evidence you will retain for **D2–D4**.

READ OR SAVE	EXPLAIN WHAT IT ESTABLISHES
Inputs and active mode	Temperature, volume and inventory constraints
Solid remaining and gas amount	Which phases are present at the selected point
Partial and total pressure	Subliming-species and inert contributions
Inventory check	Gas plus solid equals the subliming-species total
Study JSON	A reproducible parameter and result record

The actual volatile partial pressure follows $P_{sub}(T)$ wherever solid remains. The plots sweep **temperature, not time**. A plotted boundary does not mean every possible phase is present at the selected state.

Lab 10 independent investigation

Your action: Pause for about **22 minutes**. Complete **D2–D4, worksheet p. 3**, using **Lab guide pp. 1–2** and [Lab 10](#).

D2. Run cases **10A, 10B and 10C** from D1. Record phase presence, gas and solid moles, partial pressure and total pressure.

D3. Check gas capacity, the species inventory and the inert contribution by hand. Use the plots to explain the transition from solid present to solid exhausted.

D4. Export the cases. Reopen a JSON file, restore the controls, verify them, and **recalculate**. Record whether the results reproduce.

Retain one comparison table, your calculations and the saved files. Explain any discrepancy before advancing.

Lab 10 check

Your action: Compare **D2–D4** with these values and the worked solutions. Correct the reasoning as well as the arithmetic.

At 300 K and 1 L, the gas capacity is **0.00400908 mol**.

CASE	p_A (KPA)	SOLID (MOL)	P_{tot} (KPA)
10A: 0.010 mol A , no inert	10.0000	0.00599092	10.0000
10B: 0.002 mol A , no inert	4.98868	0	4.98868
10C: 0.002 mol A , 0.002 mol inert	4.98868	0	9.97736

A pressure below P_{sub} is the expected finite-inventory result after solid depletion. It is not a failed saturation calculation.

These are equilibrium endpoints. They do not give a sublimation rate or the time needed to reach equilibrium.

Break

Your action: Pause for **10 minutes**. Save your Lab 10 files and leave the screen briefly.

When you return, open **worksheet p. 4** and **Lab guide pp. 3–4**.

The next part treats gas uptake on a surface. You will calculate an isotherm value, then solve an inventory balance for a closed vessel.

The same question remains useful: **What does equilibrium determine, and what must the material balance determine?**

Adsorption and bulk phases

Your action: Read the definition of uptake before starting **E, worksheet p. 4**.

Adsorption describes material associated with a surface. An isotherm gives uptake at a specified temperature and gas pressure.

$$q(P, T) = \frac{\text{moles adsorbed}}{\text{mass of adsorbent}}$$

Here, q is **absolute uptake in mol kg⁻¹** and P is the **adsorbate partial pressure in kPa**.

Adsorbed moles are $n_{ads} = m_s q$, with adsorbent mass m_s in kg. The symbol q itself is not an amount in moles.

Bulk sublimation and surface adsorption require different state descriptions and inventory balances.

Langmuir model

Your action: Identify the parameters and dimensionless group. Use this expression for **E1–E3**.

$$q = q_s \frac{bP}{1 + bP}, \qquad \theta = \frac{q}{q_s} = \frac{bP}{1 + bP}$$

QUANTITY	MEANING	UNIT USED HERE
q_s	Saturation uptake	mol kg^{-1}
b	Affinity parameter	kPa^{-1}
bP	Dimensionless pressure group	1
θ	Fractional coverage in the model	1

The idealized model assumes a finite set of equivalent sites and no lateral interactions. A good fit alone does not establish this microscopic mechanism.

Henry limit

Your action: Derive the low-pressure slope from Langmuir. Retain the units when comparing the models.

If $bP \ll 1$:

$$q \approx q_s bP = K_H P, \quad K_H = q_s b$$

K_H has units **mol kg⁻¹ kPa⁻¹** for this adsorption convention.

The matched Henry line and Langmuir curve share the slope at $P \rightarrow 0$. The Henry line has no saturation plateau and requires a low-pressure domain.

A gas-solubility convention such as $p = Hx$ defines a different constant with different units. State the equation and concentration basis whenever using the name “Henry constant.”

Isotherm worked example

Your action: Follow this calculation, then use the same parameters for **E1–E3**.

Synthetic parameters at fixed T : $q_s = 2 \text{ mol kg}^{-1}$ and $b = 0.1 \text{ kPa}^{-1}$.

$$q = \frac{2(0.1)P}{1 + 0.1P}, \qquad K_H = 0.2 \text{ mol kg}^{-1} \text{ kPa}^{-1}$$

$P \text{ (KPA)}$	bP	LANGMUIR $q \text{ (MOL KG}^{-1}\text{)}$	HENRY $q \text{ (MOL KG}^{-1}\text{)}$
1	0.1	0.181818	0.200000
10	1	1.000000	2.000000

At $P = 1/b = 10 \text{ kPa}$, Langmuir coverage is **one half**. At this pressure, a low-pressure linear approximation is already poor.

Isotherm attempt

Your action: Pause for about **10 minutes**. Complete **E1–E3, worksheet p. 4**. Calculate before viewing slide 26.

Keep $q_s = 2 \text{ mol kg}^{-1}$ and $b = 0.1 \text{ kPa}^{-1}$. Use matched Henry $K_H = q_s b = 0.2 \text{ mol kg}^{-1} \text{ kPa}^{-1}$ for comparison.

E1. Calculate Langmuir and matched Henry uptake at **5 kPa** and **40 kPa**. Also calculate Langmuir fractional coverage.

E2. Calculate bP at each pressure and compare with the low-pressure condition $bP \ll 1$.

E3. Predict each model's high-pressure behavior. Which model can exceed q_s mathematically, and what does that mean for its use?

Show the substitutions and units. Compare your calculations with the matched Henry values on the next slide.

Isotherm check

Your action: Check **E1–E3**. Explain model disagreement using bP , not only curve shapes.

P (KPA)	bP	LANGMUIR q	θ	HENRY q
5	0.5	0.666667	0.333333	1.00000
40	4	1.60000	0.800000	8.00000

Uptake values are in **mol kg⁻¹**. As pressure increases, Langmuir uptake approaches **2 mol kg⁻¹**. The Henry line continues increasing without a plateau.

At 40 kPa, $bP = 4$ is far outside $bP \ll 1$. The large Henry value shows why a low-pressure approximation needs a stated domain.

Closed adsorption vessel

Your action: Read the balance before **F1–F3, worksheet p. 4**. Identify which pressure is unknown.

For an ideal gas and **absolute uptake** in a closed vessel:

$$n_A^{tot} = \underbrace{\frac{PV_g}{RT}}_{n_A^g} + \underbrace{m_s q(P, T)}_{n_A^{ads}}$$

Use the **accessible gas volume** V_g and adsorbent mass m_s in **kg**. The unknown P is adsorbate partial pressure.

At fixed T, V_g, m_s, n_A^{tot} , the isotherm and balance determine P together. Both terms increase with $P \geq 0$ for positive Langmuir parameters.

Excess uptake requires a gas-density and volume convention. It cannot be substituted directly for absolute uptake in this balance.

Vessel worked example

Your action: Follow this known-pressure calculation. Use its inventory to justify your predictions in **F1–F3**.

Synthetic case at **300 K, 1 L and 10 kPa**: use $m_s = 10$ g, $q_s = 2$ mol kg⁻¹ and $b = 0.1$ kPa⁻¹.

$$q = 2 \frac{0.1(10)}{1 + 0.1(10)} = 1 \text{ mol kg}^{-1}$$

$$n_A^g = \frac{10(1)}{8.314462618(300)} = 0.00400908 \text{ mol}$$

$$n_A^{ads} = 0.010(1) = 0.0100000 \text{ mol}, \quad n_A^{tot} = 0.01400908 \text{ mol}$$

The next task uses **a smaller total inventory, 0.010 mol**, with the same other parameters. That change will require a different equilibrium pressure.

Lab 11 predictions

Your action: Pause for about **5 minutes**. Complete **F1–F3, worksheet p. 4**. Read **Lab guide pp. 3–4** before watching.

Lab 11: Adsorption

Use $T = 300 \text{ K}$, $V_g = 1 \text{ L}$, $n_A^{tot} = 0.010 \text{ mol}$, $q_s = 2 \text{ mol kg}^{-1}$, $b = 0.1 \text{ kPa}^{-1}$ and initially **10 g** adsorbent.

F1. Compared with slide 28, predict whether Langmuir pressure is above or below 10 kPa. Explain using the smaller inventory.

F2. Switch to matched Henry adsorption, $K_H = 0.2 \text{ mol kg}^{-1} \text{ kPa}^{-1}$. Predict which model gives the lower pressure at this fixed inventory.

F3. Return to Langmuir and double adsorbent mass to **20 g**. Predict the pressure change.

Lab 11 demonstration

Your action: Watch the actual Lab 11 demonstration with **Lab guide pp. 3–4**. Compare results with your F1–F3 predictions.

The demonstration follows this route:

1. Set pressure and uptake units, model parameters and temperature.
2. Compare the Langmuir curve with its matched Henry limit.
3. Enter the closed-vessel inventory and accessible gas volume.
4. Compare 10 g and 20 g of adsorbent and check the inventory balance.
5. Export a study, reopen it, verify the controls, and calculate again.

Use the **independent rerun at slide 32** to build your own comparison. Record the selected model and parameter units with every result.

Adsorption evidence

Your action: Prepare the columns for **G1–G4, worksheet p. 5**, using **Lab guide pp. 3–4**.

RECORD	WHY IT MATTERS
Model, units and temperature	Parameters depend on the equation and convention
Pressure and uptake	An isotherm point is a state, not a total amount
Gas moles and adsorbed moles	Their sum must reproduce the closed inventory
Adsorbent mass in kg	$m_s q$ converts uptake to moles
Saved settings and recalculated output	The comparison can be reproduced

Shared low-pressure slope does not make models identical over a finite range. A good inventory balance also does not establish a model’s physical validity.

Lab 11 independent investigation

Your action: Pause for about **24 minutes**. Complete **G1–G4**, **worksheet p. 5**, using **Lab guide pp. 3–4** and [Lab 11](#).

G1. Run **11A: Langmuir, 10 g**; **11B: Henry, 10 g**; and **11C: Langmuir, 20 g**. Keep $T = 300$ K, $V_g = 1$ L and $n_A^{tot} = 0.010$ mol. Use $q_s = 2$, $b = 0.1$ and matched $K_H = 0.2$ in the stated units.

G2. Record pressure, uptake, gas moles and adsorbed moles. Check each inventory balance independently.

G3. Compare with your predictions and inspect the graph. Explain model choice and mass effects, including the low-pressure limitation.

G4. Save the studies, reopen one, restore and verify settings, then recalculate. Record the reproduced result.

Lab 11 check

Your action: Check **G1–G4** against these synthetic results. Use unrounded values for the balance.

CASE	P (KPA)	q (MOL KG ^{−1})	n_A^g (MOL)	n_A^{ads} (MOL)
11A: Langmuir, 10 g	6.08025	0.756238	0.00243762	0.00756238
11B: Henry, 10 g	4.16509	0.833018	0.00166982	0.00833018
11C: Langmuir, 20 g	2.84498	0.442971	0.00114057	0.00885943

Each row sums to **0.010 mol**. More adsorbent lowers pressure and increases adsorbed moles, even though uptake **per kilogram** decreases.

The Henry result illustrates model sensitivity. The finite value of bP requires caution about treating it as a valid low-pressure approximation.

Model scope

Your action: Read these limitations. Choose one that matters to your interpretation. Extensions are optional.

EXTENSION	REQUIRED QUALIFICATION
Freundlich	Empirical pressure range; no saturation plateau
BET	Relative pressure P/P_0 , a fitting range and model assumptions
Isosteric heat Q_{st}	Pressures at the same absolute loading across temperatures
Experimental fitting	Data, uncertainty, units and a defined fitting objective

Today’s tasks use **synthetic parameters**. They do not establish a material’s adsorption mechanism or validate extrapolation.

The required work is the model comparisons and inventory checks. No new fit, BET calculation or isosteric-heat calculation is required.

Optional transfer practice

H1–H4 on worksheet p. 6 is optional. It adds about 20 minutes.

Required route: go to core slide 39 for section I and the form.

If you choose H: use new gas–solid and adsorption parameters. Keep the worked solutions closed until your attempt.

For the exact case values, use worksheet p. 6. Apply the same inventory balances, units and phase-presence checks.

Choose your route

Required route: select “Go to exit ticket (slide 39)”. Complete I and submit the Session 4 form once.

Optional extension: pause for about 20 minutes to attempt H1–H4, then continue to its check.

H: gas capacity → phase amounts → partial and total pressure.

Adsorption: uptake → gas and adsorbed moles → inventory.

Use the worksheet case values. The opening review has replaced H in the required lesson budget.

Unseen check

Your action: Check **H1–H4**. Keep your original attempt and annotate corrections. The solutions show intermediate calculations.

GSE gas capacity: **0.00387975 mol**. Inert contribution: **1.28874 kPa**.

n_A^{tot} (MOL)	n_A^g (MOL)	n_A^s (MOL)	p_A (KPA)	P_{tot} (KPA)
0.002	0.00200000	0	2.57748	3.86623
0.008	0.00387975	0.00412025	5.00000	6.28874

Adsorption: $q = 1.5 \text{ mol kg}^{-1}$, gas **0.0155190 mol**, adsorbed **0.0075000 mol**, total **0.0230190 mol**.

Doubling adsorbent mass at fixed inventory lowers pressure: at the old pressure, the balance would contain too many moles.

Choosing an equilibrium description

Your action: Use these questions to prepare your reflection in **I, worksheet p. 6**.

- 1. What process occurs?** Bulk phase transfer, surface uptake or chemical reaction?
- 2. What is fixed?** Temperature, pressure, accessible volume and/or species inventory?
- 3. Which model and convention apply?** Standard states, gas ideality, uptake basis, units and pressure range?
- 4. What sets amounts?** Combine the equilibrium relation with material balances and check phase presence.

A solubility composition, sublimation pressure or isotherm loading describes part of the equilibrium state. None replaces an inventory balance.

Report a numerical result with its assumptions and a check that supports the interpretation.

Exit ticket and feedback

Your action: Pause for about **10 minutes**. Complete **I, worksheet p. 6**, then submit the **Session 4 form once**.

Explain what happens to gas pressure when bulk solid runs out. In the **evidence answer**, include **one Lab 10 comparison and one Lab 11 numerical balance**, with settings and units.

Report your **actual study time**, access problems, and what would improve the next lesson.

The form asks for no name, student ID or email. Wait for **“Response received.”**

[Open Session 4 exit ticket and feedback](#)



Session 4 exit ticket and feedback QR code.

Receipt and saved work

Your action: Verify the submission receipt and save your work. If the form shows “**Response received,**” do not submit again.

Keep these records together:

- Completed worksheet, including predictions, calculations and corrections.
- Lab 10 and Lab 11 comparison tables and study JSON exports.
- One reproduced result after reopening and recalculating a saved study.
- Your actual study time and confirmation that you submitted the form.

The recording, worksheet and Lab investigations form this week’s lesson. There is **no additional compulsory after-class task**.

[Study route](#) · [Optional appendix](#) · [Learning path](#)