EngrD 2190 – Lecture 21

Concept: Process Analysis - Graphical Modeling

Context: Combined Mass & Energy Balances for Binary Mixtures: Enthalpy-Composition (H-(x,y)) Phase Maps

Defining Question: Why are tie lines on enthalpy-composition phase maps not horizontal?

Bring a Straightedge or Ruler to Lecture 22.

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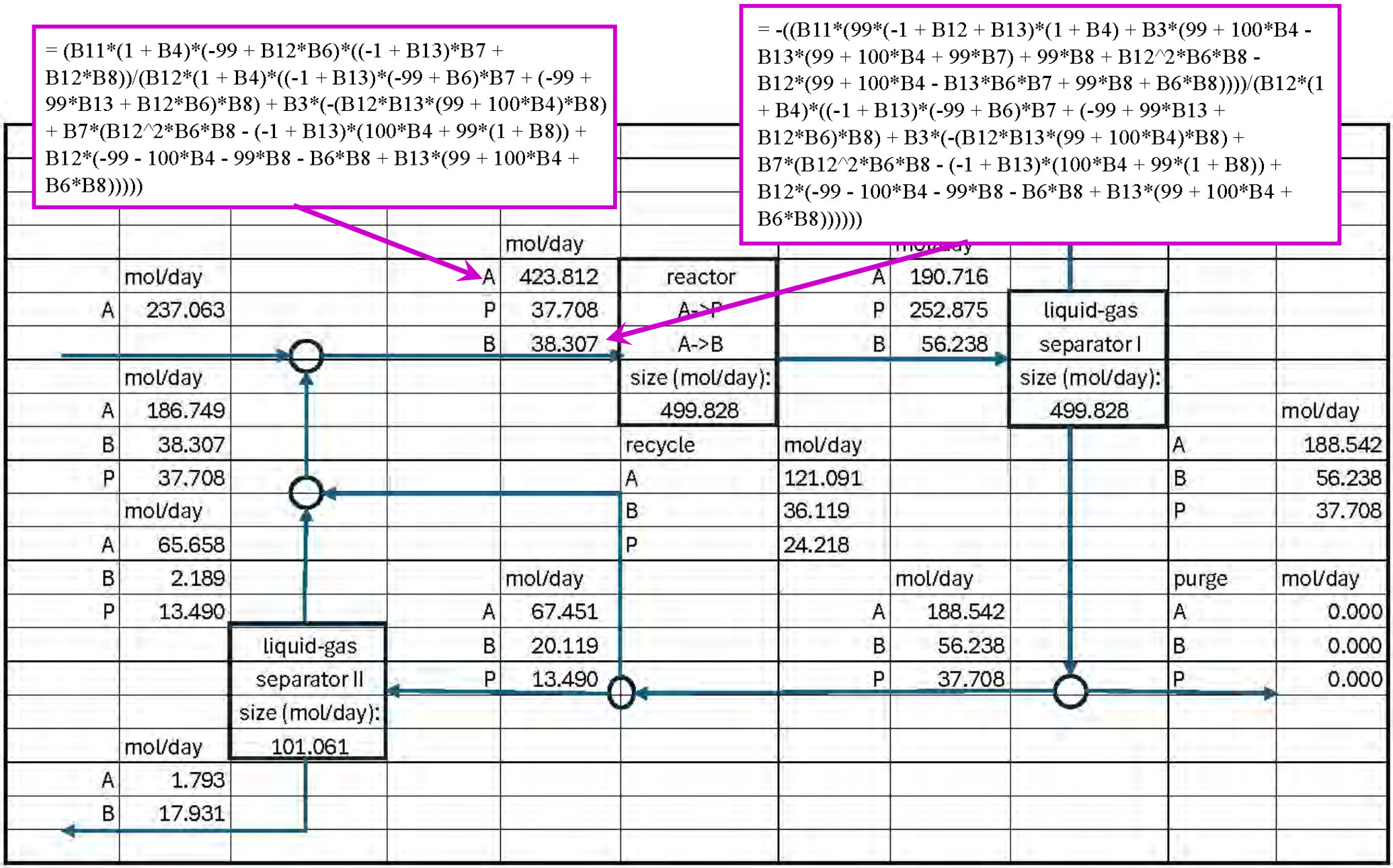

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```
In[44]:= Clear["Global`*"]

In[45]:= Assumptions = {kp ≤ 1, kr ≤ 1, kp ≥ 0, kr ≥ 0, a ≥ 0,
    b ≥ 0, p ≥ 0, k1 > 0, k2 < 1, r1 > 0, r2 > 0, r3 > 0, r4 > 0, fin > 0};
```

*** Set: Symbol Assumptions is Protected.

k1 = conversion rate of A = 0.55
r1 = ratio of P : B in reactor effluent = 12
pct1 = separator I % P tops = 0.99
r2 = separator I ratio of P : A in bottoms = 0.2
r3 = separator II ratio of A : B in tops = 30
r4 = separator II ratio of A : B in bottoms = 0.1
fin = reactant A flow rate
krem = 1-kp-kr = separator II bottoms remaining after purge and recycle

```
In[46]:= pct1 = 99 / 100;
```

Define stream relationships and overall equations

```
In[47]:= a1 = (1 - k1) * a; p1 = p + k1 * a * r1 / (r1 + 1); b1 = b + k1 * a * 1 / (r1 + 1);
a2 = (p + k1 * a * r1 / (r1 + 1) - r2 * (1 - k1) * a) / ((pct1 / (1 - pct1)) - r2);
a3 = a1 - a2; p3 = p + k1 * a * r1 / (r1 + 1) - (pct1 / (1 - pct1)) * a2;
a5 = krem * a3; b5 = krem * b1; p5 = krem * p3;
a6 = r4 * (r3 * b5 - a5) / (r3 - r4);

In[52]:= eq1 = a == fin + a5 - a6 + kr * a3;

In[53]:= eq2 = b == b5 - (1 / r4) * a6 + kr * b1;

In[54]:= eq3 = p == p5 + kr * p3;

In[55]:= eq4 = fin == 100 * a2 + (1 + 1 / r4) * a6 + kp * (a3 + b1 + p3);
```

Solve for A equation

```
In[56]:= redsA = Reduce[eq1, a]
```

Out[56]=

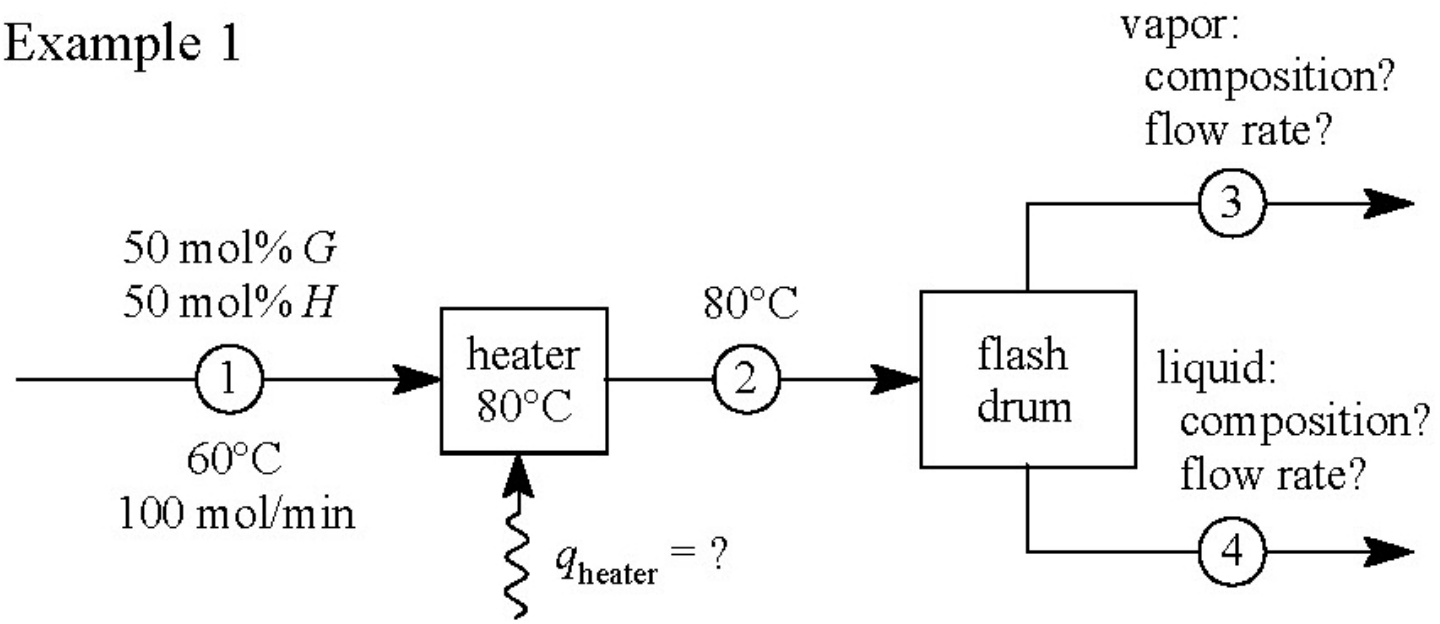
$$(99\,r3 - 99\,kr\,r3 + 99\,k1\,kr\,r3 - 99\,krem\,r3 + 99\,k1\,krem\,r3 + 99\,r1\,r3 - 99\,kr\,r1\,r3 + 100\,k1\,kr\,r1\,r3 - 99\,krem\,r1\,r3 + 100\,k1\,krem\,r1\,r3 - r2\,r3 - r1\,r2\,r3 - 99\,r4 + 99\,kr\,r4 - 99\,k1\,kr\,r4 - 99\,r1\,r4 + 99\,kr\,r1\,r4 - 100\,k1\,kr\,r1\,r4 + r2\,r4 + r1\,r2\,r4 + 99\,k1\,krem\,r3\,r4 - k1\,krem\,r2\,r3\,r4 \neq 0 \;\&\&$$
$$a == -(((1 + r1)\,(-99\,fin\,r3 + kr\,p\,r3 + krem\,p\,r3 + fin\,r2\,r3 + 99\,fin\,r4 - kr\,p\,r4 - fin\,r2\,r4 + 99\,b\,krem\,r3\,r4 - b\,krem\,r2\,r3\,r4)) / (99\,r3 - 99\,kr\,r3 + 99\,k1\,kr\,r3 - 99\,krem\,r3 + 99\,k1\,krem\,r3 + 99\,r1\,r3 - 99\,kr\,r1\,r3 + 100\,k1\,kr\,r1\,r3 - 99\,krem\,r1\,r3 + 100\,k1\,krem\,r1\,r3 - r2\,r3 - r1\,r2\,r3 - 99\,r4 + 99\,kr\,r4 - 99\,k1\,kr\,r4 - 99\,r1\,r4 + 99\,kr\,r1\,r4 - 100\,k1\,kr\,r1\,r4 + r2\,r4 + r1\,r2\,r4 + 99\,k1\,krem\,r3\,r4 - k1\,krem\,r2\,r3\,r4)) \;\&\&$$
$$-99\,r3 - 99\,r1\,r3 + r2\,r3 + r1\,r2\,r3 + 99\,r4 + 99\,r1\,r4 - r2\,r4 - r1\,r2\,r4 \neq 0) \;||$$
$$\left(r1 == -\frac{99}{100} \;\&\&\; krem == 0 \;\&\&\; kr == \frac{99 - r2}{99} \;\&\&\; fin == \frac{p}{99} \;\&\&\right.$$
$$\left.-99\,r3^2\,r4 + r2\,r3^2\,r4 + 99\,r3\,r4^2 - r2\,r3\,r4^2 \neq 0\right) \;||$$
$$\left(r3 == 0 \;\&\&\; r1 == -\frac{99}{100} \;\&\&\; kr == \frac{99 - r2}{99} \;\&\&\; fin == \frac{p}{99} \;\&\&\right.$$
$$\left.-99\,r4 + r2\,r4 \neq 0\right) \;||$$
$$\left(r4 == 0 \;\&\&\; r1 == -\frac{99}{100} \;\&\&\; kr == \frac{1}{99}\,(99 - 99\,krem - r2) \;\&\&\right.$$
$$\left.fin == \frac{p}{99} \;\&\&\; -99\,r3 + r2\,r3 \neq 0\right) \;||$$
$$\left(99\,kr\,r3 + 99\,krem\,r3 + 100\,kr\,r1\,r3 + 100\,krem\,r1\,r3 - 99\,kr\,r4 - 100\,kr\,r1\,r4 + 99\,krem\,r3\,r4 - krem\,r2\,r3\,r4 \neq 0 \;\&\&\right.$$
$$k1 == ((1 + r1)\,(-99\,r3 + 99\,kr\,r3 + 99\,krem\,r3 + r2\,r3 + 99\,r4 - 99\,kr\,r4 - r2\,r4)) / (99\,kr\,r3 + 99\,krem\,r3 + 100\,kr\,r1\,r3 + 100\,krem\,r1\,r3 - 99\,kr\,r4 - 100\,kr\,r1\,r4 + 99\,krem\,r3\,r4 - krem\,r2\,r3\,r4) \;\&\&$$
$$(99 - 99\,kr + 99\,k1\,kr + 99\,r1 - 99\,kr\,r1 + 100\,k1\,kr\,r1 - r2 - r1\,r2)\,r4 \neq 0 \;\&\&\; b == \frac{99\,fin - 99\,fin\,k1 - p + 99\,fin\,r1 - 100\,fin\,k1\,r1 - p\,r1 - 99\,fin\,k1\,r4 + k1\,kr\,p\,r4 + fin\,k1\,r2\,r4}{(99 - 99\,kr + 99\,k1\,kr + 99\,r1 - 99\,kr\,r1 + 100\,k1\,kr\,r1 - r2 - r1\,r2)\,r4} \;\&\&$$
$$\left.r3 - r4 \neq 0\right) \;||\; \left(r3 == 0 \;\&\&\; kr\,(99 + 100\,r1) \neq 0 \;\&\&\; k1 == \frac{(1 + r1)\,(-99 + 99\,kr + r2)}{kr\,(99 + 100\,r1)} \;\&\&\right.$$
$$-99 + 99\,k1 - 99\,r1 + 100\,k1\,r1 \neq 0 \;\&\&$$
$$\left.fin == \frac{-p - p\,r1}{-99 + 99\,k1 - 99\,r1 + 100\,k1\,r1} \;\&\&\; r4 \neq 0\right) \;||$$
$$\left(100\,r1) \neq 0 \;\&\&\; k1 == \frac{(1 + r1)\,(-99 + 99\,kr + 99\,krem + r2)}{(kr + krem)\,(99 + 100\,r1)} \;\&\&\right.$$
$$r1 \neq 0 \;\&\&$$
$$\left.fin == \frac{p - p\,r1}{-99 + 99\,k1 - 99\,r1 + 100\,k1\,r1} \;\&\&\; r3 \neq 0\right) \;||$$
$$\left(r3\,r4 \neq 0 \;\&\&\; krem == \frac{-99\,r3 - 100\,r1\,r3 + 99\,r4 + 100\,r1\,r4}{99\,r3\,r4} \;\&\&\right.$$
$$kr == \frac{99 + 100\,r1 + 99\,r3 - 99\,krem\,r3 - r2\,r3}{99\,r3} \;\&\&\; 99 + 100\,r1 \neq 0 \;\&\&\; b == \frac{-99\,fin + p}{99 + 100\,r1} \;\&\&$$
$$\left.-99\,r3 - 99\,r1\,r3 + r2\,r3 + r1\,r2\,r3 + 99\,r4 + 99\,r1\,r4 - r2\,r4 - r1\,r2\,r4 \neq 0\right) \;||$$
$$\left(r1 == -\frac{99}{100} \;\&\&\; kr == \frac{99 - r2}{99} \;\&\&\; (-99 + r2)\,r4 \neq 0 \;\&\&\; k1 == -\frac{99}{100\,(-99 + r2)\,r4} \;\&\&\right.$$
$$krem\,r3 \neq 0 \;\&\&\; b == \frac{1}{9801\,krem\,r3}(-9801\,fin + 99\,p + 980100\,fin\,k1\,r3 - 9900\,k1\,p\,r3 - 9900\,k1\,krem\,p\,r3 - 9900\,fin\,k1\,r2\,r3 + 100\,k1\,p\,r2\,r3) \;\&\&\; r3 - r4 \neq 0\Big) \;||$$
$$\left(r4 \neq 0 \;\&\&\; kr == \frac{99 + 100\,r1 + 99\,r4 - r2\,r4}{99\,r4} \;\&\&\; 99 + 100\,r1 + 99\,r4 - r2\,r4 \neq 0 \;\&\&\right.$$

Plus 6 more pages …

Combined Mass & Energy Balances on Binary Mixtures

Graphical Methods Examples

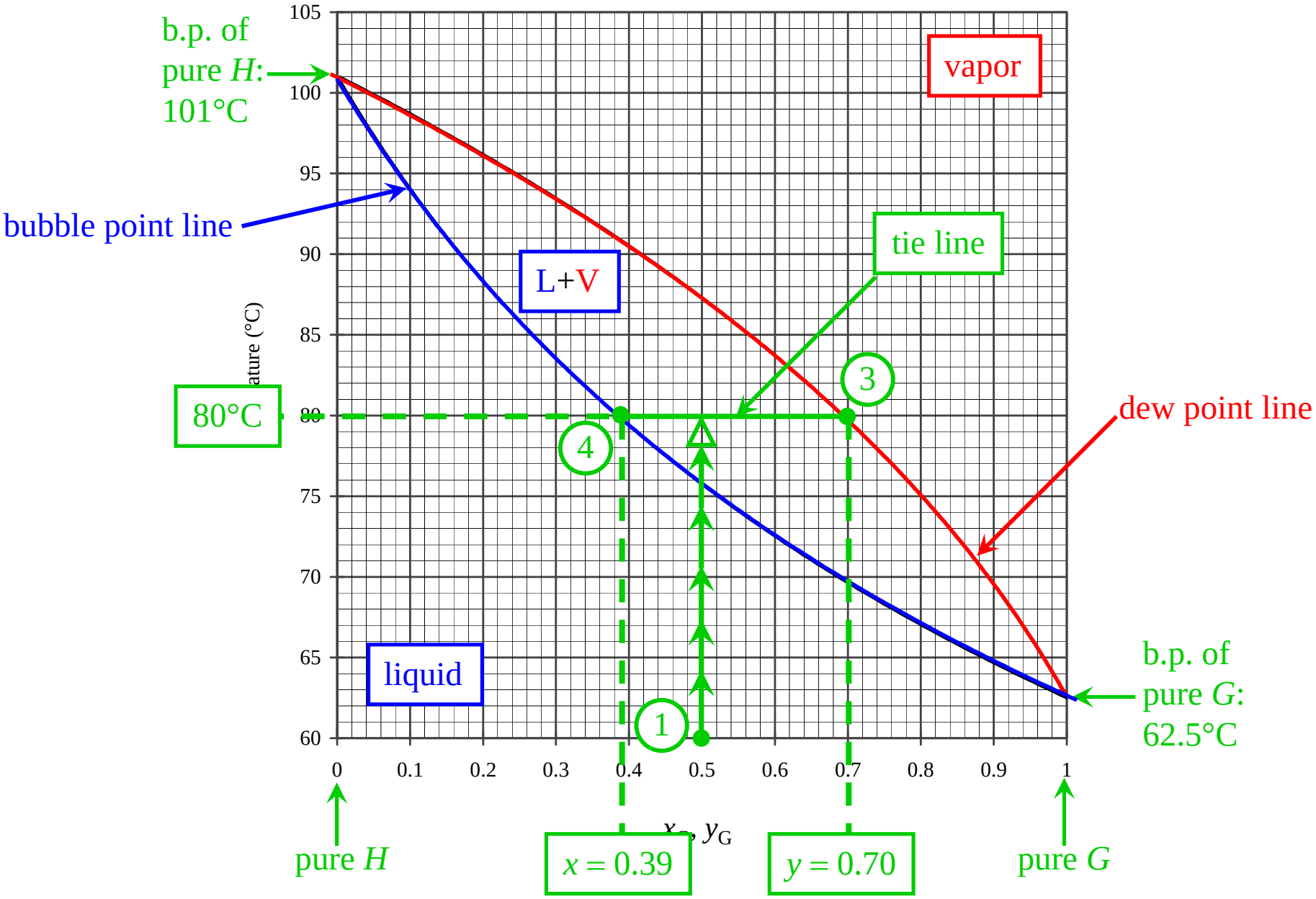
Example 1



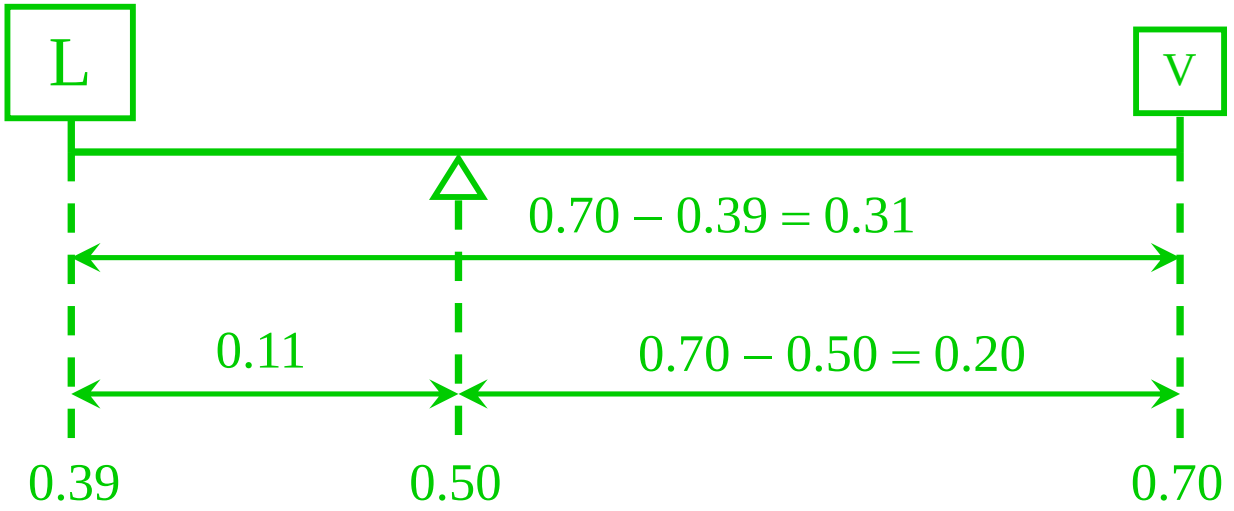
Temperature-Composition Phase Diagram for *G*–*H* Mixtures at 1 atm

G – more volatile component

Example 1.



Example 1: Apply the Lever Rule to the Tie Line



$$\text{liquid flow rate} = \left(\frac{0.20}{0.31}\right) \times 100 \text{ mol/min} = 65 \text{ mol/min}$$

vapor flow rate = 35 mol/min.

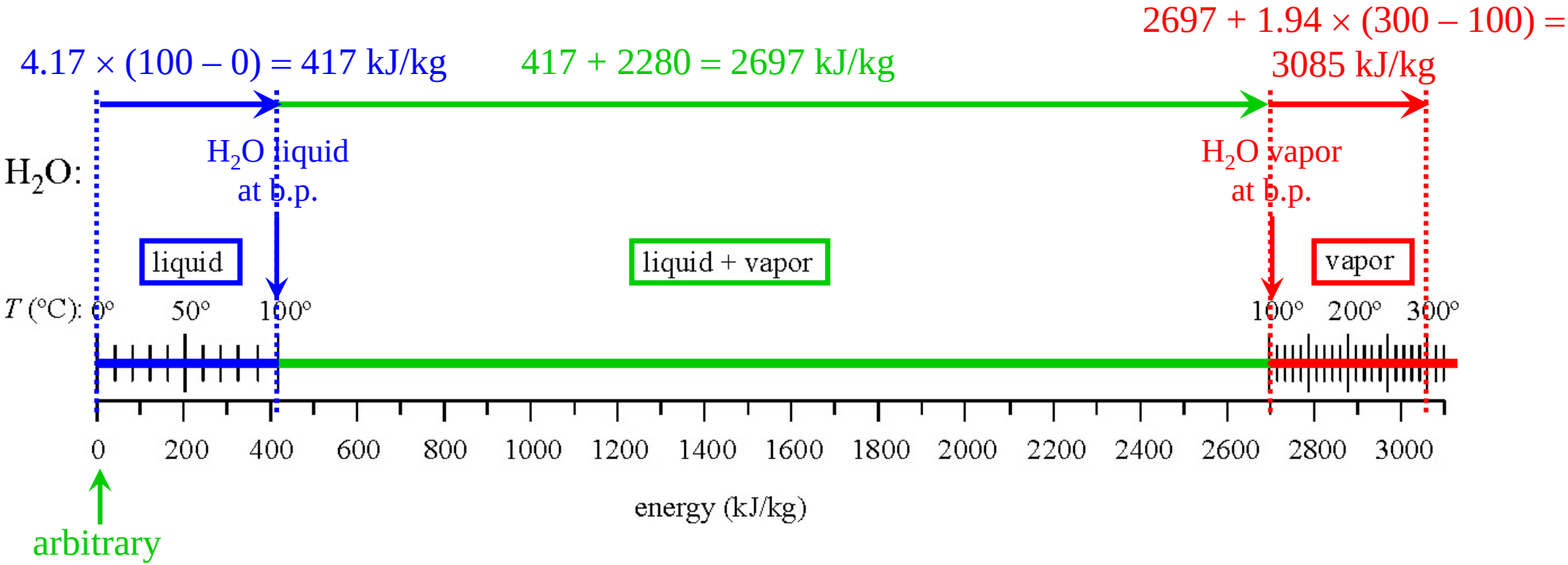
We need a graphical method for energy balances on binary mixtures.

Recall our number line for energy balances on a pure substance: H_2O.

Graphical Modeling - Energy Balance Lines

Thermodynamic Data:

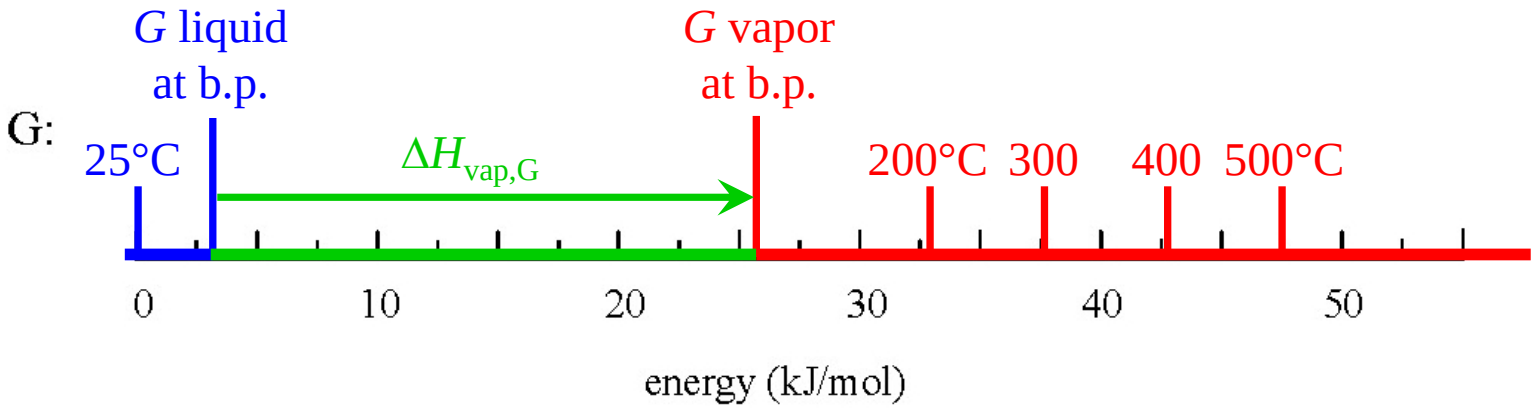
	H_2O
boiling point	100°C
ΔH_{vap}	2280 kJ/kg = 41 kJ/mol
$C_{P,\,liquid}$	4.17 kJ/(kg °C) = 75 J/(mol °C)
$C_{P,\,vapor}$	1.94 kJ/(kg °C) = 33 J/(mol °C)



Create a number line for energy balances on pure *G*.

Thermodynamic Data:

	H_2O	G
boiling point	100°C	62.5°C
ΔH_{vap}	2280 kJ/kg = 41 kJ/mol	23 kJ/mol
$C_{P,\ liquid}$	4.17 kJ/(kg °C) = 75 J/(mol °C)	80 J/(mol °C)
$C_{P,\ vapor}$	1.94 kJ/(kg °C) = 33 J/(mol °C)	50 J/(mol °C)



Arbitrarily set $\overline{H} = 0$ kJ/mol for *G* liquid at 25°C

Calculate $\overline{H}$ for *G* liquid at b.p. $\quad \overline{H} = 0 + \overline{C}_{P,G\ liquid}(\Delta T)$

$= 0 + 80\ \text{J/mol°C} \times (62.5 - 25°C) = 3.0\ \text{kJ/mol}$

Calculate $\overline{H}$ for *G* vapor at b.p. $\quad \overline{H} = 3.0 + \Delta\overline{H}_{vap,G} = 3.0 + 23\ \text{kJ/mol} = 26\ \text{kJ/mol}$

Calculate $\overline{H}$ for *G* vapor at 200°C. $\quad \overline{H} = 26 + \overline{C}_{P,G\ vapor}(\Delta T)$

$= 26 + 50\ \text{J/mol°C} \times (200 - 62.5\ °C) = 32.9\ \text{kJ/mol}$

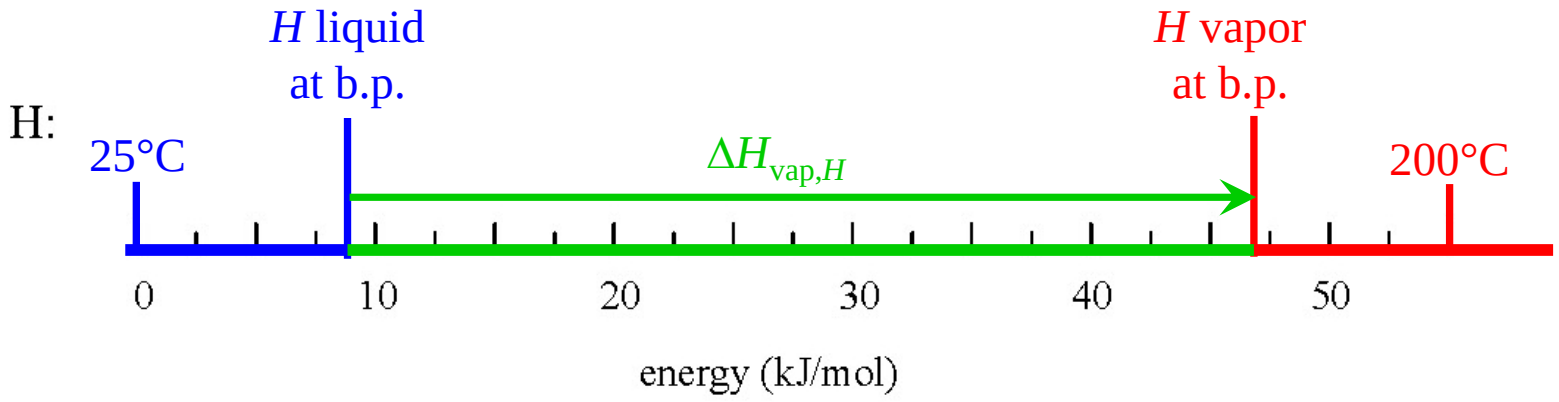
Calculate $\overline{H}$ for *G* vapor at 300°C. $\quad \overline{H} = 32.9 + \overline{C}_{P,G\ vapor}(\Delta T)$

$= 32.9 + 50\ \text{J/mol°C} \times (300 - 200\ °C) = 37.9\ \text{kJ/mol}$

Create a number line for energy balances on pure *H*.

Thermodynamic Data:

	H_2O	G	H
boiling point	100°C	62.5°C	101°C
ΔH_{vap}	2280 kJ/kg = 41 kJ/mol	23 kJ/mol	38 kJ/mol
$C_{P,\ liquid}$	4.17 kJ/(kg °C) = 75 J/(mol °C)	80 J/(mol °C)	120 J/(mol °C)
$C_{P,\ vapor}$	1.94 kJ/(kg °C) = 33 J/(mol °C)	50 J/(mol °C)	80 J/(mol °C)



Arbitrarily set $\overline{H}$ = 0 kJ/mol for *H* liquid at 25°C

Calculate $\overline{H}$ for *H* liquid at b.p. $\overline{H} = 0 + \overline{C}_{P,H\ liquid}(\Delta T)$

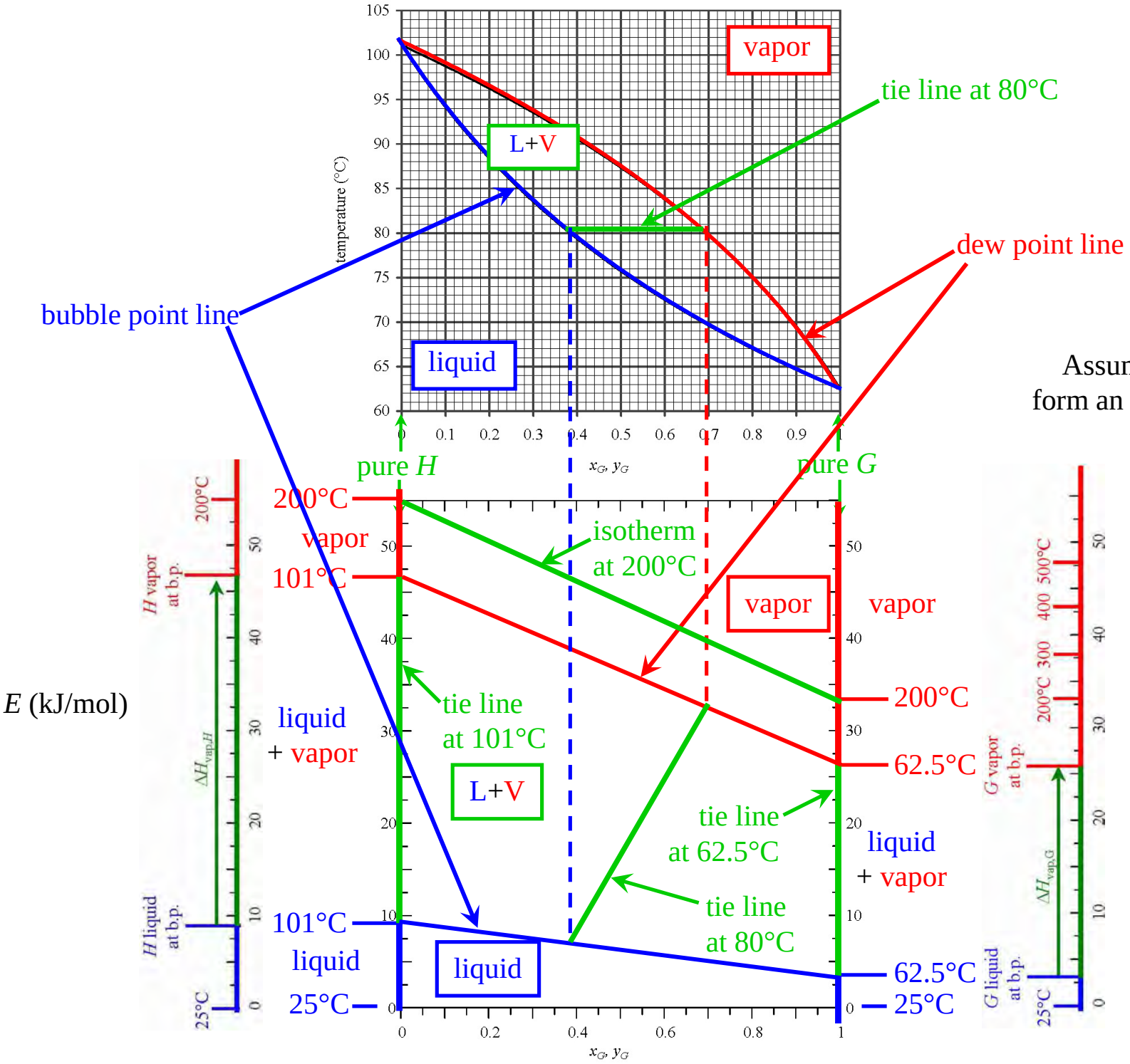
$= 0 + 120\ J/mol°C \times (101 - 25°C) = 9.1\ kJ/mol$

Calculate $\overline{H}$ for *H* vapor at b.p. $\overline{H} = 9.1 + \Delta\overline{H}_{vap,H} = 9.1 + 38\ kJ/mol = 47.1\ kJ/mol$

Calculate $\overline{H}$ for *H* vapor at 200°C. $\overline{H} = 47.1 + \overline{C}_{P,H\ vapor}(\Delta T)$

$= 47.1 + 80\ J/mol°C \times (200 - 101\ °C) = 55\ kJ/mol$

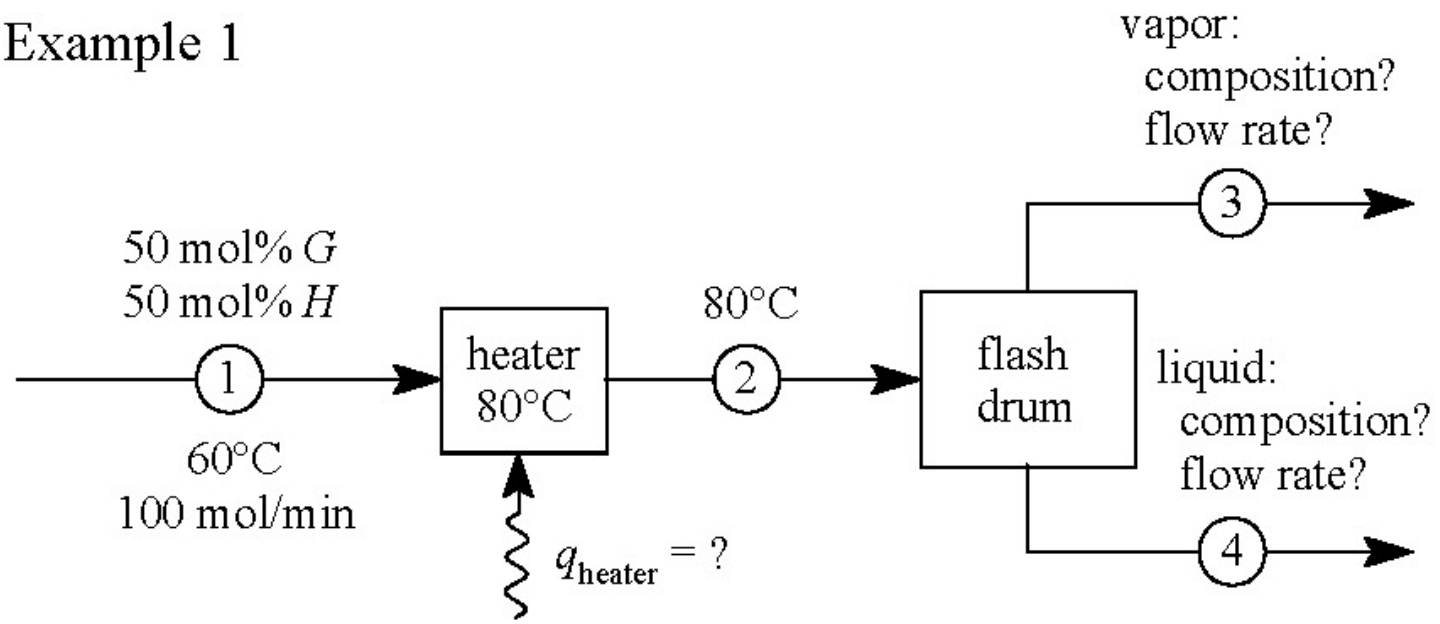
Temperature-Composition Phase Diagram for *G*+*H* Mixtures at 1 atm



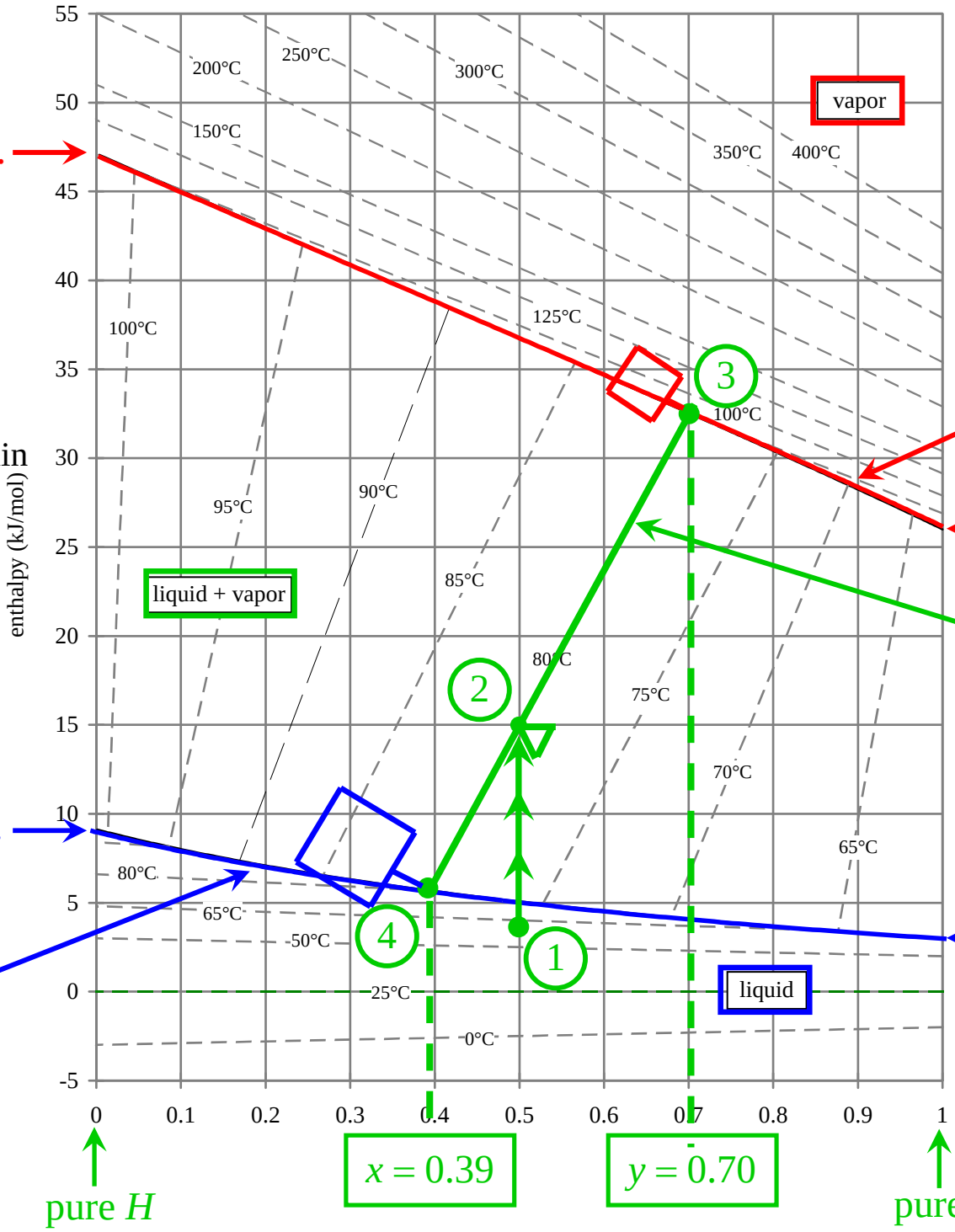
Combined Mass & Energy Balances on Binary Mixtures

Graphical Methods Examples

Example 1



Enthalpy-Composition Phase Diagram for *G*+*H* Mixtures at 1 atm



H vapor at b.p.

G vapor at b.p.

dew point line

tie line at 80°C

H liquid at b.p.

G liquid at b.p.

bubble point line

q_{heater}:
stream 1: 3.6 kJ/mol
stream 2: 15 kJ/mol

$\Delta H = 15 - 3.6$
$= 11.4$ kJ/mol

$q_{heater} = 11.4 \times 100$ mol/min
$= 1{,}140$ kJ/min

$q_{heater} = 1100$ kJ/min

Tie Line:
total length = 81.5 mm
liquid arm = 29 mm

$$\text{vapor} = \frac{29\text{ mm}}{81.5\text{ mm}} \times 100$$

$= 36$ mol/min

liquid = 64 mol/min