ABE 201
Biological Thermodynamics 1

Module 5:

Linear Algebra for Mass Balances

Summary

- Material (and energy!) balances are systems of linear equations
- Systems of linear equations can be represented and solved in matrix form
- MatLAB and other computer tools make easy the tedious and repetitive work of solving

  `inv(A)*B, A\B, or linsolve(A,B)`
- The challenge is <u>translating</u> an engineering problem into mathematics

Procedure

- Write out your mass balance equations
- Pick which ones you will use
- Re-arrange so that all of your <u>constants</u> are on 1 side of the = and coefficients*variables on the other
- Segregate coefficients (known values) into matrix
- Solve

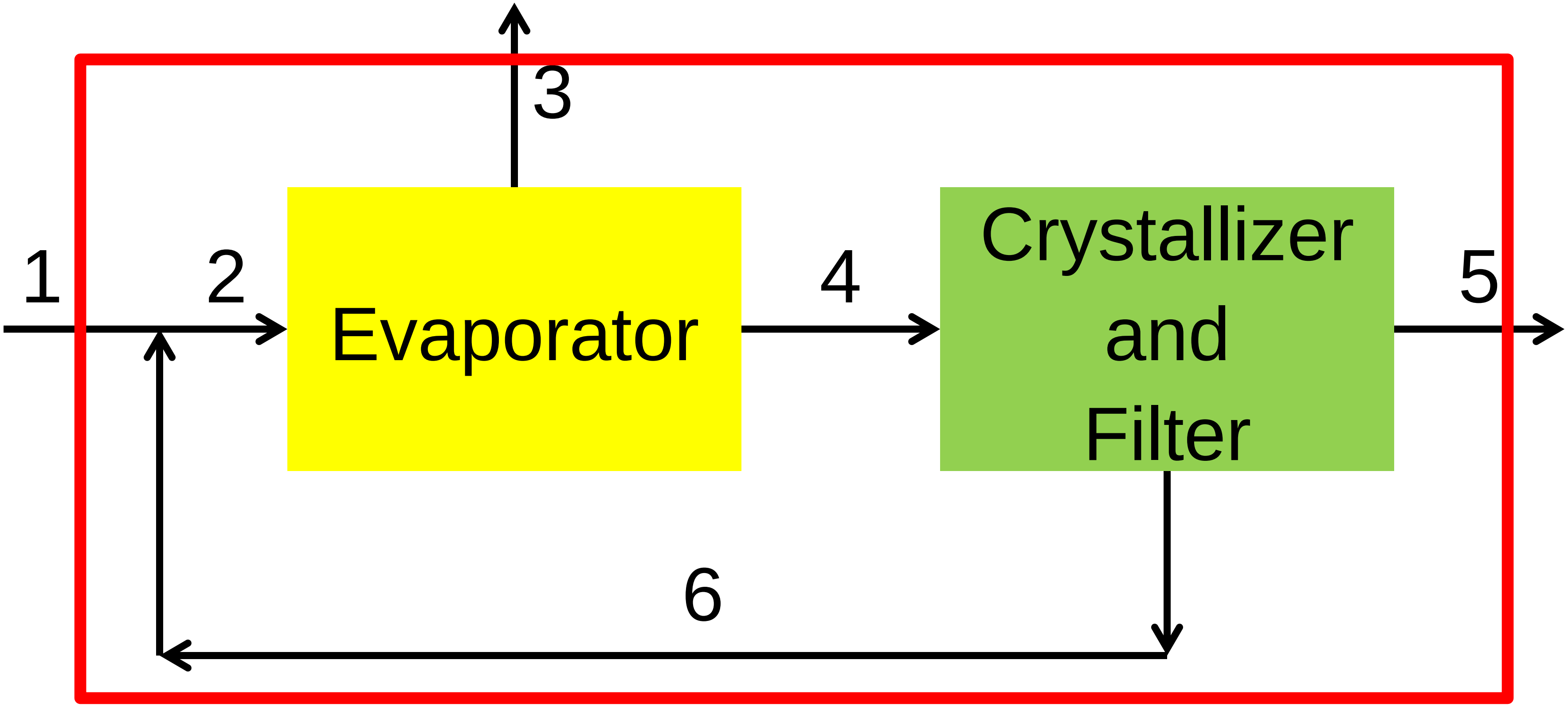
Pharmaceutical Recovery

After synthesis, a pharmaceutical is recovered from solvent. The feed is 4521 kg/h and contains 3% (w/w) drug and the remainder solvent.

In the first step, 50% of the solvent entering the evaporator is removed, leaving the drug behind in the remaining solvent.

In the second step, the mixture (2573 kg/h) is cooled causing 95% of the drug entering the second step to crystalize and be filtered out. The filter cake is 75% drug and 25% solvent. The remaining solvent with un-crystalized drug is recycled back to step 1 where it is blended with the feed and fed to the evaporator.

What is the recycle rate?



	1	2	3	4	5	6
m (kg/h)	4521	m_2	m_3	2573	m_5	m_6
x_d	0.03	x_{2d}	0	x_{4d}	0.75	x_{6d}
x_s	0.97	x_{2s}	1	x_{4s}	0.25	x_{6s}

DOF = V – B – P – C = 2 – 2 – 0 – 0 = 0

$Acc = In - Out + Gen - Con$

Total Mass

$$0 = (m_1) - (m_3 + m_5)$$

$$0 = 4521 - (m_3 + m_5)$$

Drug Mass

$$0 = (x_{1d}*m_1) - (x_{3d}*m_3 + x5d*m5)$$

$$0 = (0.03*4521) - (0 + 0.75*m5)$$

Solvent Mass

$$0 = (x_{1s}*m_1) - (x_{3s}*m_3 + x_{5s}*m_5)$$

$$0 = (0.97*4521) - (m_3 + 0.25*m_5)$$

0 = 4521 – (m3 + m5)

0 = (0.03*4521) – (0 + 0.75*m5)

$4521 = 1^* m_3 + 1^*m_5$

$135.6 = 0^*m_3 + 0.75^*m_5$

$$\begin{bmatrix} 4521 \\ 135.6 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 0.75 \end{bmatrix} \bullet \begin{bmatrix} m_3 \\ m_5 \end{bmatrix} \qquad \begin{bmatrix} m_3 \\ m_5 \end{bmatrix} = \begin{bmatrix} 4340.2 \\ 180.8 \end{bmatrix}$$

What happens if you cannot segregate?

Change Variables!

- If you cannot segregate your variables, you will need to define new ones that enable you to segregate

- Defining new masses (specific substances) is often useful

- Uses these to define mass fraction constraint!

ABE Fermentation

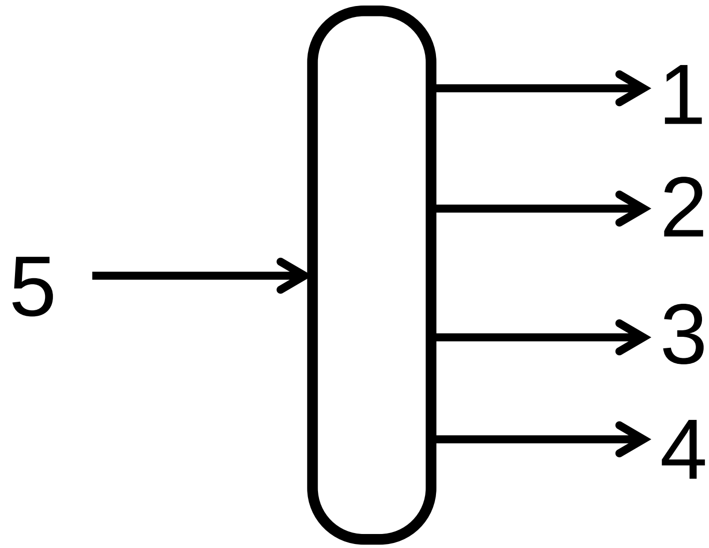
Clostridium acetylbutylicum is used to ferment sugar to a mixture of acetone, butanol, and ethanol. Distillation is used to recover and purify the products from the fermentation liquid (water).

At steady state, 1,575 kg of liquid enters the distillation column per minute. This liquid is 3.5% (w/w) acetone, 4.5% (w/w) butanol, 3.7% (w/w) ethanol, and the remainder water.

Four streams leave the column with the following compositions:

1. 93.2% acetone, 3.1% ethanol, 1.1% butanol with water
2. 92.1% ethanol, with residual acetone, butanol and water
3. 93.3% butanol, with water
4. 1.0% butanol with water

If stream 1 is produced at 58.3 kg/min and stream 4 at 1398 kg/min, what are the rates of production for the other product streams?



	1	**2**	**3**	**4**	**5**
m (kg/min)	58.3	m_2	m_3	1398	1575
x_a	0.932	x_{2a}	0	0	0.035
x_e	0.031	0.921	0	0	0.037
x_b	0.011	x_{2b}	0.933	0.010	0.045
x_w	0.026	x_{2w}	0.067	0.990	0.883

$$DOF = V - B - P - C = 5 - 4 - 0 - 1 = 0$$

$$acc = in - out + gen - con$$

$$0 = (m_5) - (m_1 + m_2 + m_3 + m_4)$$

Acetone Balance

$$0 = (x_{5a}*m_5) - (x_{1a}*m_1 + x_{2a}*m_2 + x_{3a}*m_3 + x_{4a}*m_4)$$

$$0 = (55.13) - (54.34 + \boxed{x_{2a}*m_2} + 0*m_3 + 0*1398)$$

$$0 = (55.13) - (54.34 + m_{2a} + 0*m_3)$$

Ethanol Balance

$$0 = (x_{5e}*m_5) – (x_{1e}*m_1 + x_{2e}*m_2 + x_{3e}*m_3 + x_{4e}*m_4)$$

$$0 = (58.28) – (1.807 + 0.921*m_2 + 0*m_3 + 0)$$

Butanol Balance

$$0 = (x_{5b}*m_5) – (x_{1b}*m_1 + \boxed{x_{2b}*m_2} + x_{3b}*m_3 + x_{4b}*m_4)$$

$$0 = (70.88) – (0.6413 + m_{2b} + 0.933*m_3 + 13.98)$$

Water Balance

$$0 = (x_{5w}*m_5) – (x_{1w}*m_1 + \boxed{x_{2w}*m_2} + x_{3w}*m_3 + x_{4w}*m_4)$$

$$0 = (1391) – (1.516 + m_{2w} + 0.067*m_3 + 1384)$$

Stream 2 Constraint

$$1 = m_{2a}/ m_2 + 0.921 + m_{2b}/ m_2 + m_{2w} / m_2$$

$$m_2 = m_{2a} + 0.921^* m_2 + m_{2b} + m_{2w}$$

$$0 = 0.079^*m_2 - m_{2a} - m_{2b} - m_{2w}$$

$0 = (55.13) – (54.34 + m_{2a} + 0*m_3)$ acetone

$0 = (58.28) – (1.807 + 0.921*m_2 + 0*m_3 + 0)$ ethanol

$0 = (70.88) – (0.6413 + m_{2b} + 0.933*m_3 + 13.98)$ buOH

$0 = (1391) – (1.516 + m_{2w} + 0.067*m_3 + 1384)$ H2O

$0 = 0.079*m_2 - m_{2a} - m_{2b} - m_{2w}$ constraint

$0.79 = 1*m_{2a} + 0*m_3$

$56.47 = 0.921*m_2 + 0*m_3$

$56.26 = 1*m_{2b} + 0.933*m_3$

$5.484 = 1*m_{2w} + 0.067*m_3$

$0 = 0.079*m_2 – 1*m_{2a} – 1*m_{2b} – 1*m_{2w}$

$$
\begin{array}{lccccc}
 & m_{2a} & m_{2b} & m_{2w} & m_2 & m_3 \\
0.79 = & 1*m_{2a} & & & & + 0*m_3 \\
56.47 = & & & & 0.921*m_2 & + 0*m_3 \\
56.26 = & & m_{2b} + & & & 0.933*m_3 \\
5.484 = & & & m_{2w} + & & 0.067*m_3 \\
0 = & -1*m_{2a} & -1*m_{2b} & 1*m_{2w} & + 0.079*m_2 &
\end{array}
$$

$$\begin{bmatrix} 0.79 \\ 56.47 \\ 56.26 \\ 5.484 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.921 & 0 \\ 0 & 1 & 0 & 0 & 0.933 \\ 0 & 0 & 1 & 0 & 0.067 \\ -1 & -1 & -1 & 0.079 & 0 \end{bmatrix} \bullet \begin{bmatrix} m_{2a} \\ m_{2b} \\ m_{2w} \\ m_2 \\ m_3 \end{bmatrix}$$

$$\begin{bmatrix} m_{2a} \\ m_{2b} \\ m_{2w} \\ m_2 \\ m_3 \end{bmatrix} = \begin{bmatrix} 0.790 \\ 2.435 \\ 1.6188 \\ 61.31 \\ 58.69 \end{bmatrix}$$

$$\begin{bmatrix} x_{2a} \\ x_{2b} \\ x_{2w} \end{bmatrix} = \begin{bmatrix} m_{2a} / \mathrm{m}_2 \\ m_{2b} / \mathrm{m}_2 \\ m_{2w} / \mathrm{m}_2 \end{bmatrix} = \begin{bmatrix} 0.013 \\ 0.040 \\ 0.026 \end{bmatrix}$$

Review for Exam 1

- Module 1: Dimensions
- Module 2: Pressure and Temperature
- Module 3: Material Balances
- Module 4: Complex Systems and DOF`