Analysis of Degrees of Freedom

Reference: D.M. Himmelblau, Basic Principles and Calculations in Chemical Engineering, 6th Edition, Prentice-Hall, 1996. Chapter 6.1, Solving Simultaneous Material and Energy Balances.

Objectives:

1. Identify stream variables entering and leaving a unit; identify variables that describe the unit.

2. Determine the number of independent equations for each unit.

3. Calculate the degrees of freedom or number of decision variables.

4. Specify the values of variables equal to the number of degrees of freedom.

To obtain a solution to a process model, we need to formulate a well-posed problem.

The degrees of freedom (DOF) are the variables in a set of independent equations which must have their values assigned.

$$\text{DOF} = \#\ \text{variables} - \#\ \text{equations}$$
$$N_d = N_v - N_c$$

Equations include material and energy balances, unit constraints, composition constraints.

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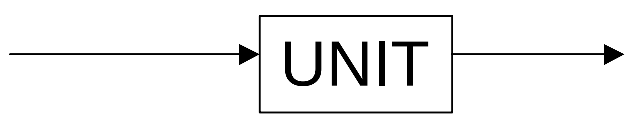
Important process variables include:

- temperature
- pressure
- mass (mole) component flow rates concentration and total flow rates
- specific enthalpies
- heat flow
- work
- flow ratios (e.g. recycle, feed/product, reflux)

To define the state of a stream with N_{sp} species:



F, x_i, T, P
or
n_i or m_i, T, P

The number of variables to describe a stream is given by:

$$N_v = N_{sp} + 2$$

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Where do the constraints (balances) come from?

1. independent material balances for each species or a total flow balance and (N_{sp}-1) species balances

2. energy

3. phase equilibrium relationships that link the compositions between phases

4. chemical equilibrium relationships

5. implicit constraints, e.g. a species concentration is zero

6. explicit constraints, e.g. a given stream fraction is condensing

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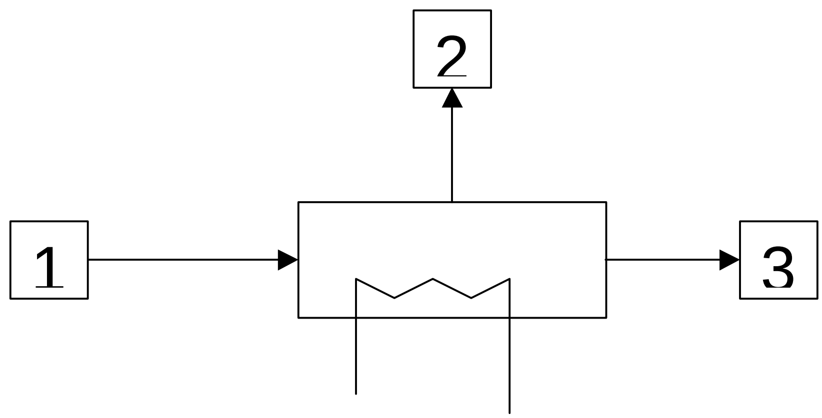
Example - water heater



In each stream, j =1,2,3, we have :
n^j_{water}, n^j_{air}, T^j, P^j

The heater is isothermal, isobaric, with heating Q.

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Example - water heater (Continued)

Number of variables:

3 (N_{sp} +2)	12
Q	1
	13

Number of constraints:

Material balances (N_{sp})	2
Energy	1
Phase equilibrium (water)	1
Isothermal spec ($T^1=T^2=T^3$)	2
Isobaric spec ($P^1=P^2=P^3$)	2
	8

$$\boxed{N_d = 13 - 8 = 5 \text{ DOF}}$$

We can choose 5 variables and specify them to have a well-posed problem.

Q? Can we specify <u>any</u> 5 variables arbitrarily?

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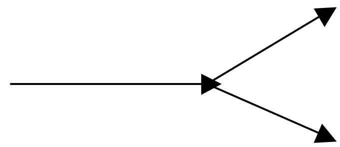
Common Units:

Stream Splitter (adiabatic)



N_v : Stream variables $3(N_{sp}+2)$

N_c :	Material balance	1
	Composition spec	$2(N_{sp} - 1)$
	Temperature spec	2
	Pressure spec	2

$$N_d=\{3(N_{sp}+2)\} - \{2N_{sp}+3\}= N_{sp}+3$$

Q? Give an example specification for a well-posed problem.

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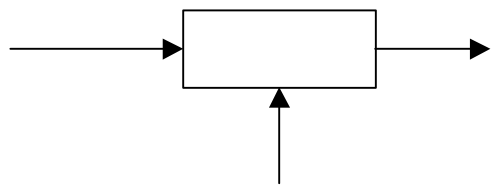
Common Units:

Mixer (not adiabatic)



N_v :	Stream variables	$3(N_{sp}+2)$
	Heat gain/loss (Q)	1
N_c :	Component balance	N_{sp}
	Energy balance	1

$$N_d = \{3(N_{sp}+2) + 1\} - \{N_{sp}+1\} = 2N_{sp}+6$$

Q? Give example specification for a well-posed problem.

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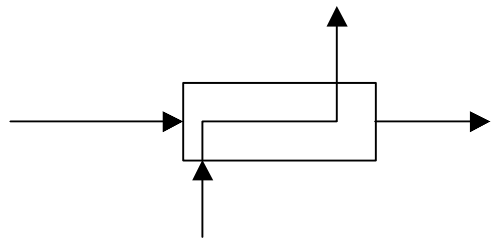
Common Units:
Heat exchanger (not adiabatic)



N_v :	Stream variables	$4(N_{sp}+2)$
	Heat gain/loss (Q)	1
N_c :	Flow balance	2
	Energy balance	1
	Composition spec	$2(N_{sp}-1)$

$$N_d = \{4(N_{sp}+2) + 1\} - \{2N_{sp}+1\} = 2N_{sp}+8$$

Note: model assumes you have total flows for each stream (F) and mass/mole fractions for components (x_i).

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Common Units:
Heat exchanger (not adiabatic)

Q1? Give example specification for a well-posed problem for $N_{sp} = 2$.

Q2? What would change in the model if the number of components in each stream is not the same?

Q3? Heat exchangers do have hydraulic pressure losses on the shell and tube sides. How would we incorporate this information into the model?

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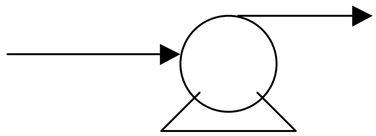
Common Units:
Pump



N_v :	Stream variables	$2(N_{sp}+2)$
	Work (W)	1
N_c :	Flow balance	1
	Energy balance	1
	Composition spec	$N_{sp}-1$

$$N_d = \{2(N_{sp}+2) + 1\} - \{N_{sp}+1\} = N_{sp}+4$$

Note: model assumes you have total flows for each stream and mass/mole fractions for components.

Q? Give example specification for a well-posed problem.

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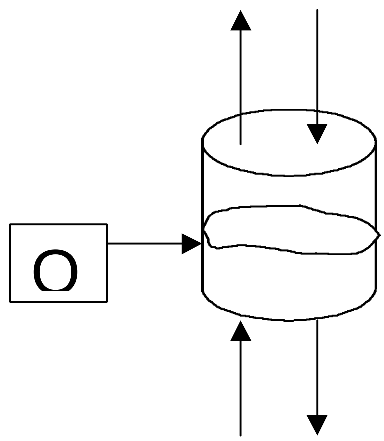
Common units:
Flash tank (single phase streams)



N_v :	Stream variables	$4(N_{sp}+2)$
	Heat (Q)	1
N_c :	Component balance	N_{sp}
	Energy balance	1
	Phase equilibrium	N_{sp}
	Temperature (exit)	1
	Pressure (exit)	1

$$N_d = \{4(N_{sp}+2) + 1\} - \{2N_{sp}+3\} = 2N_{sp}+6$$

Note: model assumes you have component flow rates.

Q? Give an example specification for a well-posed problem.

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