Computer Applications in Chemical Engineering

Priv.-Doz. Dr. Roland Dittmeyer
Karl-Winnacker-Institut der DECHEMA e.V., Frankfurt am Main

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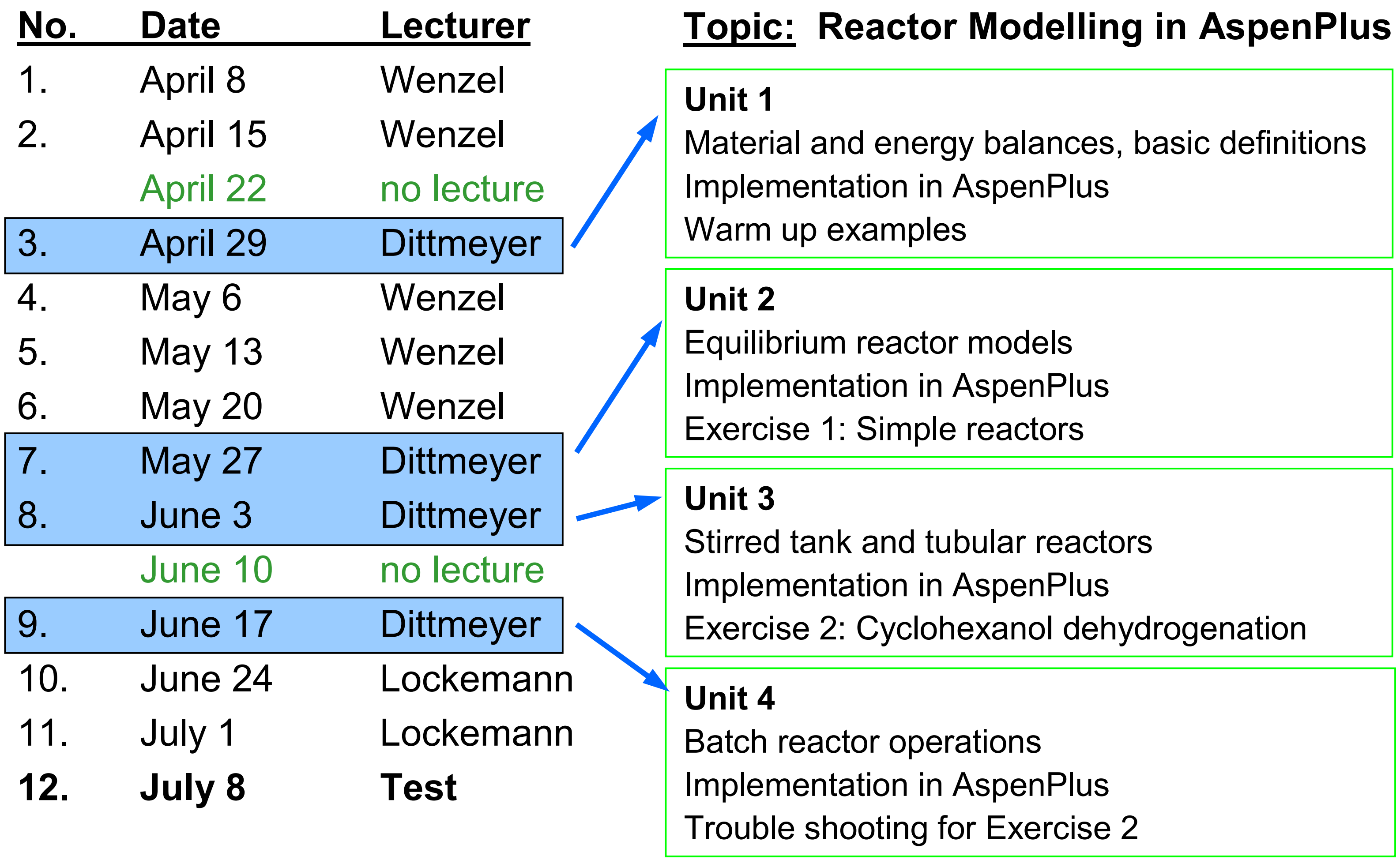


No.	Date	Lecturer
1.	April 8	Wenzel
2.	April 15	Wenzel
	April 22	no lecture
3.	April 29	Dittmeyer
4.	May 6	Wenzel
5.	May 13	Wenzel
6.	May 20	Wenzel
7.	May 27	Dittmeyer
8.	June 3	Dittmeyer
	June 10	no lecture
9.	June 17	Dittmeyer
10.	June 24	Lockemann
11.	July 1	Lockemann
12.	**July 8**	**Test**

Topic: Reactor Modelling in AspenPlus

Unit 1
Material and energy balances, basic definitions
Implementation in AspenPlus
Warm up examples

Unit 2
Equilibrium reactor models
Implementation in AspenPlus
Exercise 1: Simple reactors

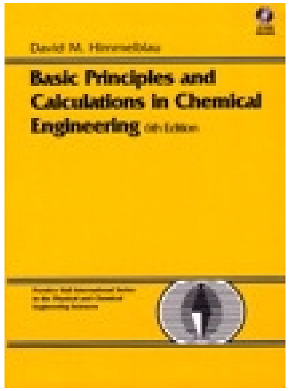
Unit 3
Stirred tank and tubular reactors
Implementation in AspenPlus
Exercise 2: Cyclohexanol dehydrogenation

Unit 4
Batch reactor operations
Implementation in AspenPlus
Trouble shooting for Exercise 2

Process Simulation: Required Knowledge, Recommended Books

Required knowledge:

- Chemical Engineering Thermodynamics
- Unit Operations
- Chemical Reaction Engineering

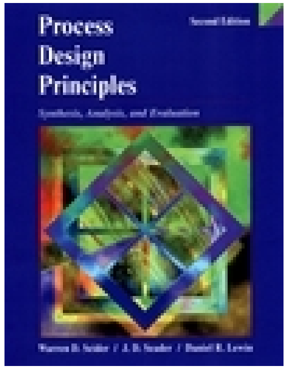


David M. Himmelblau

Basic Principles and Calculations in Chemical Engineering

Books:

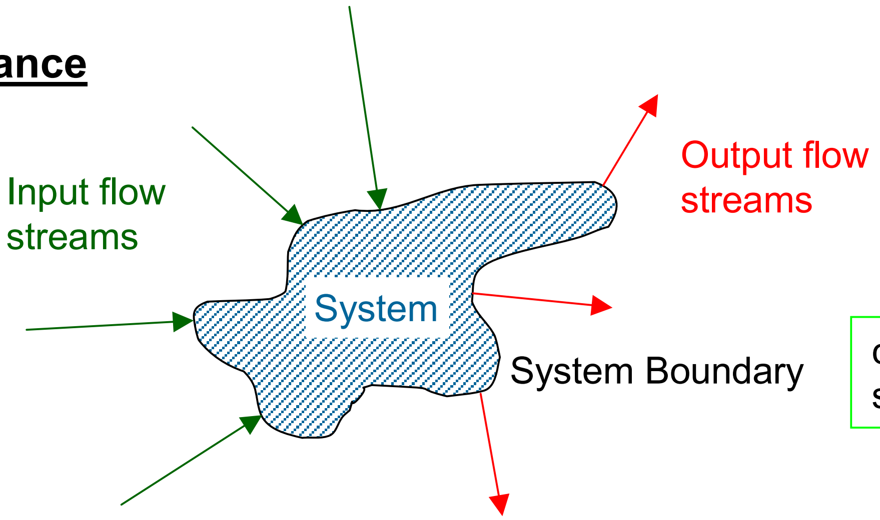
- David M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, 6th edition, Prentice-Hall, Upper Saddle River, 1996
- Warren D. Seider, J.D. Seader, Daniel R. Lewin, *Process Design Principles: Synthesis, Analysis, and Evaluation*, Wiley, New York, 1999



Process Design Principles

Unit 1 Material Balances

1. The Material Balance



not only convective flow, but all other relevant mass transfer processes !

careful choice of system boundary !

In words:

$$\left\{\begin{matrix}\text{accumulation}\\ \text{within the}\\ \text{system}\end{matrix}\right\} = \left\{\begin{matrix}\text{input through}\\ \text{system}\\ \text{boundaries}\end{matrix}\right\} - \left\{\begin{matrix}\text{output through}\\ \text{system}\\ \text{boundaries}\end{matrix}\right\} + \left\{\begin{matrix}\text{generation}\\ \text{within the}\\ \text{system}\end{matrix}\right\} - \left\{\begin{matrix}\text{consumption}\\ \text{within the}\\ \text{system}\end{matrix}\right\}$$

General Principle:

Conservation of: **Requirements:**

1. Total mass .... no nuclear reactions !
2. Total moles .... no net change of moles due to chemical reactions !
3. Mass of an atomic species }
4. Moles of an atomic species } see 1.
5. Moles of a chemical compound }
6. Mass of a chemical compound } no chemical reactions !

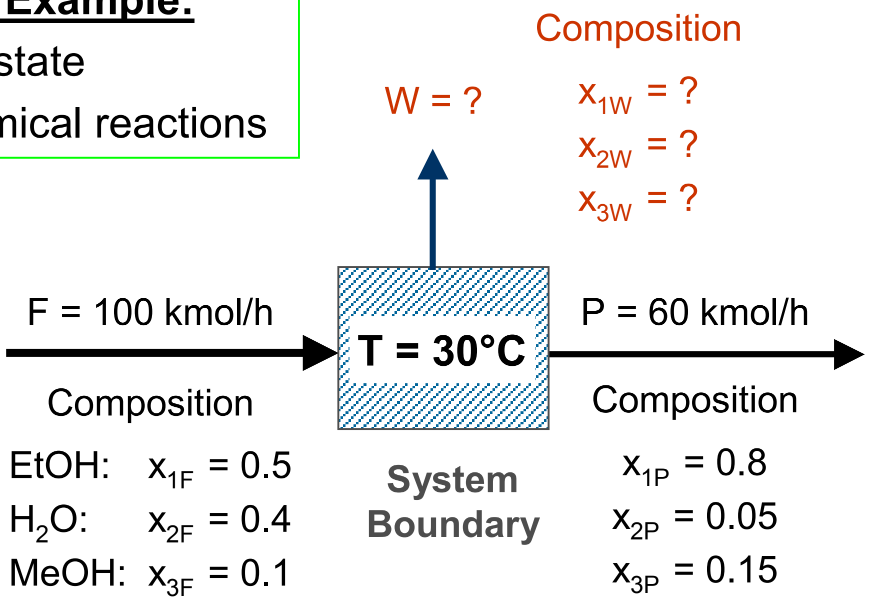
Task:

Find mathematical expressions for these terms that accurately describe the particular situation

Solve the resulting system of equations (linear, nonlinear)

2. Determining the Number of Independent Equations

General Example:
- steady state
- no chemical reactions



Composition

W = ?

x_{1W} = ?
x_{2W} = ?
x_{3W} = ?

F = 100 kmol/h

T = 30°C

P = 60 kmol/h

Composition

EtOH: $x_{1F} = 0.5$
H_2O: $x_{2F} = 0.4$
MeOH: $x_{3F} = 0.1$

System Boundary

Composition

$x_{1P} = 0.8$
$x_{2P} = 0.05$
$x_{3P} = 0.15$

Rule:

The number of variables whose values are unknown equals the number of independent equations !

Total Mole Balance:

$0 = F - P - W$

Component Mole Balances:

EtOH: $0 = F \cdot x_{1F} - P \cdot x_{1P} - W \cdot x_{1W}$
H_2O: $0 = F \cdot x_{2F} - P \cdot x_{2P} - W \cdot x_{2W}$
MeOH: $0 = F \cdot x_{3F} - P \cdot x_{3P} - W \cdot x_{3W}$

Balance of Mole Fractions:

$\Sigma x_{iF} = 1$
$\Sigma x_{iP} = 1$
$\Sigma x_{iW} = 1$

Systems of Linear Equations:

The rank of the coefficient matrix equals the number of independent variables !

rank = order of the largest nonzero determinant in a matrix (can be determined by Gauss-Jordan method)

Component Mole Balances in Matrix Form:

$$\begin{pmatrix} F \cdot x_{1F} - P \cdot x_{1P} \\ F \cdot x_{2F} - P \cdot x_{2P} \\ F \cdot x_{3F} - P \cdot x_{3P} \end{pmatrix} = \begin{pmatrix} W & 0 & 0 \\ 0 & W & 0 \\ 0 & 0 & W \end{pmatrix} \times \begin{pmatrix} x_{1W} \\ x_{2W} \\ x_{3W} \end{pmatrix}$$

3. Number of Degrees of Freedom

$$\left\{\begin{matrix}\text{number of}\\ \text{degrees}\\ \text{of freedom}\end{matrix}\right\} = \left\{\begin{matrix}\text{number of}\\ \text{variables}\\ \text{whose values}\\ \text{are unknown}\end{matrix}\right\} - \left\{\begin{matrix}\text{number of}\\ \text{independent}\\ \text{equations}\end{matrix}\right\}$$

$$f = n - r$$

f	Problem is	Meaning
0	properly specified	unique solution exists
< 0	underspecified	infinite number of solutions
> 0	overspecified	no solution, equations are inconsistent

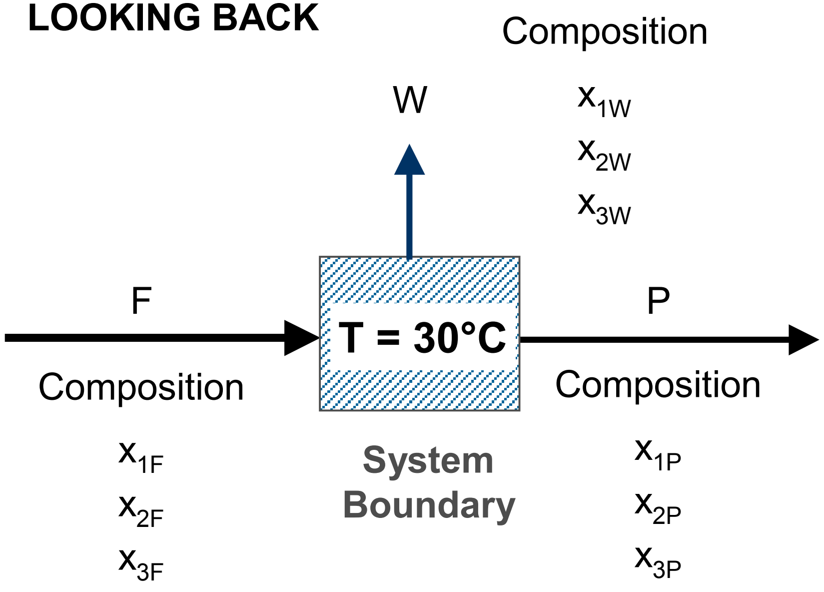
Nonlinear Equations:

more than one solution may exist even for f = 0

if so, the physics of the process tell which solution (s) is (are) relevant

no general statement can be made

LOOKING BACK



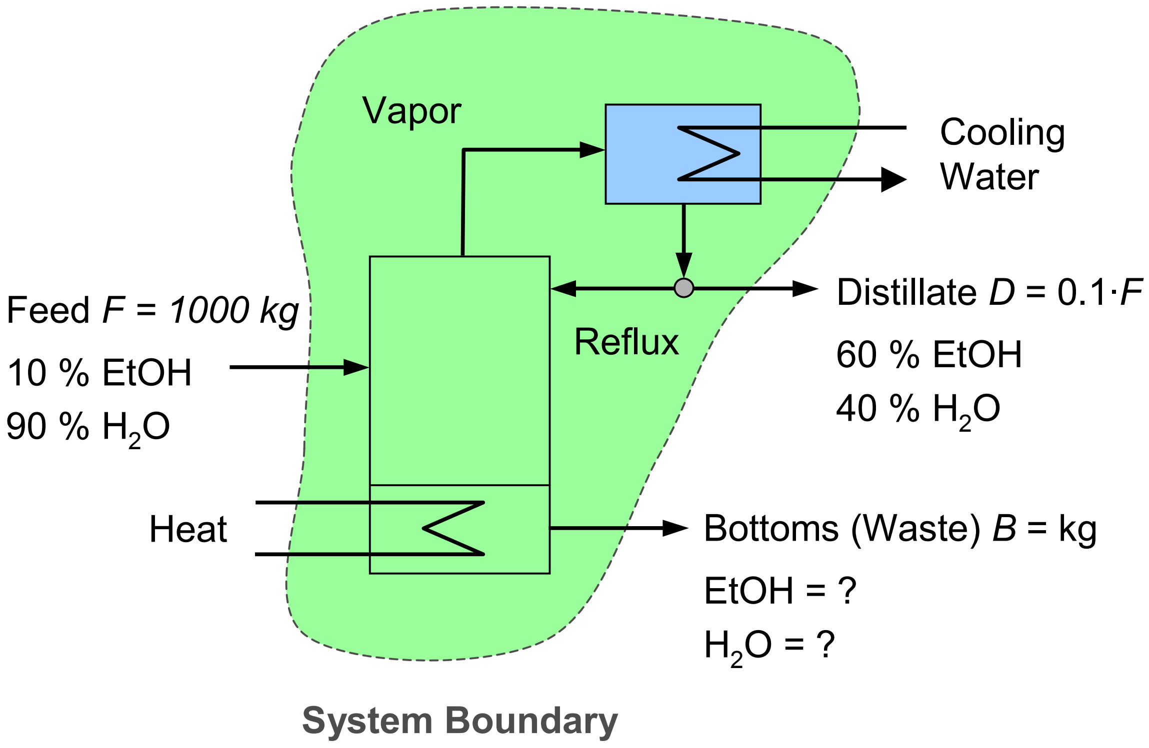
- 12 variables in total
- 7 equations, of which 1 is not independent
- 6 variables have to be specified
- choice of these independent variables is not at will

  → selection must leave a number of independent material balances equal to the number of unknown variables

Unit 1 Material Balances

General Strategy for Analyzing Material Balance Problems	
1.	Read the problem and clarify what is to be accomplished.
2.	Draw a sketch of the process; define the system by a boundary.
3.	Label with symbols the flow of each stream and the associated compositions and other information that is unknown.
4.	Put all the known values of compositions and stream flows on the figure by each stream; calculate additional compositions from the given data as necessary. Or, at least initially identify the known parameters in some fashion.
5.	Select a basis.
6.	Make a list by symbols for each of the unknown values of the stream flows and compositions, or at least mark them distinctly in some fashion, and count them.
7.	Write down the names of an appropriate set of balances to solve; write the balances down with type of balance listed by each one. Do not forget the implicit balances for mass or mole fractions.
8.	Count the number of independent balances that can be written; ascertain that a unique solution is possible. If not, look for more information or check your assumptions.
9.	Solve the equations. Each calculation must be made on a consistent basis.
10.	Check your answers by introducing them, or some of them, into any redundant material balances. Are the equations satisfied? Are the answers reasonable?

Distillation Unit:



Vapor

Cooling Water

Feed F = *1000 kg*

10 % EtOH

90 % H_2O

Reflux

Distillate $D = 0.1 \cdot F$

60 % EtOH

40 % H_2O

Heat

Bottoms (Waste) B = kg

EtOH = ?

H_2O = ?

System Boundary

Task:

Calculate composition of bottoms and mass of lost alcohol

Steps 1–3: Symbols and data placed in flow sheet

Step 4: Evaluate $D = 0.1 \cdot F = 100$ *kg*

Step 5: Select as the basis the given feed F = *1000 kg*

Steps 6–8: The remaining unknowns are $w_{EtOH,B}$, $w_{H2O,B}$ and B.
Two components exist, yielding two independent component mass balances, and $w_{EtOH,B} + w_{H2O,B} = 1$, so that the problem has a unique solution.

Step 9: The total mass balance yields:
$B = F - D = 100$ *kg*

The solution for the composition of the bottoms can be computed directly by subtraction:

	kg in Feed	kg Distillate out	kg Bottoms	percent
EtOH	*0.1·1000*	*– 0.6 ·100*	= 40	4.4
H_2O	*0.9 ·1000*	*– 0.4·100*	= 860	95.6
			900	100.0

Material Balance Problem Involving Chemical Reactions

$$\left\{\begin{matrix}\text{accumulation}\\ \text{within the}\\ \text{system}\end{matrix}\right\} = \left\{\begin{matrix}\text{input through}\\ \text{system}\\ \text{boundaries}\end{matrix}\right\} - \left\{\begin{matrix}\text{output through}\\ \text{system}\\ \text{boundaries}\end{matrix}\right\}$$

$$+\left\{\begin{matrix}\text{generation}\\ \text{within the}\\ \text{system}\end{matrix}\right\} - \left\{\begin{matrix}\text{consumption}\\ \text{within the}\\ \text{system}\end{matrix}\right\}$$

Combustion of Coal:

- Steady state
- Coal elemental composition is given
- Moisture content of the coal is 3.9 %
- Moisture content of the air is 0.0048 lb H_2O/lb dry air
- Stack gas analysis is given on a dry basis
- Refuse shows 14 % unburned coal with the remainder being ash

Tasks:

Check data for consistency

Determine the average percentage excess air used

Coal Composition

	%
C	83.05
H	4.45
O	3.36
N	1.08
S	0.7
Ash	7.36
	100

Gas Composition

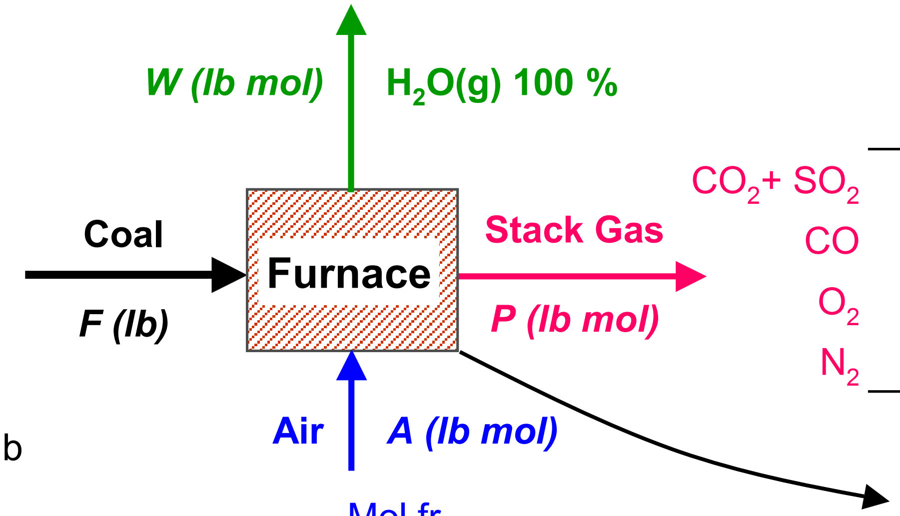
	%
CO_2+ SO_2	15.4
CO	0.0
O_2	4.0
N_2	80.6
	100

Refuse Composition

	%
C+H+O+N+S	14.0
Ash	86.0
	100

Unit 1 Material Balances

Steps 1– 4:



	lb
C	83.05
H	4.45
O	3.36
N	1.08
S	0.7
Ash	7.36
	100

Added H_2O 3.9 lb

Coal

F (lb)

Furnace

W (lb mol) **H_2O(g) 100 %**

Stack Gas

P (lb mol)

	%
CO_2+ SO_2	15.4
CO	0.0
O_2	4.0
N_2	80.6
	100

Air ***A (lb mol)***

	Mol fr
N_2	0.79
O_2	0.21
	100

Added H_2O 0.0048 lb/lb Air

Refuse *R (lb)*

	%
C+H+N+O+S	14.0
Ash	86.0
	100

Step 5: Pick a basis of *F = 100 lb* as convenient.

Unit 1 Material Balances

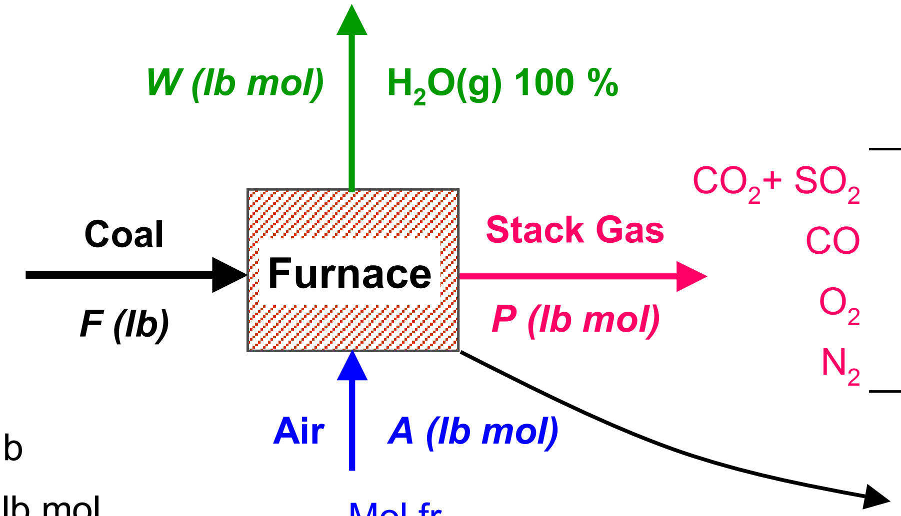
3.9 lb H_2O	1 lb mol H_2O	2 lb mol H	= 0.433 lb mol H
	18 lb H_2O	1 lb mol H_2O	

Steps 1– 4:

	lb
C	83.05
H	4.45
O	3.36
N	1.08
S	0.7
Ash	7.36
	100

Added H_2O 3.9 lb

Containing { H: 0.433 lb mol
O: 0.217 lb mol



	%
CO_2+ SO_2	15.4
CO	0.0
O_2	4.0
N_2	80.6
	100

	Mol fr
N_2	0.79
O_2	0.21
	100

Refuse *R (lb)*

	%
C+H+N+O+S	14.0
Ash	86.0
	100

Added H_2O 0.0048 lb/lb Air

Containing { H: 0.0154 lb mol/mol A
O: 0.0077 lb mol/mol A

Step 5: Pick a basis of *F = 100 lb* as convenient.

Step 6: *A, W, P, R* remain unknown. Mass balance on the elements in lb mol.

0.0048 lb H_2O	29 lb air	1 lb mol H_2O	= 0.0077	lb mol H_2O
lb air	1 lb mol air	18 lb H_2O		lb mol air

Unit 1 Material Balances

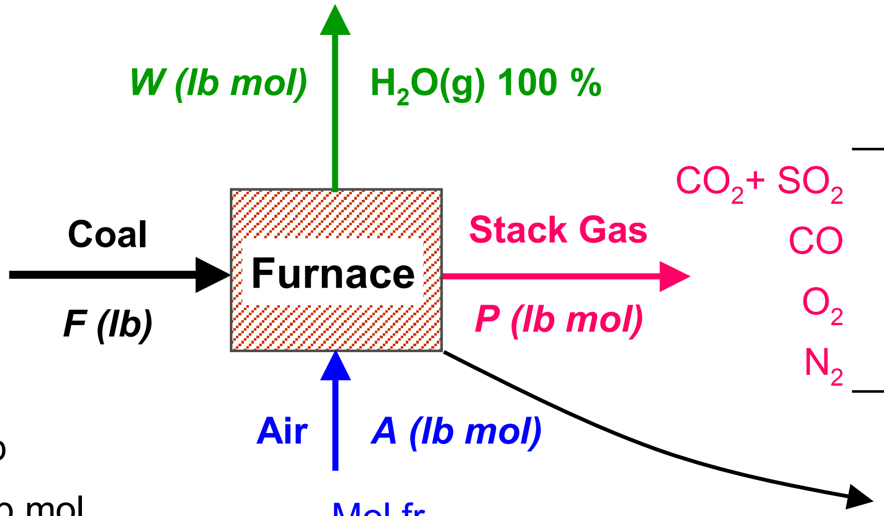
3.9 lb H_2O	1 lb mol H_2O	2 lb mol H	= 0.433 lb mol H
	18 lb H_2O	1 lb mol H_2O	

Steps 1– 4:

	lb
C	83.05
H	4.45
O	3.36
N	1.08
S	0.7
Ash	7.36
	100

Added H_2O 3.9 lb

Containing { H: 0.433 lb mol
O: 0.217 lb mol



	%
CO_2+ SO_2	15.4
CO	0.0
O_2	4.0
N_2	80.6
	100

	Mol fr
N_2	0.79
O_2	0.21
	100

Added H_2O 0.0048 lb/lb Air

Containing { H: 0.0154 lb mol/mol A
O: 0.0077 lb mol/mol A

Refuse *R (lb)*

	%
C+H+N+O+S	14.0
Ash	86.0
	100

Step 5: Pick a basis of *F = 100 lb* as convenient.

Step 6: *A, W, P, R* remain unknown. Mass balance on the elements in lb mol.

0.0048 lb H_2O	29 lb air	1 lb mol H_2O	= 0.0077	lb mol H_2O
lb air	1 lb mol air	18 lb H_2O		lb mol air

Ash Material Balance

7.36 lb = R·0.86

→ *R = 8.56 lb*

Unit 1 Material Balances

C, H, O, N, S in **unburned coal** (assumption: proportions may not change)

Mass of unburned coal: $0.14 \cdot R = 1.2\ lb$

Component	**Mass %***	**lb**	**lb mol**
C	89.65	1.076	0.0897
H	4.8	0.058	0.0537
O	3.63	0.0436	0.0027
N	1.17	0.014	0.0010
S	0.76	0.009	0.0003
	100.00	1.20	0.1474
*on an ash-free basis			

Step 6 (repeated): *A, W, P* remain unknown. Only four mole balances on the elements can be written, because S + C must be combined as these elements are linked in the stack gas analysis (SO_2 + CO_2).

		Input			*Output*		
		F	*A*		*W*	*P*	*R*
1.	C+ S	$83.05/12 + 0.70/32$	$+ 0$	=	0	$+ 0.154 \cdot P$	$+ 0.0897 + 0.0003$
3.	H	$4.45/1.008 + 0.433$	$+ 0.0154 \cdot A$	=	$2 \cdot W$	$+ 0$	$+ 0.0537$
Test	O	$3.36/16 + 0.217$	$+ 0.21 \cdot 2 \cdot A + 0.0077 \cdot A$	=	W	$+ 2 \cdot (0.154+0.04) \cdot P$	$+ 0.0027$
2.	N	$1.08/14$	$+ 2 \cdot 0.79 \cdot A$	=	0	$+ 2 \cdot 0.806 \cdot P$	$+ 2 \cdot 0.001$

$C+S \rightarrow P = 50\ lb\ mol$ $N \rightarrow A = 45.35\ lb\ mol$ $H \rightarrow W = 2.746\ lb\ mol$ $O \rightarrow 19.8 \approx 20$

Average percentage excess air:

$$\% \text{ excess air } = 100 \times \frac{O_2 \text{ entering} - O_2 \text{ required}}{O_2 \text{ required}}$$

O_2 required is calculated from reaction stoichiometry:

Component	Reaction	lb	lb mol	Required O_2 (lb mol)
C	$C + O_2 \rightarrow CO_2$	83.05	6.921	6.921
H	$H_2 + 0.5\ O_2 \rightarrow H_2O$	4.45	4.415	1.104
O	-	3.36	0.210	-0.105
N	-	1.08	0.077	-
S	$S + O_2 \rightarrow SO_2$	0.70	0.022	0.022
				7.942

O_2 coming with the coal !

O_2 entering with the air: 45.35 lb mol × 0.21 = 9.524 lb mol.

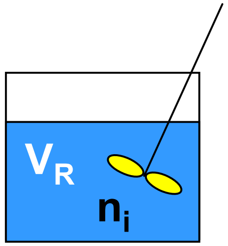
$$\% \text{ excess air } = 100 \times \frac{9.524 - 7.942}{7.942} = 19.9\%$$

Unit 1 Basic definitions

Extent of Reaction, Reaction Rate and Fractional Conversion in Single Reactions:

stoichiometric coefficients

Batch Reactor:



Reaction: $$|\nu_A|A+|\nu_B|B \rightarrow |\nu_C|C+|\nu_D|D$$

Molar extent: $$\xi=\frac{n_A-n_A^0}{\nu_A}\ [\mathrm{kmol}] \Rightarrow n_A=n_A^0+\nu_A\xi$$

if there is no volume change due to the reaction you better divide by the volume of the reaction mixture and work with concentrations

$$\lambda=\frac{\xi}{V_R}\left[\frac{\mathrm{kmol}}{\mathrm{m}^3}\right] \Rightarrow c_A=c_A^0+\nu_A\lambda$$

Rate of Consumption: $$R_A=-\boxed{r_A}=-\frac{1}{V_R}\frac{dn_A}{dt}\left[\frac{\mathrm{kmol}}{\mathrm{m}^3\mathrm{s}}\right]$$

Rate of Reaction:

ν_A = -1

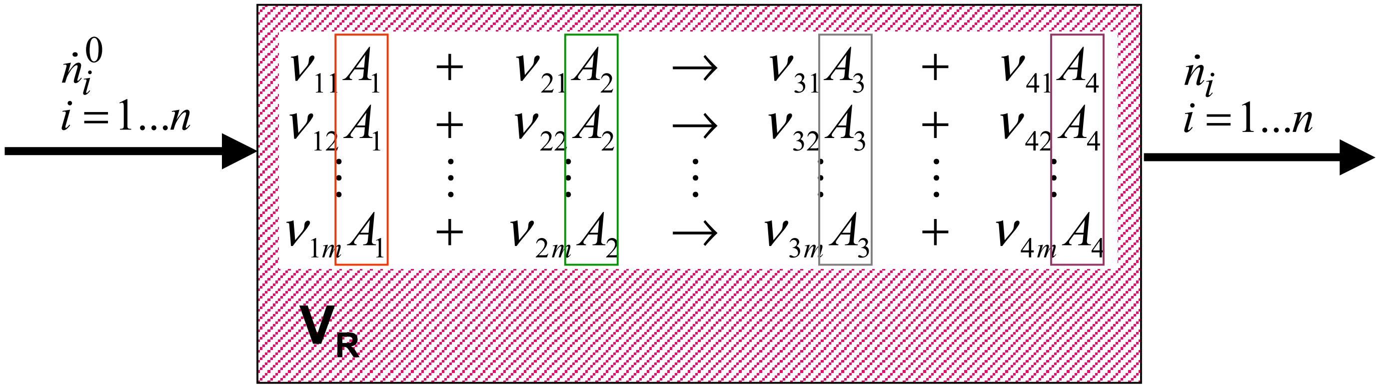
Fractional Conversion of *A*: $$X_A=\frac{n_A^0-n_A}{n_A^0}=1-\frac{n_A}{n_A^0}=-\frac{\overbrace{\nu_A\xi}^{\boxed{f_A}}}{n_A^0}\ [-]$$

Remaining fraction of A

$$=1-\frac{c_A}{c_A^0}=-\frac{\nu_A\lambda}{c_A^0}\ [-]$$ for V_R=const.

Unit 1 Basic definitions

Rate of Consumption/Formation, Yield and Selectivity in Multiple Reactions:



$\dot{n}_i^0$
$i = 1 \ldots n$

$$\begin{array}{ccccccc}
\nu_{11}A_1 & + & \nu_{21}A_2 & \rightarrow & \nu_{31}A_3 & + & \nu_{41}A_4 \\
\nu_{12}A_1 & + & \nu_{22}A_2 & \rightarrow & \nu_{32}A_3 & + & \nu_{42}A_4 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\nu_{1m}A_1 & + & \nu_{2m}A_2 & \rightarrow & \nu_{3m}A_3 & + & \nu_{4m}A_4
\end{array}$$

V_R

$\dot{n}_i$
$i = 1 \ldots n$

$$\dot{n}_A = \dot{n}_A^0 + V_R \sum_{j=1}^{m} \nu_{Aj} \xi_j$$

Matrix Form: $\dot{\mathbf{n}} = \dot{\mathbf{n}}_0 + V_R \boldsymbol{\nu} \boldsymbol{\xi}$

$$c_A = c_A^0 + \sum_{j=1}^{m} \nu_{Aj} \lambda_j$$

for V_R=const.

$\mathbf{c} = \mathbf{c}_0 + \boldsymbol{\nu} \boldsymbol{\lambda}$

Rate of Consumption/Formation: $R_i = \sum_{j=1}^{m} \nu_{ij} r_j \quad \left[\frac{\text{kmol}}{\text{m}^3\text{s}} \right]$

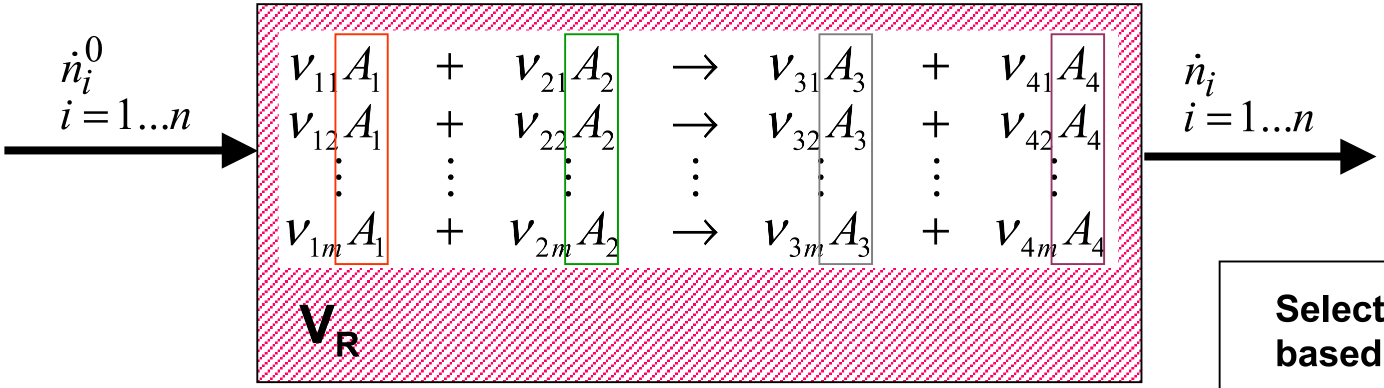
stoichiometric coefficient of compound i in reaction j

Fractional Conversion of A:

$$X_A = \frac{\dot{n}_A^0 - \dot{n}_A}{\dot{n}_A^0} = 1 - \frac{\dot{n}_A}{\dot{n}_A^0}$$

Same definition, but more than one reaction contribute to the consumption of A.

Rate of Consumption/Formation, Yield and Selectivity in Multiple Reactions:



$$\begin{array}{ccccccc} \nu_{11} A_1 & + & \nu_{21} A_2 & \rightarrow & \nu_{31} A_3 & + & \nu_{41} A_4 \\ \nu_{12} A_1 & + & \nu_{22} A_2 & \rightarrow & \nu_{32} A_3 & + & \nu_{42} A_4 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \nu_{1m} A_1 & + & \nu_{2m} A_2 & \rightarrow & \nu_{3m} A_3 & + & \nu_{4m} A_4 \end{array}$$

Yield of Product P based on consumption of A:

$$Y_{P,A} = \frac{P \text{ formed} - P \text{ supplied with feed}}{A \text{ supplied with feed}} \times \left(\begin{array}{c} \text{moles of P formed} \\ \text{when all moles of A} \\ \text{are converted to P} \end{array} \right)$$

$$Y_{P,A} = \frac{\dot{n}_P - \dot{n}_P^0}{\dot{n}_A^0} \times \frac{\beta_{A,ref}}{\beta_{P,ref}}$$

Stoichiometric ratio between A and P based on a common reference, e.g. an atomic species

(**β** = matrix of chemical compounds vs. atomic species)

Selectivity to product P based on reactant A:

$$S_{PA} = \frac{Y_{PA}}{X_A} \quad [-]$$

Differential selectivity:

$$s_{PA} = \frac{R_P}{-R_A} = \frac{\sum_{j=1}^{m} \nu_{Pj} r_j}{\sum_{j=1}^{m} \nu_{Aj} r_j} \quad [-]$$

Unit 1 Basic definitions

Example:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$CH_4 + CO_2 \rightarrow CO + 2H_2$$

$$\beta = \begin{array}{c|cccccc} & \text{reactants} & & & & \text{product} & \\ & CH_4 & O_2 & CO_2 & H_2O & CO & H_2 \\ \hline C & 1 & 0 & 1 & 0 & 1 & 0 \\ H & 4 & 0 & 0 & 2 & 0 & 2 \\ O & 0 & 2 & 2 & 1 & 1 & 0 \end{array}$$

Yield of CO either based on CH_4 or on O_2:

$$\underbrace{Y_{CO,CH_4}}_{\text{common basis for comparison}} = \frac{\dot{n}_{CO} - \dot{n}_{CO}^0}{\dot{n}_{CH_4}^0} \times \underbrace{\frac{\beta_{CO,C}}{\beta_{CH_4,C}}}_{1}$$

how many moles (or kg*) product do I get from one mole (or kg*) reactant ?

$$Y_{CO,O_2} = \frac{\dot{n}_{CO} - \dot{n}_{CO}^0}{\dot{n}_{O_2}^0} \times \overbrace{\frac{\beta_{CO,O}}{\beta_{O_2,O}}}^{0.5}$$

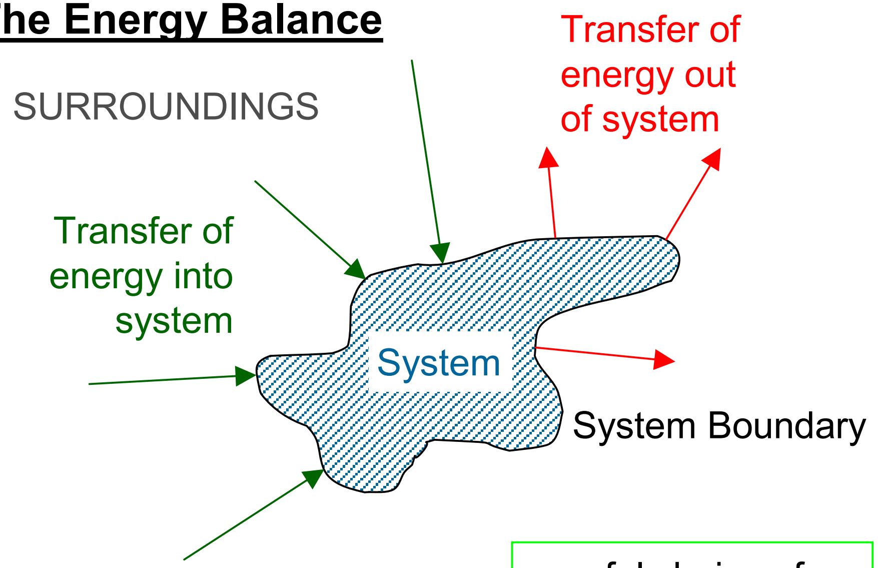
ATTENTION

The definitions based on moles – as given here – is convenient for most applications in chemical reaction engineering, but an analogeous definition of extent of reaction, reaction rate, rate of formation/consumption, conversion, yield and selectivity *based on mass** is used frequently as well.

Sometimes even *mixed definitions*, e.g. moles produced per mass of feed.

Unit 1 Energy Balances

1. The Energy Balance



careful choice of system boundary !

General Principle:

Conservation of total energy

In words:

$$\left\{\begin{matrix}\text{accumulation}\\ \text{of energy}\\ \text{within the}\\ \text{system}\end{matrix}\right\} = \left\{\begin{matrix}\text{transfer of energy}\\ \text{into system}\\ \text{through system}\\ \text{boundary}\end{matrix}\right\} - \left\{\begin{matrix}\text{transfer of energy}\\ \text{out of system}\\ \text{through system}\\ \text{boundary}\end{matrix}\right\}$$

$$+\left\{\begin{matrix}\text{energy}\\ \text{generation}\\ \text{within the}\\ \text{system}\end{matrix}\right\} - \left\{\begin{matrix}\text{energy}\\ \text{consumption}\\ \text{within the}\\ \text{system}\end{matrix}\right\}$$

Six Types of Energy		
Type	**Symbol**	**Function**
Work	$W = \int F\cdot ds$ [kJ]	Path
Heat	$Q = k\cdot A\cdot \Delta T$ [kJ]	Path
Kinetic Energy	$K = \frac{1}{2}\cdot m\cdot v^2$ [kJ]	State
Potential Energy	$P = m\cdot g\cdot h$ [kJ}	State
Internal Energy	$\hat{U} = \hat{U}(T,p)$ [kJ/kg]	State
Enthalpy	$\hat{H} = \hat{U} + p\cdot\hat{V} = \hat{H}(T,p)$ [kJ/kg]	State

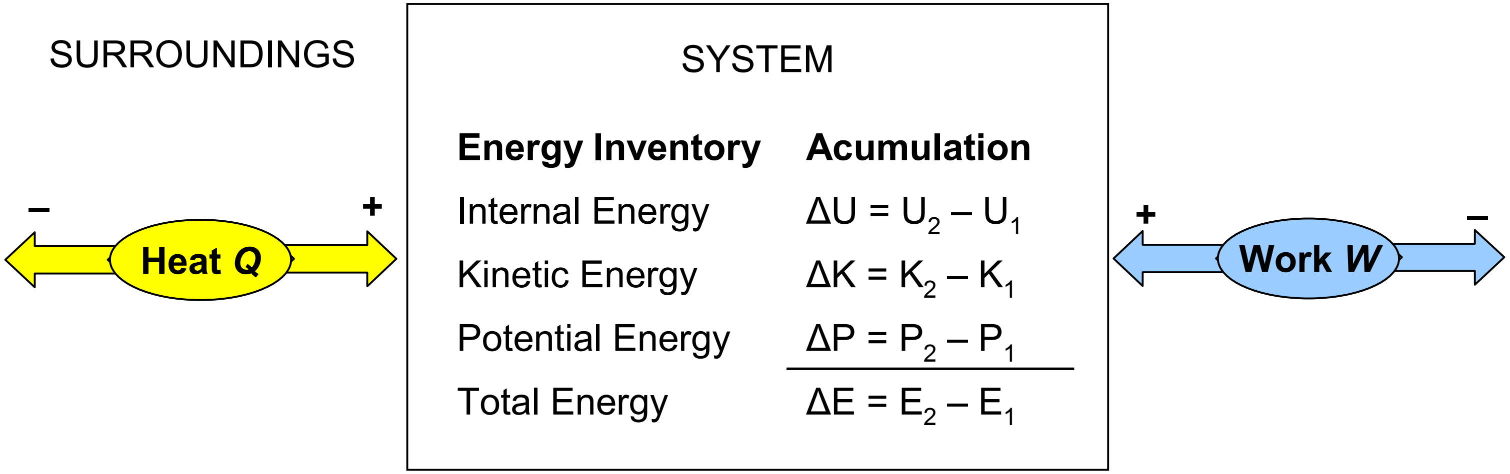
Task:

Find mathematical expressions for these terms that accurately describe the particular situation

Solve the resulting system of equations (linear, nonlinear)

Unit 1 Energy Balances

1. Closed System (without Chemical Reactions)

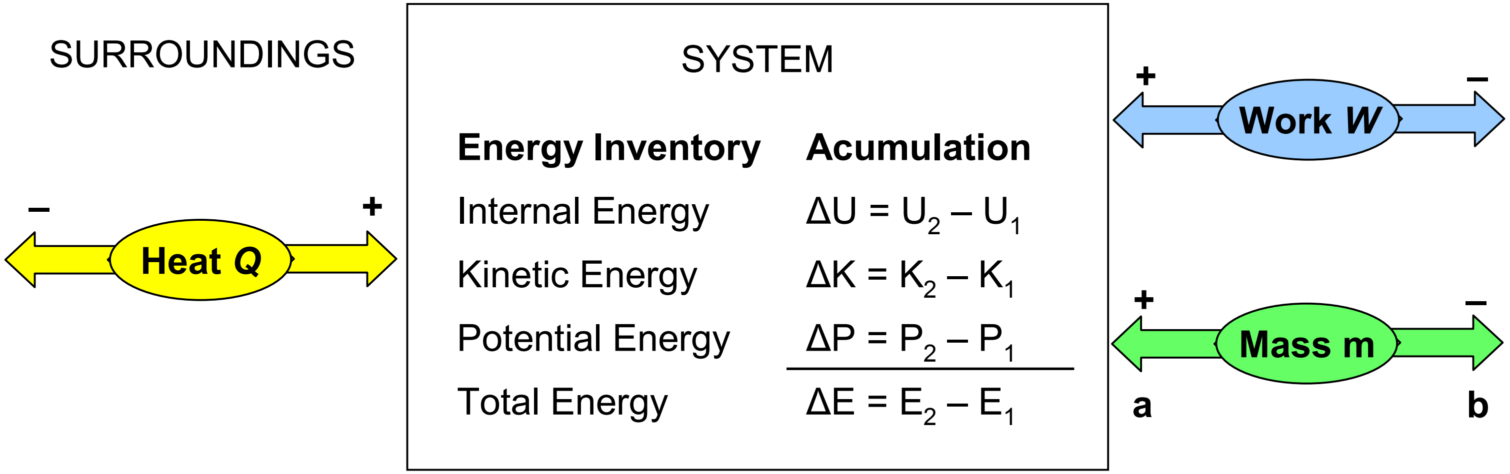


Energy Inventory	**Acumulation**
Internal Energy	$\Delta U = U_2 - U_1$
Kinetic Energy	$\Delta K = K_2 - K_1$
Potential Energy	$\Delta P = P_2 - P_1$
Total Energy	$\Delta E = E_2 - E_1$

Energy Balance:

$$\boxed{\Delta E = E(t_2) - E(t_1) = \Delta U + \Delta P + \Delta K = Q + W}$$

2. Open System (without Chemical Reactions)



Energy Inventory	**Acumulation**
Internal Energy	$\Delta U = U_2 - U_1$
Kinetic Energy	$\Delta K = K_2 - K_1$
Potential Energy	$\Delta P = P_2 - P_1$
Total Energy	$\Delta E = E_2 - E_1$

Energy Balance:

$$\Delta E = E(t_2) - E(t_1) = \left(\hat{U}_2 + \hat{K}_2 + \hat{P}_2\right)m_2 - \left(\hat{U}_1 + \hat{K}_1 + \hat{P}_1\right)m_1$$

$$= \left(\hat{U}_a + \hat{K}_a + \hat{P}_a\right)m_a - \left(\hat{U}_b + \hat{K}_b + \hat{P}_b\right)m_b + Q + W + p_a\hat{V}_a m_a - p_b\hat{V}_b m_b$$

Energy transfer due to mass tranport

Work performed to transfer mass (Volume Work)

net heat input to system

net work done on system by surroundings

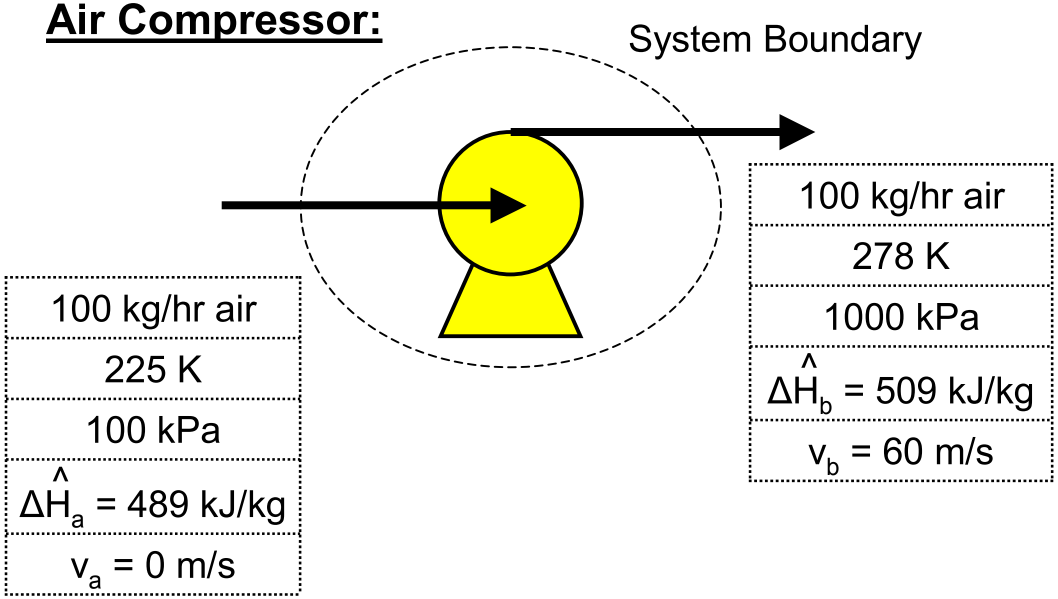
$$\boxed{\Delta E = E(t_2) - E(t_1) = Q + W - \Delta[H + K + P]}$$

Δ means „t_2 vs. t_1“ **Δ means „a minus b“**

Summary of the Symbols to be Used in the General Energy Balance

Accumulation term				
Type of Energy	At time t_1		At time t_2	
Internal	U_1	$E(t_1)$	U_2	$E(t_2)$
Kinetic	K_1		K_2	
Potential	P_1		P_2	
Mass	m_1		m_2	
Energy accompanying mass transport				
Type of Energy	Transport in		Transport out	
Internal	$U_a = \hat{U} \cdot m_a$		$U_b = \hat{U} \cdot m_b$	
Kinetic	$K_a = \hat{K} \cdot m_a$		$K_b = \hat{K} \cdot m_b$	
Potential	$P_a = \hat{P} \cdot m_a$		$P_b = \hat{P} \cdot m_b$	
Net heat input to system	Q			
Net work done on system by surroundings	W			
Work to introduce material into system, or work recovered on removing material from system	$m_a(p_a\hat{V}_a)$		$-m_b(p_b\hat{V}_b)$	

Air Compressor:



100 kg/hr air
225 K
100 kPa
$\Delta\hat{H}_a = 489$ kJ/kg
$v_a = 0$ m/s

100 kg/hr air
278 K
1000 kPa
$\Delta\hat{H}_b = 509$ kJ/kg
$v_b = 60$ m/s

Task:

determine the required power in kW for the compressor

Steps 1 – 4: Steady state flow process (open system) without chemical reactions. Available data and unknowns listed.

Step 5: Basis 100 kg/hr of air

Steps 6 – 7: Simplification of the general energy balance.

$$\Delta E = E(t_2) - E(t_1) = Q + W - \Delta[H + K + P]$$

(1) The process is at steady state, hence $\Delta E = 0$.
(2) $m_a = m_b = m$.
(3) Potential Energy is not changed: $\Delta P = 0$.
(4) $Q = 0$ by assumption (insulation).
(5) $v_a = 0$ by assumption (unknown but will be small)

Result: $0 = W - \Delta H - \Delta K$

Steps 6 (repeated): We have one equation and one unknown W (ΔH and ΔK can be calculated), hence a unique solution exists.

Steps 7 – 9: Calculate the solution.

$$\Delta H = \frac{(509-489)\ \text{kJ}}{\text{kg}} \Big| \, 100\ \text{kg} = 2000\ \text{kJ}$$

$$\Delta K = \tfrac{1}{2}\, m(v_b^2 - v_a^2) = 50\ \text{kg} \times 3600\ (\text{m/s})^2$$
$$= 180\ \text{kJ}$$

$W = 2180$ kJ

Required Power :

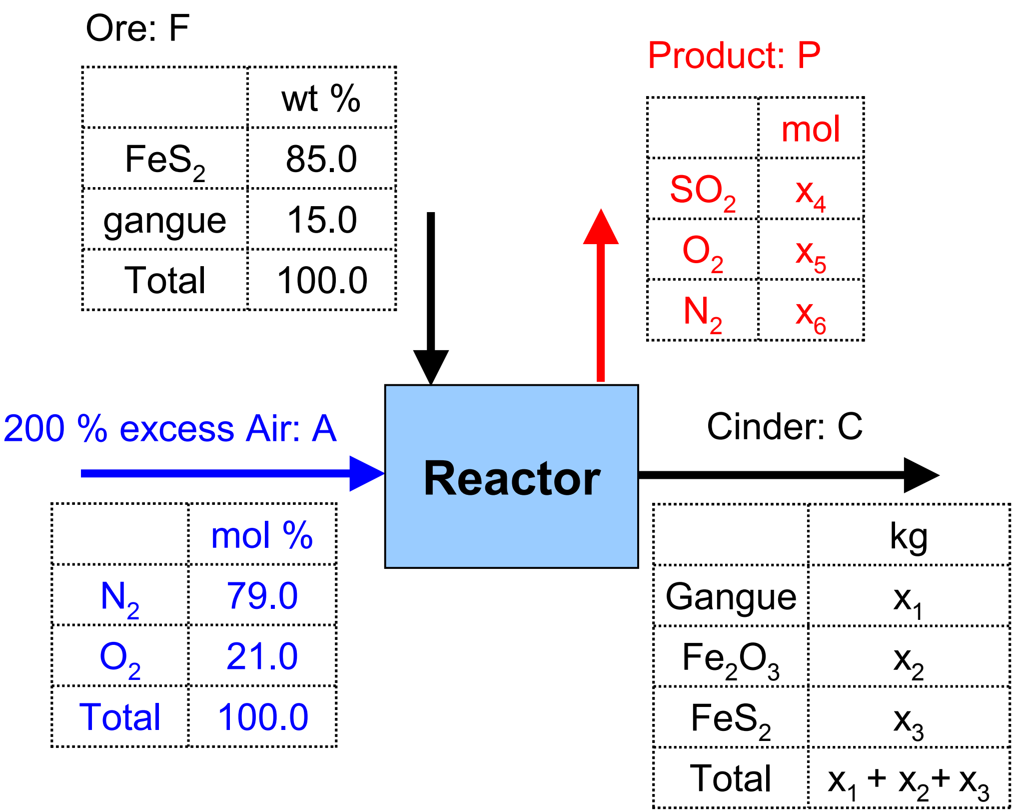
2180 kJ / 3600 s = 0.61 kW

Roasting of Iron Ore:

An iron pyrite ore containing 85 % FeS_2 and 15 % inert dirt, rock, etc. (gangue) is roasted with an amount of air equal to 200 % excess air according to the reaction:

$$4\ FeS_2 + 11\ O_2 \rightarrow 2\ Fe_2O_3 + 8\ SO_2$$

In order to produce SO_2. All the gangue plus the Fe_2O_3 end up in the solid waste product (cinder), which analyses 4% FeS_2.



Ore: F

	wt %
FeS_2	85.0
gangue	15.0
Total	100.0

Product: P

	mol
SO_2	x_4
O_2	x_5
N_2	x_6

200 % excess Air: A

	mol %
N_2	79.0
O_2	21.0
Total	100.0

Cinder: C

	kg
Gangue	x_1
Fe_2O_3	x_2
FeS_2	x_3
Total	$x_1 + x_2 + x_3$

Task:

Determine the heat transferred per kg of ore to keep the product stream at 25°C if the entering streams are at 25°C

Material balance:

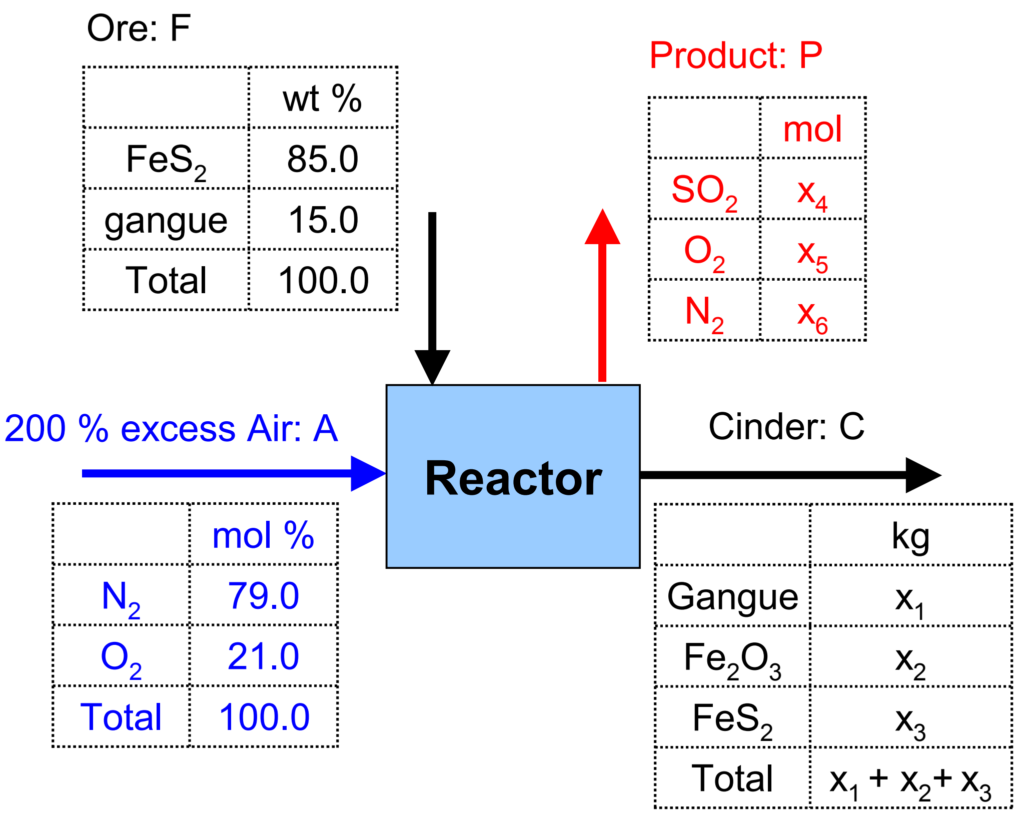
Steps 1 – 4: Steady state flow process (open system) with reaction. The system is the reactor. Available data and unknowns listed.

Step 5: Basis 100 kg of pyrite ore.

Step 6: Six unknowns exist. We can write 5 component mass balances (O, N, S, gangue, and Fe). With the information on FeS_2 in the gangue six equations are available, hence the problem should have a unique solution.

continue exact way ▶

Roasting of Iron Ore:



Ore: F

	wt %
FeS_2	85.0
gangue	15.0
Total	100.0

Product: P

	mol
SO_2	x_4
O_2	x_5
N_2	x_6

200 % excess Air: A

	mol %
N_2	79.0
O_2	21.0
Total	100.0

Cinder: C

	kg
Gangue	x_1
Fe_2O_3	x_2
FeS_2	x_3
Total	$x_1 + x_2 + x_3$

The excess air is calculated based on the stated reaction as if all the FeS_2 reacted to Fe_2O_3 even though some FeS_2 will not.

Required O_2:

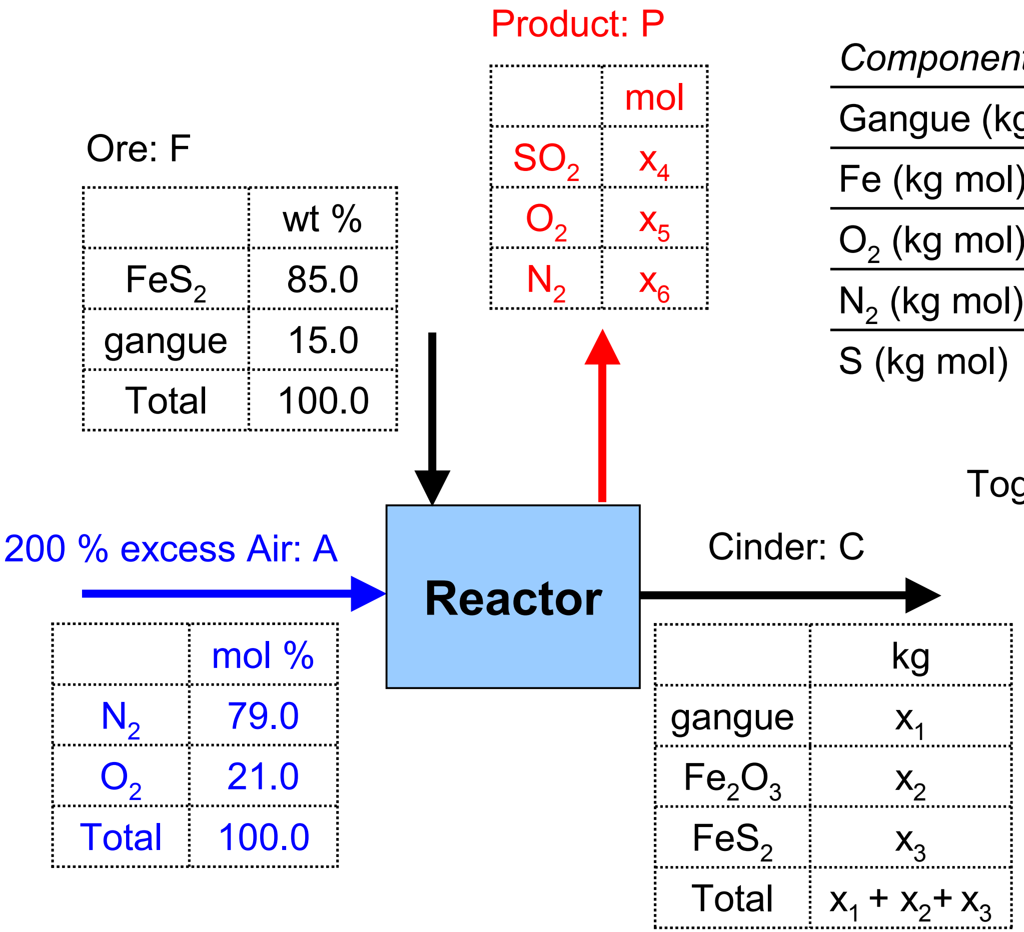
0.85·100/120·11/4 = 1.9479 kg mol

Excess O_2: 2·1.9479 = <u>3.8958 kg mol</u>

Total O_2: 5.8438 kg mol

Total N_2: 5.8438·21/79 = 21.983 kg mol

Roasting of Iron Ore:



Product: P

	mol
SO_2	x_4
O_2	x_5
N_2	x_6

Ore: F

	wt %
FeS_2	85.0
gangue	15.0
Total	100.0

200 % excess Air: A

	mol %
N_2	79.0
O_2	21.0
Total	100.0

Cinder: C

	kg
gangue	x_1
Fe_2O_3	x_2
FeS_2	x_3
Total	$x_1 + x_2 + x_3$

Step 7 – 9: The component mass balances are:

Component	*In*	*Out*
Gangue (kg)	15.0	x_1
Fe (kg mol)	0.85·100/120	$2 \cdot x_2/159.7 + x_3/120$
O_2 (kg mol)	5.8437	$x_4 + x_5 + 1.5 \cdot x_2/159.7$
N_2 (kg mol)	21.983	x6
S (kg mol)	0.85·100/120·2	$x_4 + 2 \cdot x_3/120$

Together with $$0.04 = \frac{x_3}{15 + x_2 + x_3}$$

the solution is:

C	x_1	15.0 kg
	x_2	54.63 kg mol
	x_3	2.90 kg mol
P	x_4	1.368 kg mol
	x_5	3.938 kg mol
	x_6	21.938 kg mol

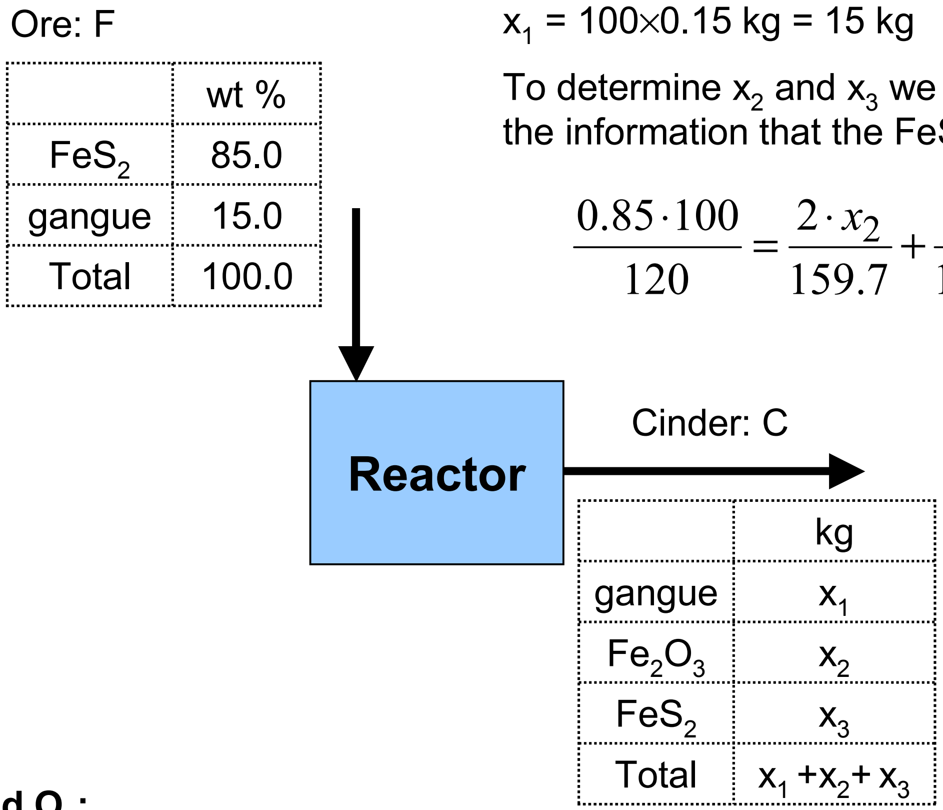
Energy Balance:

With ΔE = 0, ΔK = 0, ΔP = 0 and W = 0, the general energy balance

$\Delta E = E(t_2) - E(t_1) = Q + W - \Delta[H + K + P]$ reduces to: $Q = \Delta H$

skip exact way ▶

Roasting of Iron Ore:



Ore: F

	wt %
FeS_2	85.0
gangue	15.0
Total	100.0

Cinder: C

	kg
gangue	x_1
Fe_2O_3	x_2
FeS_2	x_3
Total	$x_1 + x_2 + x_3$

Steps 7 – 9: Gangue goes completely to Cinder, hence:

$x_1 = 100 \times 0.15$ kg = 15 kg

To determine x_2 and x_3 we use the Fe component mass balance and the information that the FeS_2 content in C is 4%.

$$\frac{0.85 \cdot 100}{120} = \frac{2 \cdot x_2}{159.7} + \frac{x_3}{120} \qquad 0.04 = \frac{x_3}{15 + x_2 + x_3}$$

The equations can be solved easily by substitution, which gives:

$x_2 = 57.7455$ kg

$x_3 = 3.0311$ kg

Step 6 (repeated): We have 3 unknowns left and 3 component mass balances.

The excess air is calculated from the stated reaction while taking into account that not all the FeS_2 will react to Fe_2O_3.

Required O_2:

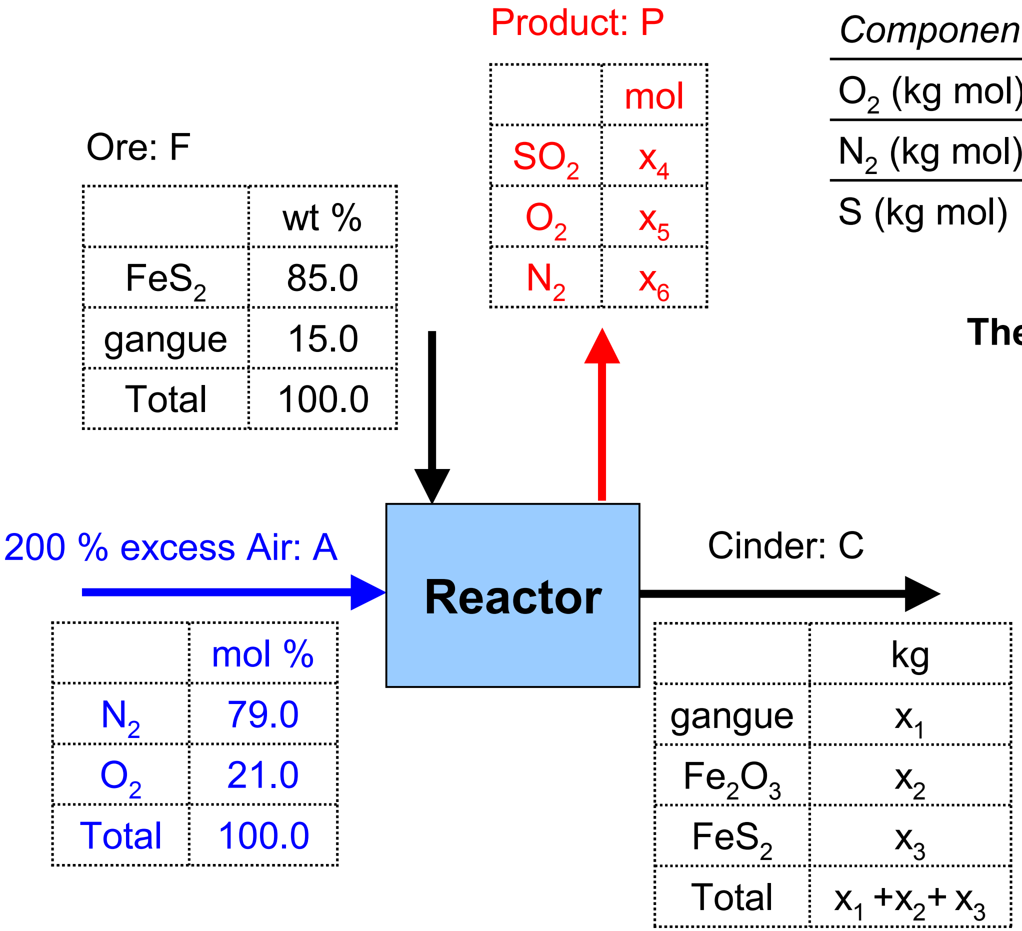
(0.85·100 – 3.0311)/120·11/4 = 1.8785 kg mol

Excess O_2: 2·1.8785 = <u>3.7569 kg mol</u>

Total O_2: 5.6354 kg mol

Total N_2: 5.7023·0.21/0.79 = 21.200 kg mol

Roasting of Iron Ore:



Product: P

	mol
SO_2	x_4
O_2	x_5
N_2	x_6

Ore: F

	wt %
FeS_2	85.0
gangue	15.0
Total	100.0

200 % excess Air: A

	mol %
N_2	79.0
O_2	21.0
Total	100.0

Cinder: C

	kg
gangue	x_1
Fe_2O_3	x_2
FeS_2	x_3
Total	$x_1 + x_2 + x_3$

Step 7 – 9: The component mass balances are:

Component	*In*	*Out*
O_2 (kg mol)	5.6354	$x_4 + x_5 + 1.5 \cdot 57.7445/159.7$
N_2 (kg mol)	21.200	x_6
S (kg mol)	$0.85 \cdot 100/120 \cdot 2$	$x_4 + 3.0311/120 \cdot 2$

The solution is:

	kg mol
x_4	1.3661
x_5	3.7269
x_6	21.200

Energy Balance:

Since $\Delta E = 0$, $\Delta K = 0$, $\Delta P = 0$ and $W = 0$, the general energy balance

$$\Delta E = E(t_2) - E(t_1) = Q + W - \Delta[H + K + P]$$

reduces to: $Q = \Delta H$

Reactants and products are at the same temperature and pressure of 25°C and 1 atm. Hence this is chosen as reference state, so that the temperature dependent term becomes zero.

$$\Delta\hat{H}_{\text{mixture}} = \left(\sum_{\text{i}} n_i \Delta\hat{H}^0_{fi} + \cancel{\sum_{\text{i}} \int_{T_{ref}}^{T} n_i c_{p,i}\,dT}\right) \Longrightarrow Q = \sum_{\text{products}} n_i \Delta\hat{H}^0_{fi} - \sum_{\text{reactants}} n_i \Delta\hat{H}^0_{fi}$$

	Products			**Reactants**		
Component	$10^{-3} \times$ g mol	ΔH_f^0 kJ/g mol	$n_i \Delta H_f^0$ kJ	$10^{-3} \times$ g mol	ΔH_f^0 kJ/g mol	$n_i \Delta H_f^0$ kJ
FeS_2	0.0253	-177.9	-4.494	0.7083	-177.9	-126.007
Fe_2O_3	0.3616	-822.156	-297.281	0	-822.156	0
N_2	21.200	0	0	21.200	0	0
O_2	3.7269	0	0	5.6354	0	0
SO_2	1.3661	-296.60	-405.185	0	-296.90	0
		Total	**-706.96**		**Total**	**-126.007**

Result:

Q = [–706.96 – (–126.007)] × 10^3 = –580.953 × 10^3 kJ / 100 kg ore = –5.801 × 10^3 kJ/kg ore

The negative sign indicates that heat is removed from the process.

Unit 1 Final Word

Many more instructive examples are contained in the book by D.M. Himmelblau (Basic Principles and Caculations in Chemical Engineering), which is an excellent textbook for self-instruction.

The last wisdom:

Take care of your units and they will take care of you !