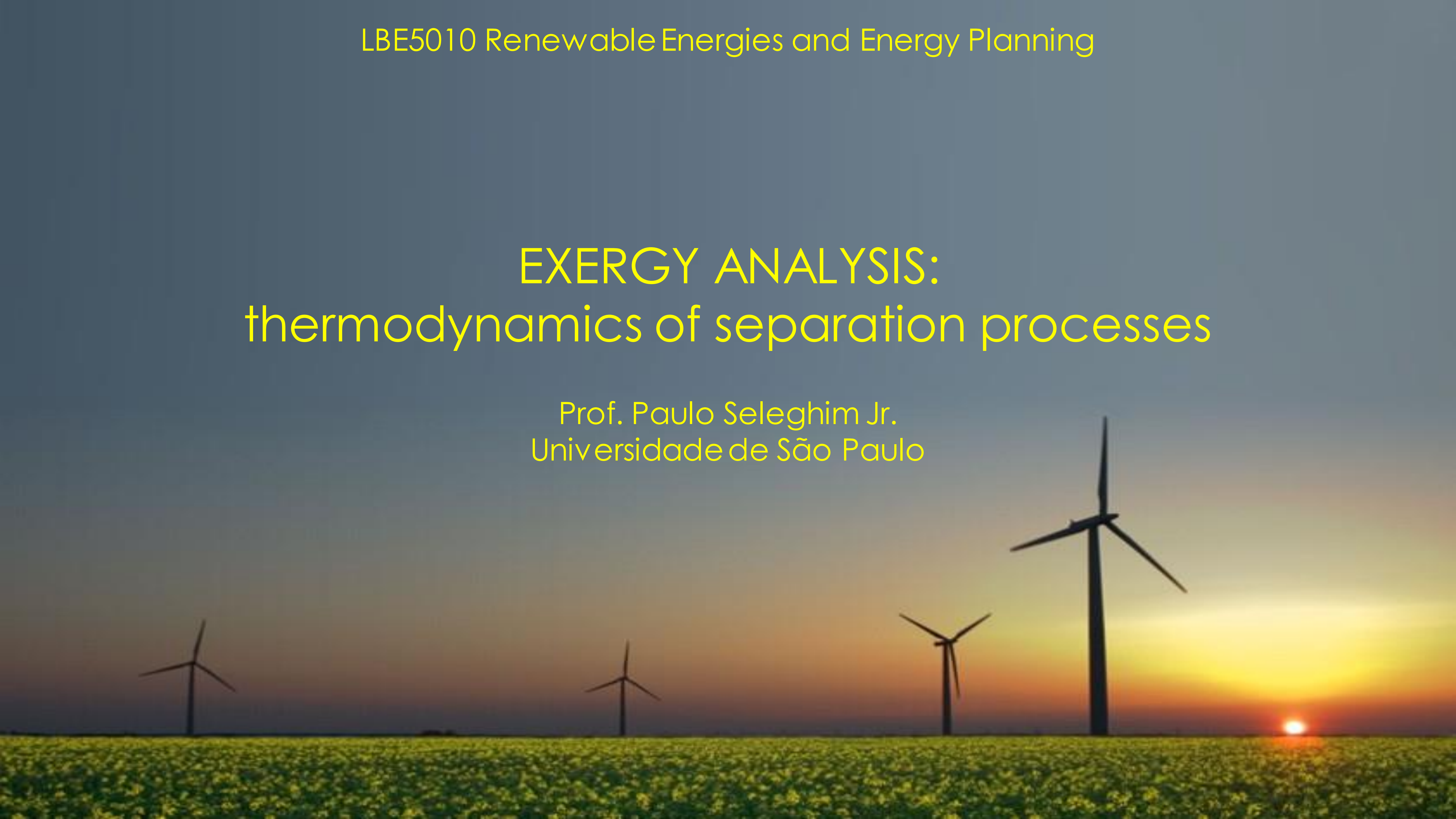
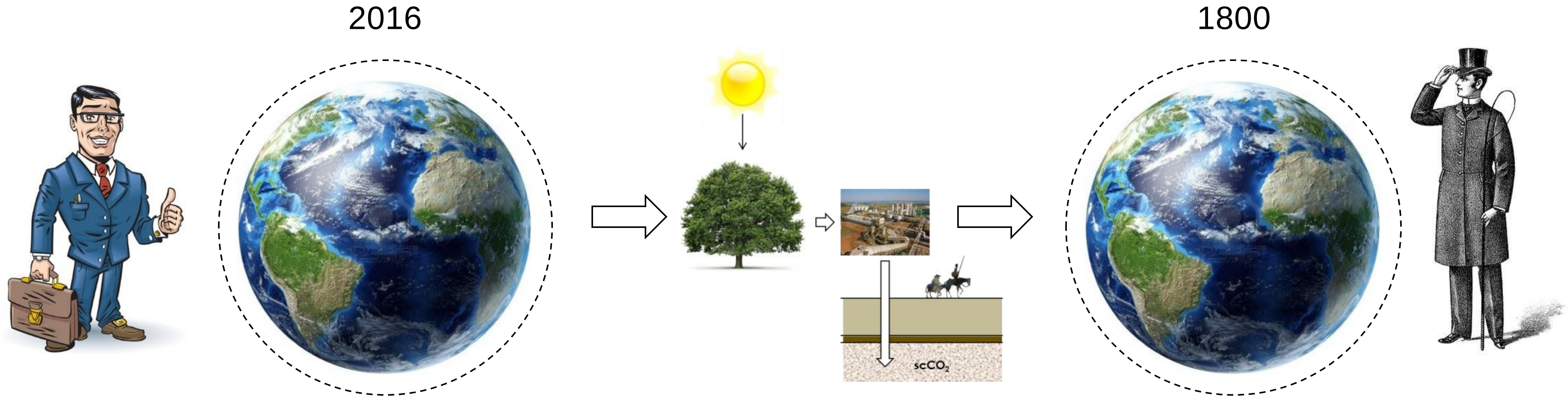
LBE5010 Renewable Energies and Energy Planning

EXERGY ANALYSIS:
thermodynamics of separation processes

Prof. Paulo Seleghim Jr.
Universidade de São Paulo



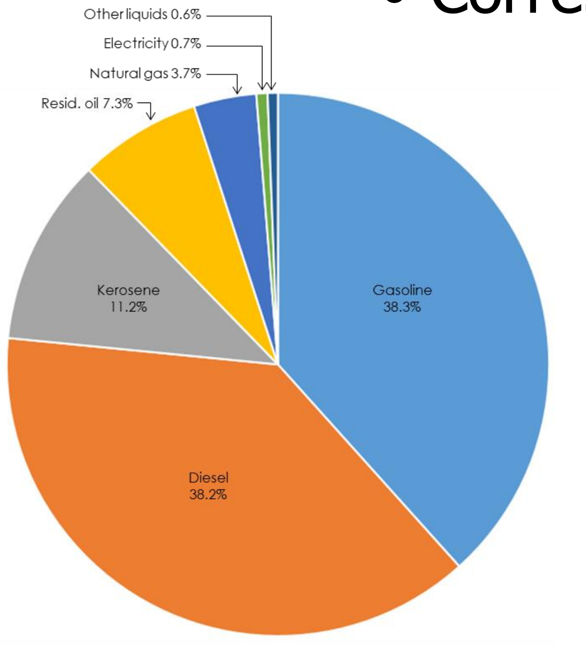
“Sun Powered CCS Industrial Plants”



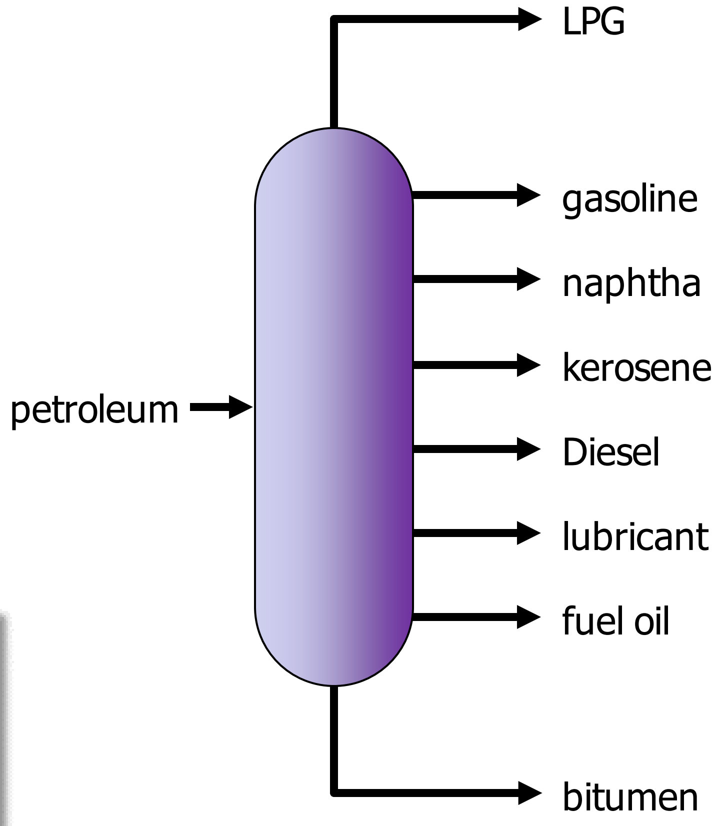
How much exergy is necessary to reconstitute earth’s atmosphere to its original composition prior to the industrial revolution...exergy analysis of separation processes.

Separation operations in the process industry:

- Correspond to approximately 40 – 90 % of total costs



International Energy Outlook 2017



petroleum

LPG

gasoline

naphtha

kerosene

Diesel

lubricant

fuel oil

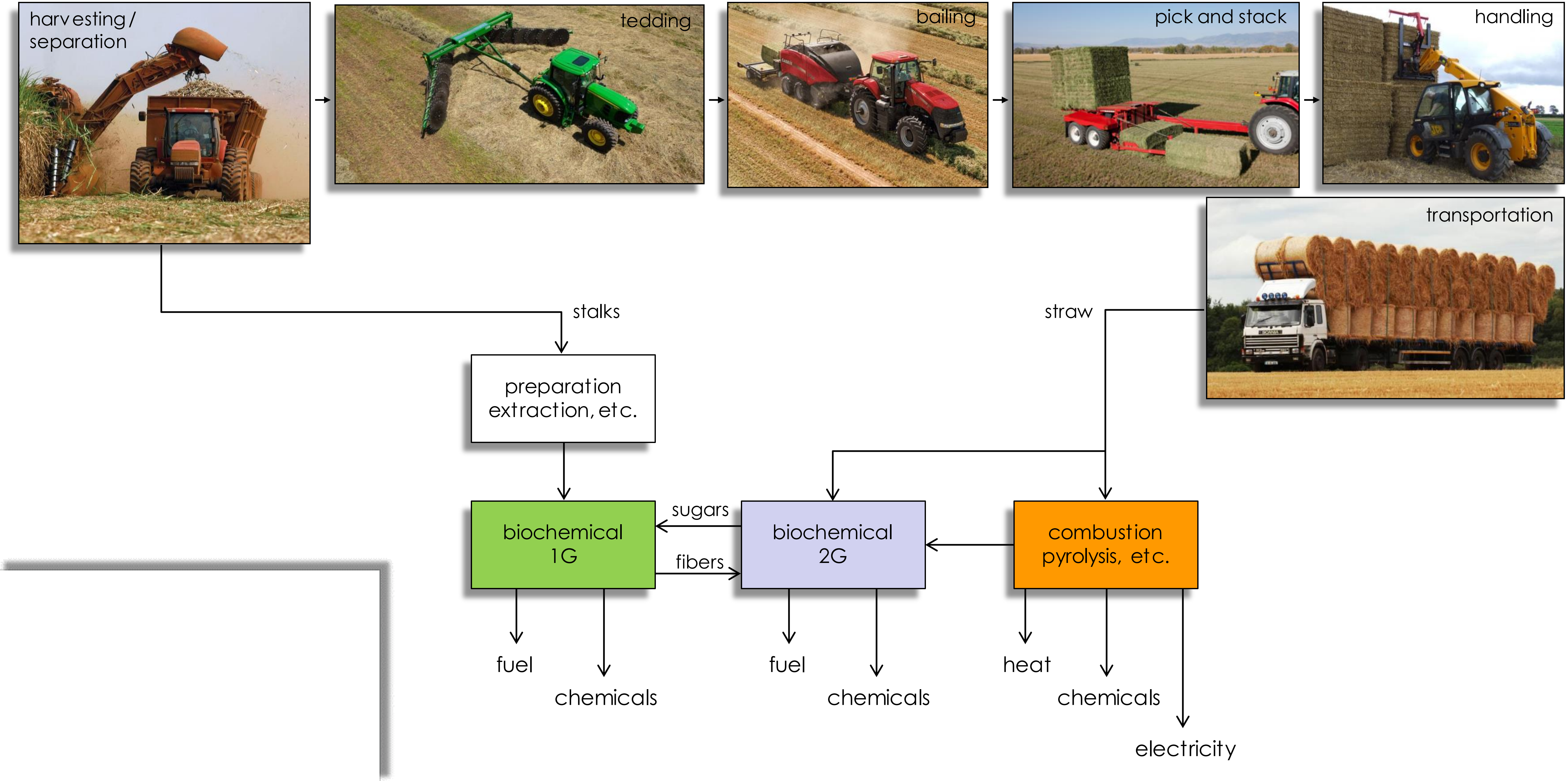
bitumen

Refinaria Duque de Caxias – RJ

MOTIVATION:

what is the minimum amount of work necessary for the separation of the components of a given mixture ?

BIOMASS PRODUCTION AND PROCESSING SYSTEM



harvesting / separation → tedding → bailing → pick and stack → handling → transportation

stalks

preparation extraction, etc.

straw

biochemical 1G

sugars

fibers

biochemical 2G

combustion pyrolysis, etc.

fuel

chemicals

fuel

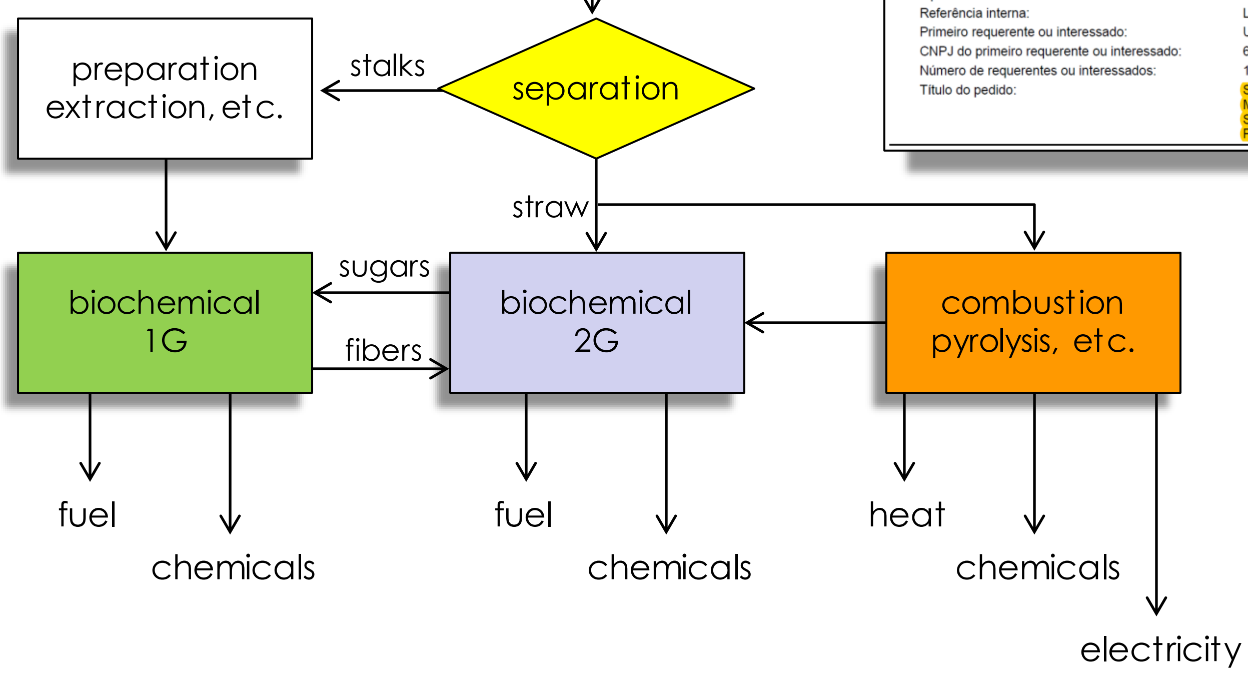
chemicals

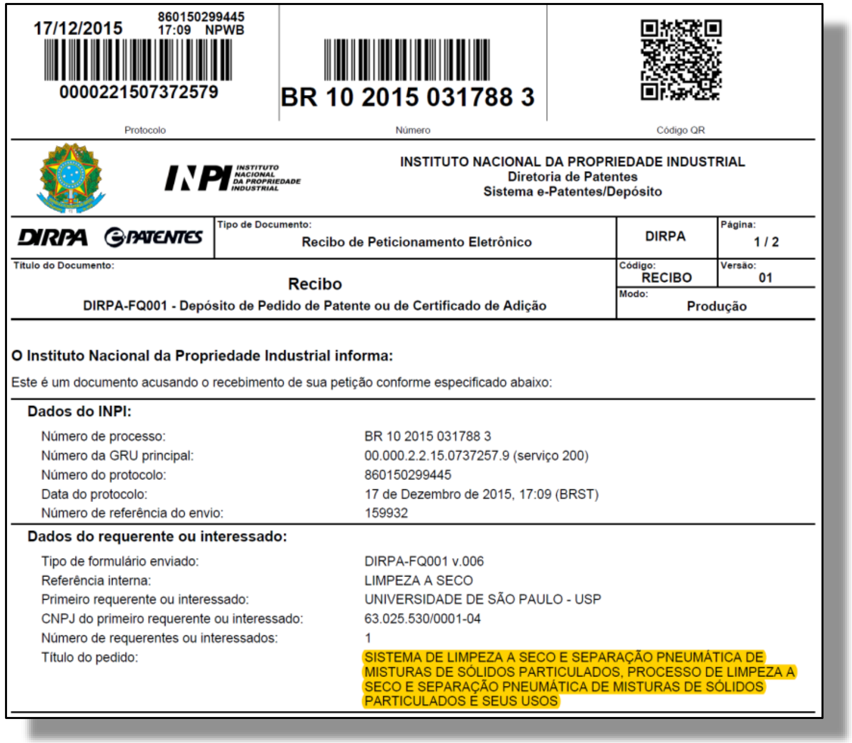
heat

chemicals

electricity

BIOMASS PRODUCTION AND PROCESSING SYSTEM





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Protocolo

BR 10 2015 031788 3

Número

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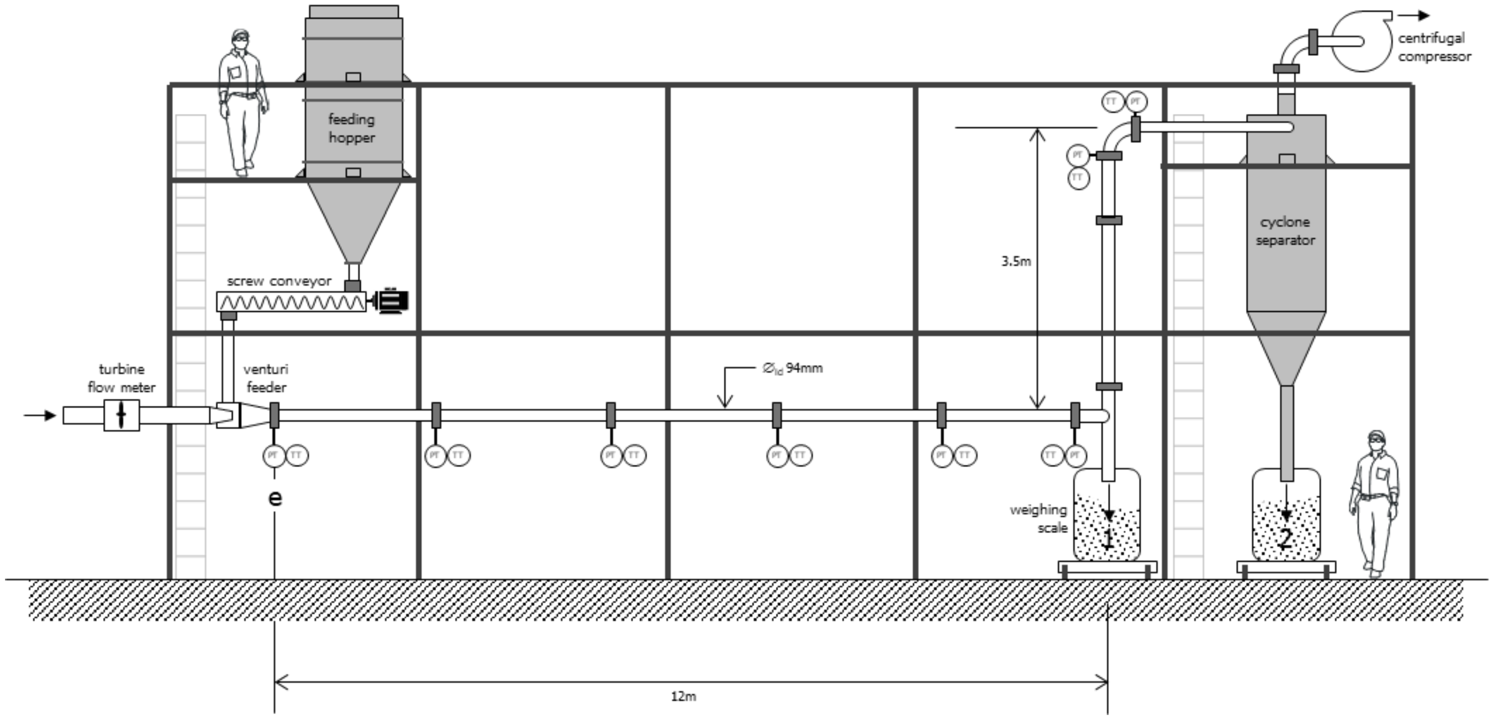
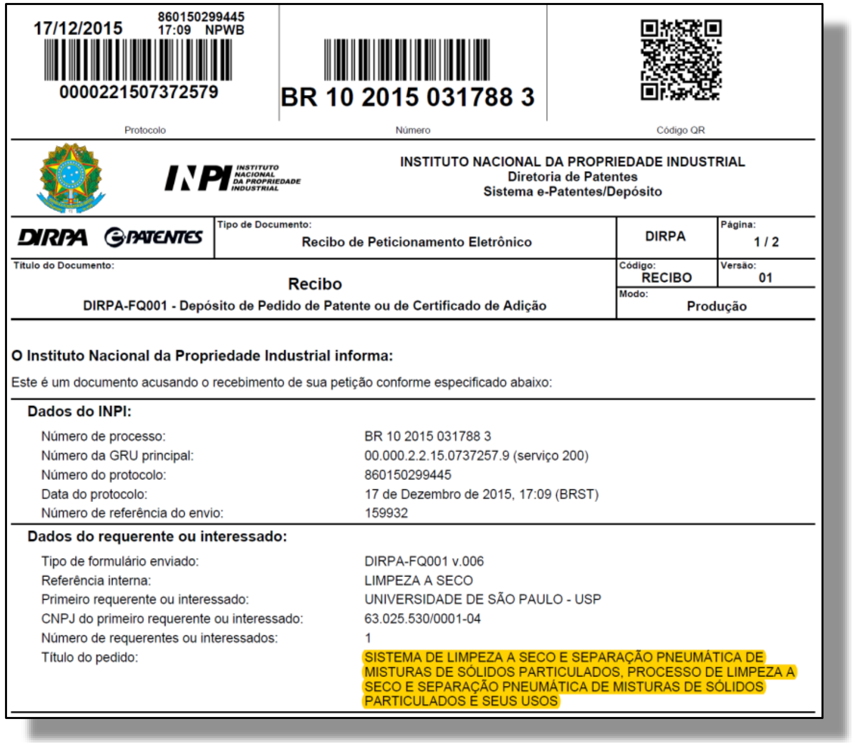
Dados do requerente ou interessado:

Tipo de formulário enviado:	DIRPA-FQ001 v.006
Referência interna:	LIMPEZA A SECO
Primeiro requerente ou interessado:	UNIVERSIDADE DE SÃO PAULO - USP
CNPJ do primeiro requerente ou interessado:	63.025.530/0001-04
Número de requerentes ou interessados:	1
Título do pedido:	SISTEMA DE LIMPEZA A SECO E SEPARAÇÃO PNEUMÁTICA DE MISTURAS DE SÓLIDOS PARTICULADOS, PROCESSO DE LIMPEZA A SECO E SEPARAÇÃO PNEUMÁTICA DE MISTURAS DE SÓLIDOS PARTICULADOS E SEUS USOS





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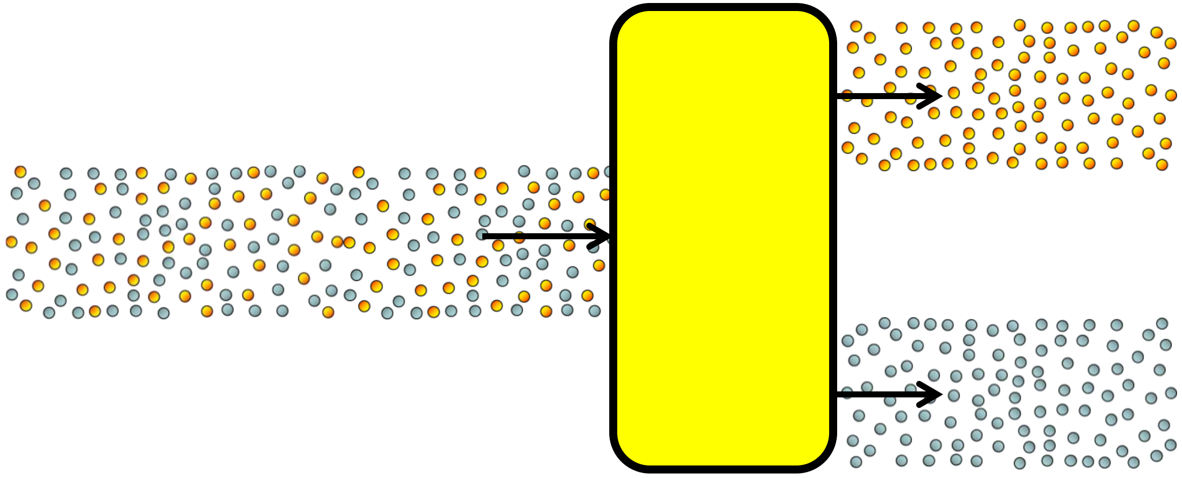
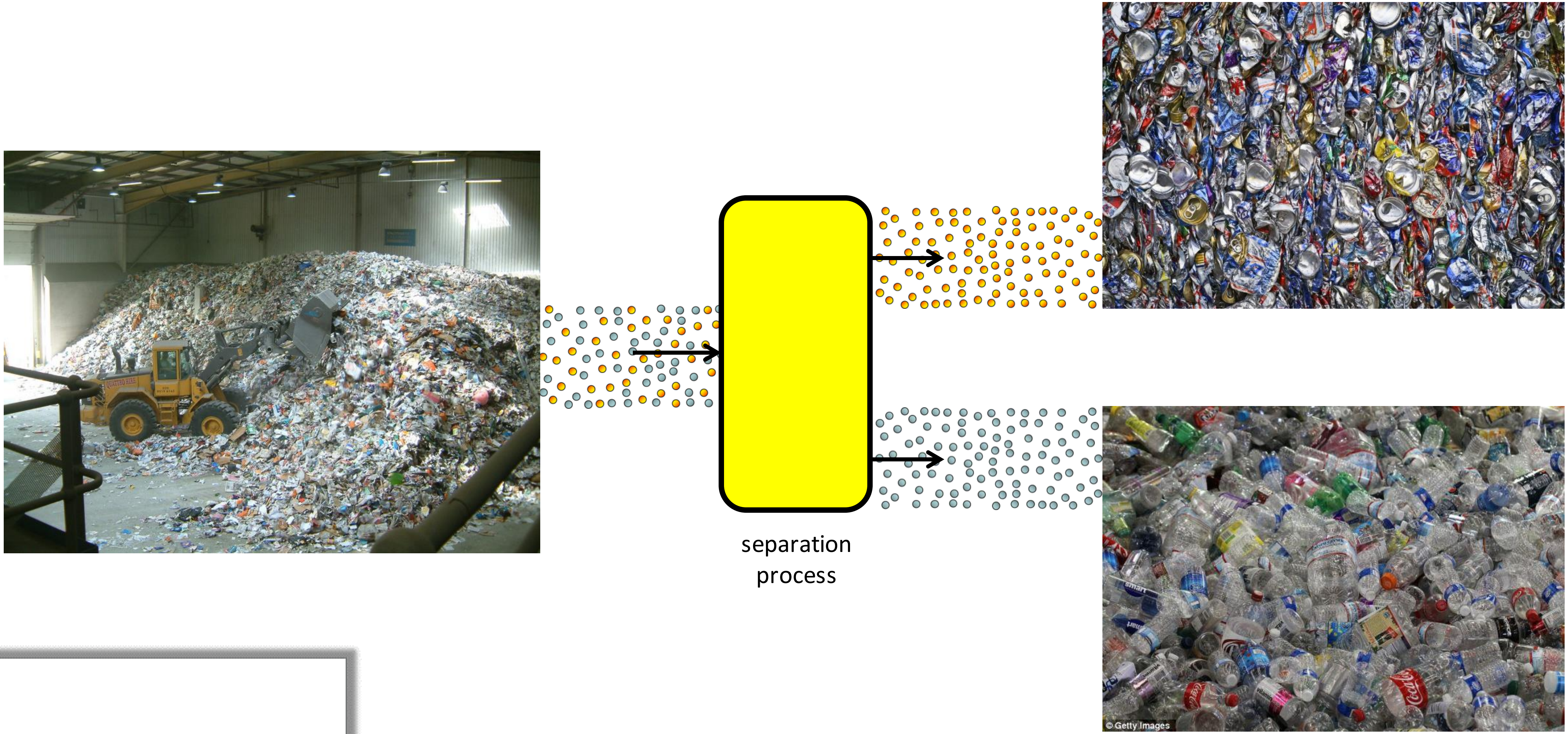
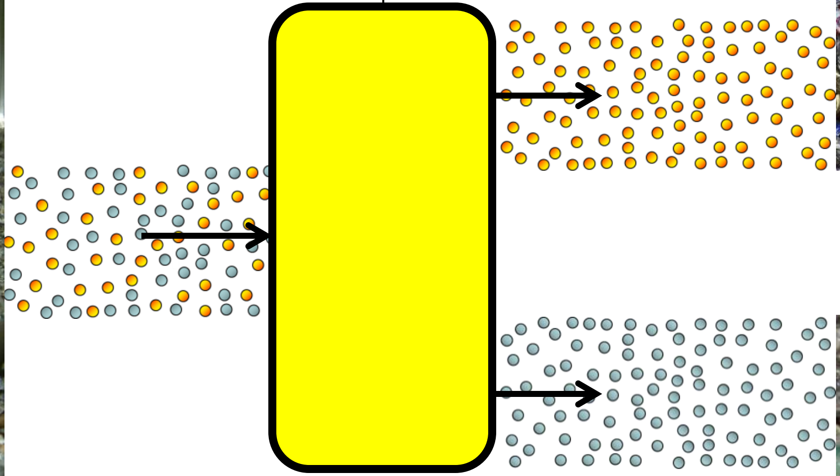


separation process



separation process

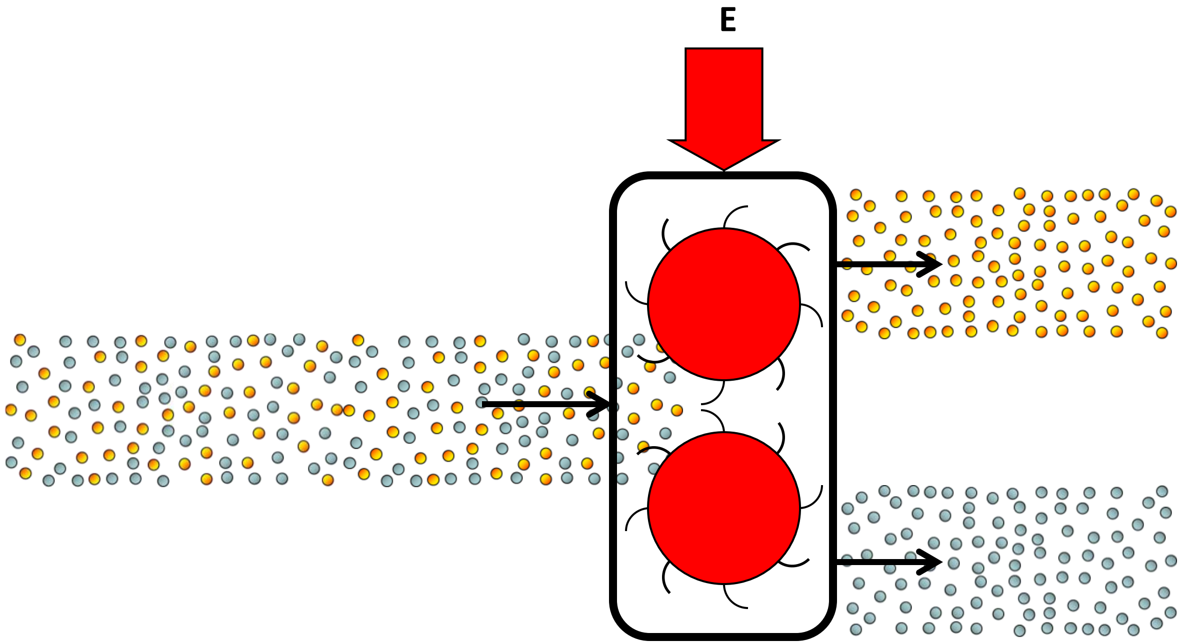


separation
process

© Getty Images

high level
of disorder

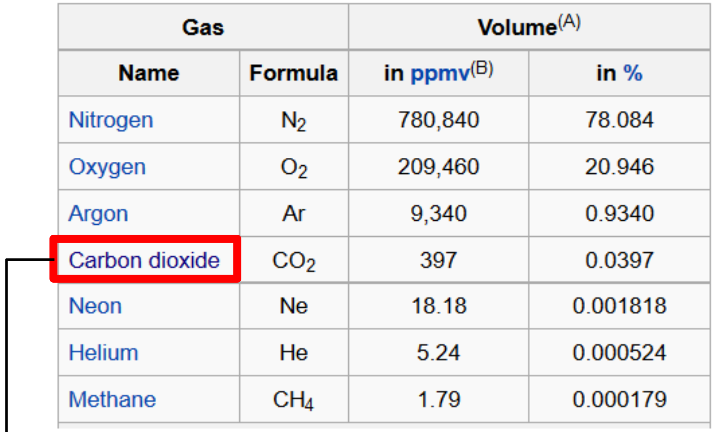
low level
of disorder



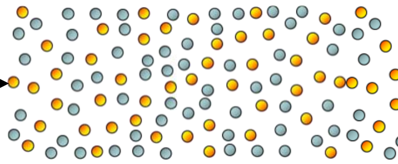
separation process

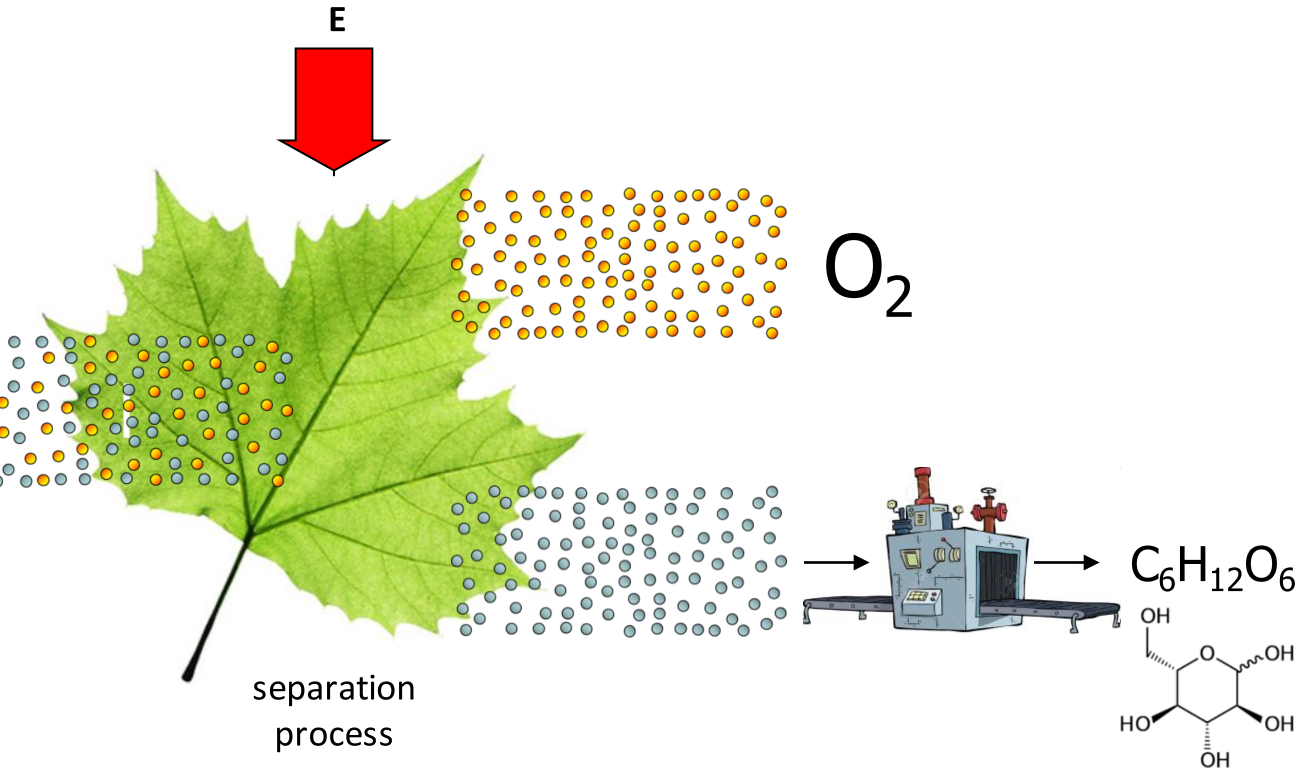
high level of disorder

low level of disorder



Gas		Volume[A]	
Name	Formula	in ppmv[B]	in %
Nitrogen	N_2	780,840	78.084
Oxygen	O_2	209,460	20.946
Argon	Ar	9,340	0.9340
Carbon dioxide	CO_2	397	0.0397
Neon	Ne	18.18	0.001818
Helium	He	5.24	0.000524
Methane	CH_4	1.79	0.000179





separation process

high level of disorder	low level of disorder
lower level of energy	higher level of energy

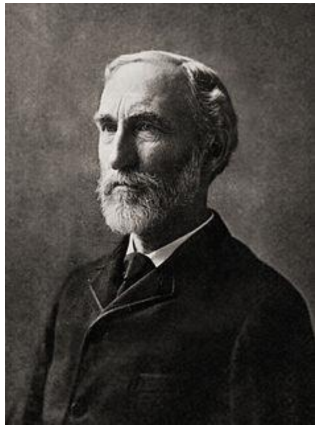
The first law enforces the energy balance of the process…

The second law assesses the efficiency of the process…

⇨ Combining the 1st and 2nd laws...

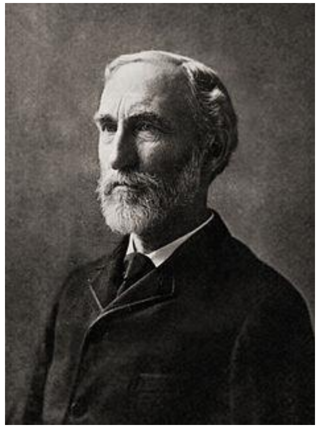
⇨ Exergy, Gibbs, etc.

AVAILABLE ENERGY:


J. Willard Gibbs

“The greatest amount of mechanical work which can be obtained from a given quantity of a certain substance in a given initial state, without increasing its total volume or allowing heat to pass to or from external bodies, except such as at the close of the processes are left in their initial condition…”

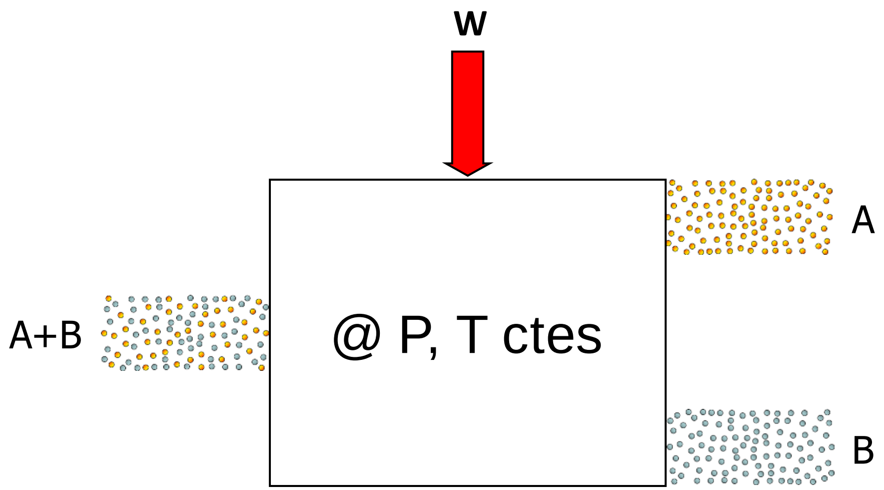
DEFINITIONS


J. Willard Gibbs

"Useful work potential": is the maximum amount of mechanical energy that one can obtain from a system, the difference being inevitably lost to the environment due to the implications of the 2nd law.

EXERGY ⇨

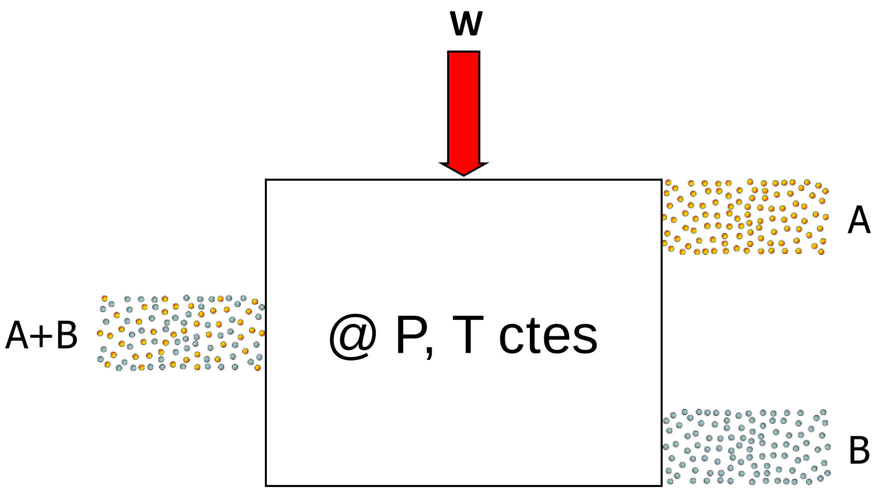
Available energy
Exergetic energy
Availability
Reversible work
Etc.



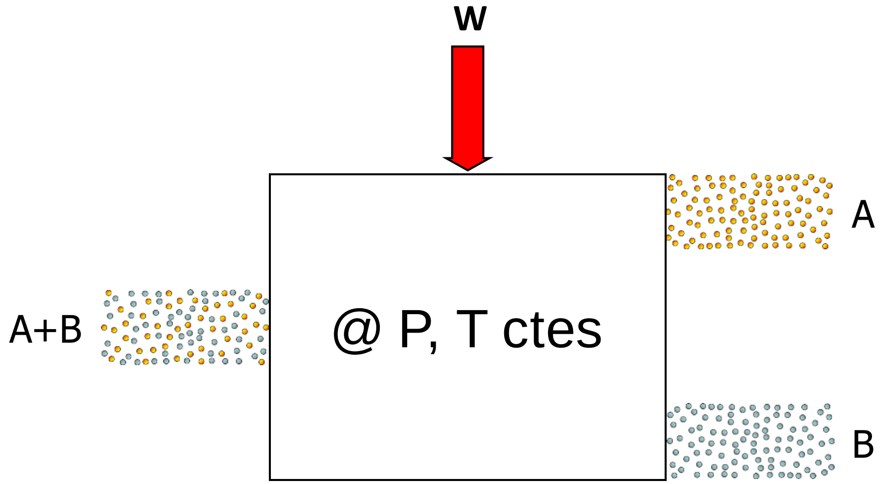
$$\sum_{k}\left(1-\frac{T_0}{T_k}\right)\dot{Q}_k-\left(\dot{W}-P_0\frac{dV_{vc}}{dt}\right)+\sum_{entra}\dot{m}_k x_k-\sum_{saída}\dot{m}_k x_k-\dot{X}_{dest}=\frac{dX_{vc}}{dt}$$

Obs: by convention W>0
= going out of the cv

Obs: by convention Q>0
= going into the cv



$$\sum_k \underbrace{\cancel{\left(1-\frac{T_0}{T_k}\right)}}_{\text{adiabatic process}}\dot{Q}_k - \left(\dot{W} - P_0 \underbrace{\cancel{\frac{dV_{vc}}{dt}}}_{\text{permanent regime}}\right) + \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k - \dot{X}_{dest} = \underbrace{\cancel{\frac{dX_{vc}}{dt}}}_{\text{permanent regime}}$$



$$\sum_k \cancel{\left(1-\frac{T_0}{T_k}\right)\dot{Q}_k} - \left(\dot{W} - P_0 \cancel{\frac{dV_{vc}}{dt}}\right) + \sum_{entra} \dot{m}_k x_k - \sum_{saída} \dot{m}_k x_k - \cancel{\dot{X}_{dest}} = \cancel{\frac{dX_{vc}}{dt}}$$

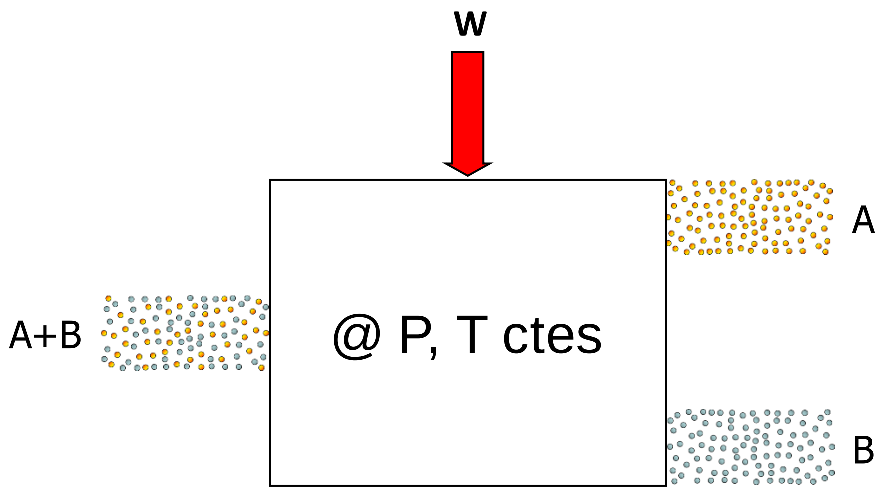
adiabatic process

minimum separation work

permanent regime

absence of irreversibilities

permanent regime



$$\cancel{\sum_k \left(1-\frac{T_0}{T_k}\right)\dot{Q}_k} - \left(\dot{W} - \cancel{P_0\frac{dV_{vc}}{dt}}\right) + \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k - \cancel{\dot{X}_{dest}} = \cancel{\frac{dX_{vc}}{dt}}$$

adiabatic process

minimum separation work

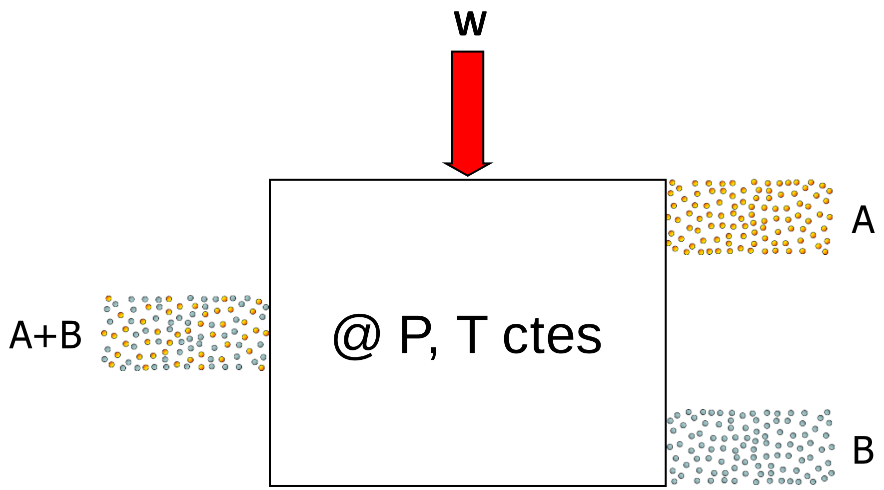
permanent regime

absence of irreversibilities

permanent regime

$$\dot{W} = \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k$$

$$x = (h-h_0) - T_0(s-s_0) + \cancel{ep} + \cancel{ec} + \cancel{eq}$$



$$\cancel{\sum_k\left(1-\frac{T_0}{T_k}\right)\dot{Q}_k} - \left(\dot{W} - P_0\cancel{\frac{dV_{vc}}{dt}}\right) + \sum_{\text{entra}}\dot{m}_k x_k - \sum_{\text{saída}}\dot{m}_k x_k - \cancel{\dot{X}_{dest}} = \cancel{\frac{dX_{vc}}{dt}}$$

adiabatic process

minimum separation work

permanent regime

absence of irreversibilities

permanent regime

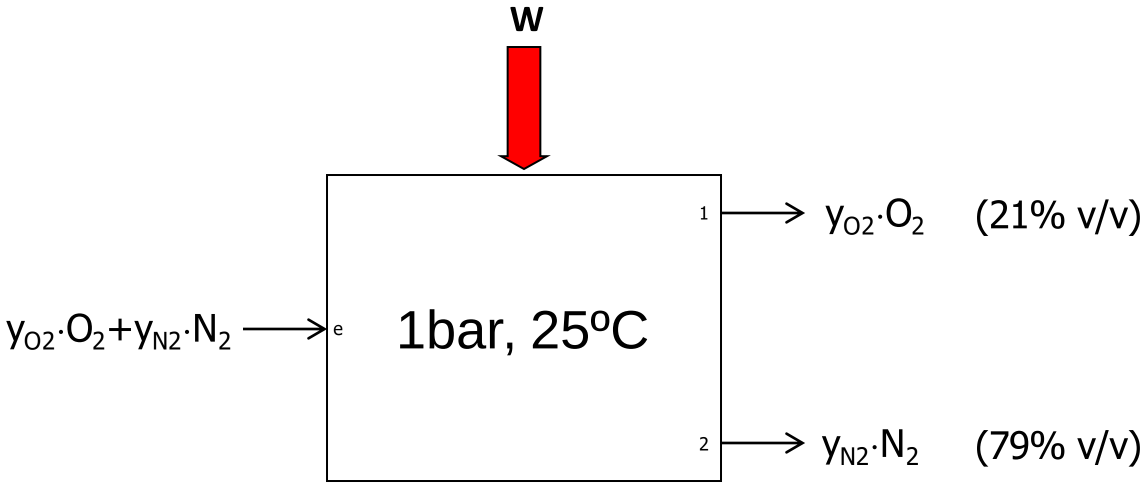
$$\dot{W} = \sum_{\text{entra}}\dot{m}_k x_k - \sum_{\text{saída}}\dot{m}_k x_k$$

$$x = \cancel{(h - h_0)} - T_0(s - s_0) + \cancel{ep} + \cancel{ec} + \cancel{eq}$$

T=cte; gases ideais

Exergy associated to the process of reduction of the level of disorder...

Example: specific demand of energy necessary to separate oxygen from the atmosphere



W

$y_{O2} \cdot O_2 + y_{N2} \cdot N_2$ → e

1bar, 25ºC

1 → $y_{O2} \cdot O_2$ (21% v/v)

2 → $y_{N2} \cdot N_2$ (79% v/v)

$$\dot{W} = \sum_{entra} \dot{m}_k x_k - \sum_{saída} \dot{m}_k x_k$$

$$\dot{W} = \left(\dot{m}_{O_2} x_{O_2} + \dot{m}_{N_2} x_{N_2}\right)_e - \left[\left(\dot{m}_{O_2} x_{O_2}\right)_1 + \left(\dot{m}_{N_2} x_{N_2}\right)_2\right]$$

$$\dot{W} = \dot{m}_{O_2} \cdot (x_{O_2,e} - x_{O_2,1}) + \dot{m}_{N_2} \cdot (x_{N_2,e} - x_{N_2,2})$$

Example: specific demand of energy necessary to separate oxygen from the atmosphere

$$\dot{W} = \dot{m}_{O_2} T_0 \cdot (s_{O_2,1} - s_{O_2,e}) + \dot{m}_{N_2} T_0 \cdot (s_{N_2,2} - s_{N_2,e})$$

$$\frac{\dot{W}}{\dot{m}_{ar}} = T_0 \cdot \left[\frac{\dot{m}_{O_2}}{\dot{m}_{ar}} (s_{O_2,1} - s_{O_2,e}) + \frac{\dot{m}_{N_2}}{\dot{m}_{ar}} (s_{N_2,2} - s_{N_2,e}) \right]$$

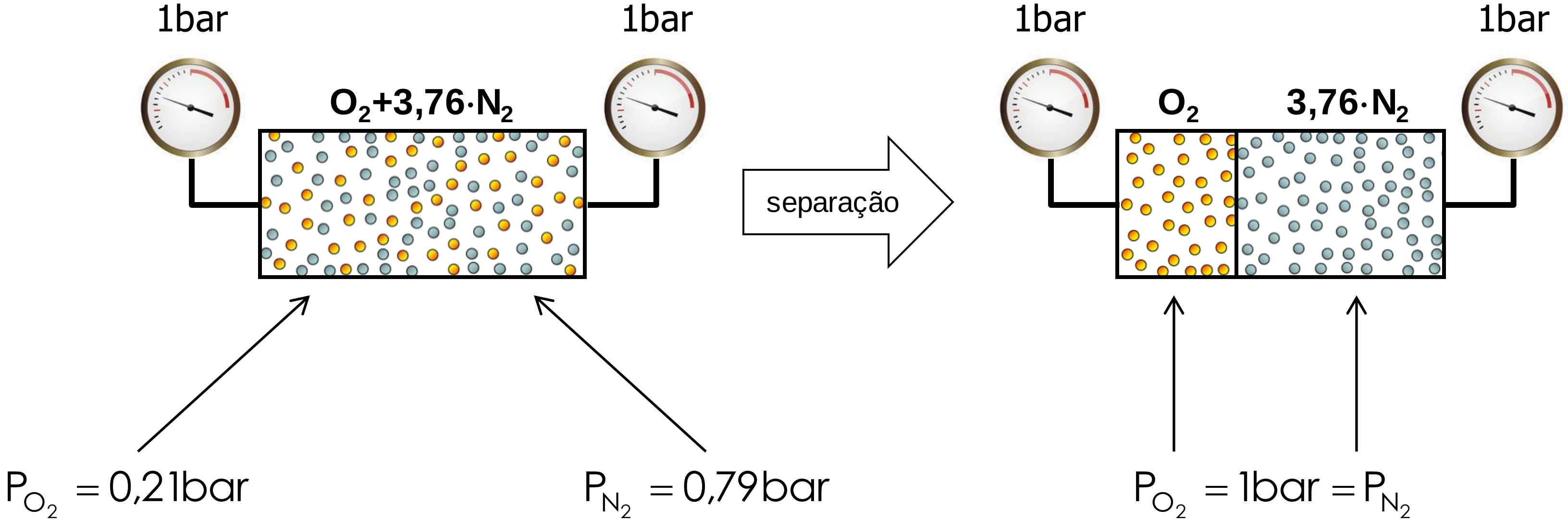
specific work→ $$w = T_0 \cdot \left[y_{O_2} (s_{O_2,1} - s_{O_2,e}) + y_{N_2} (s_{N_2,2} - s_{N_2,e}) \right]$$

$$w = T_0 \cdot \underbrace{\left[y_{O_2} \cdot \Delta s_{O_2} + y_{N_2} \cdot \Delta s_{N_2} \right]}$$

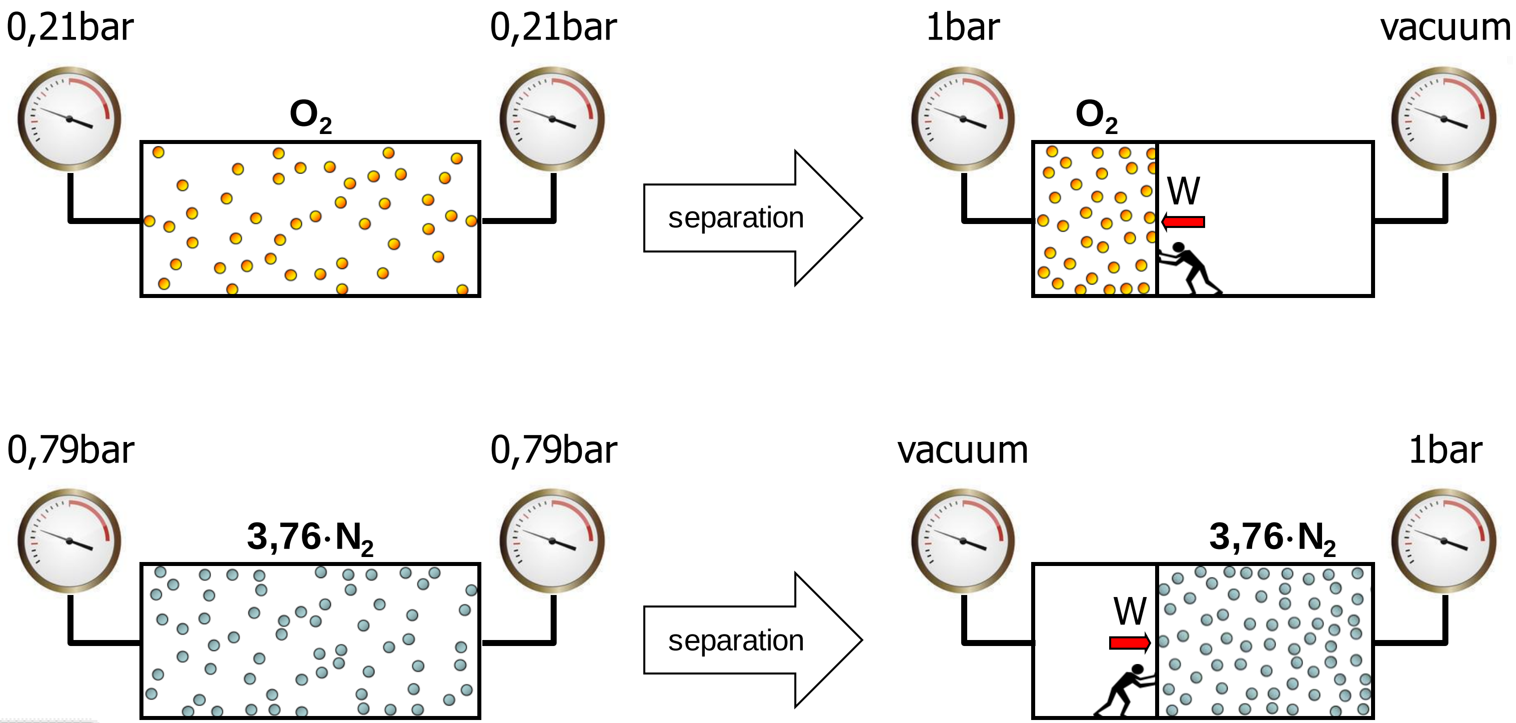
Exergy necessary for the disorder level reduction process (separation)...

THE TOTAL ENTROPY REDUCES DUE TO THE SEPARATION PROCESS !

$$w = T_0 \cdot \left[y_{O_2} \left(\underset{\substack{\downarrow \\ 1\text{bar}}}{s_{O_2,1}} - \underset{\substack{\downarrow \\ P_{O2}}}{s_{O_2,e}} \right) + y_{N_2} \left(\underset{\substack{\downarrow \\ 1\text{bar}}}{s_{N_2,2}} - \underset{\substack{\downarrow \\ P_{N2}}}{s_{N_2,e}} \right) \right]$$



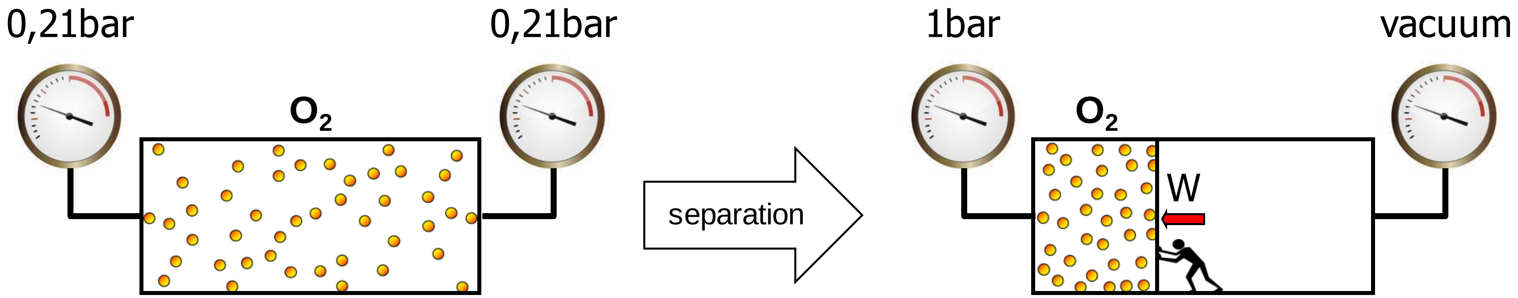
$$w = T_0 \cdot \left[y_{O_2} \left(s_{O_2,1} - s_{O_2,e} \right) + y_{N_2} \left(s_{N_2,2} - s_{N_2,e} \right) \right]$$

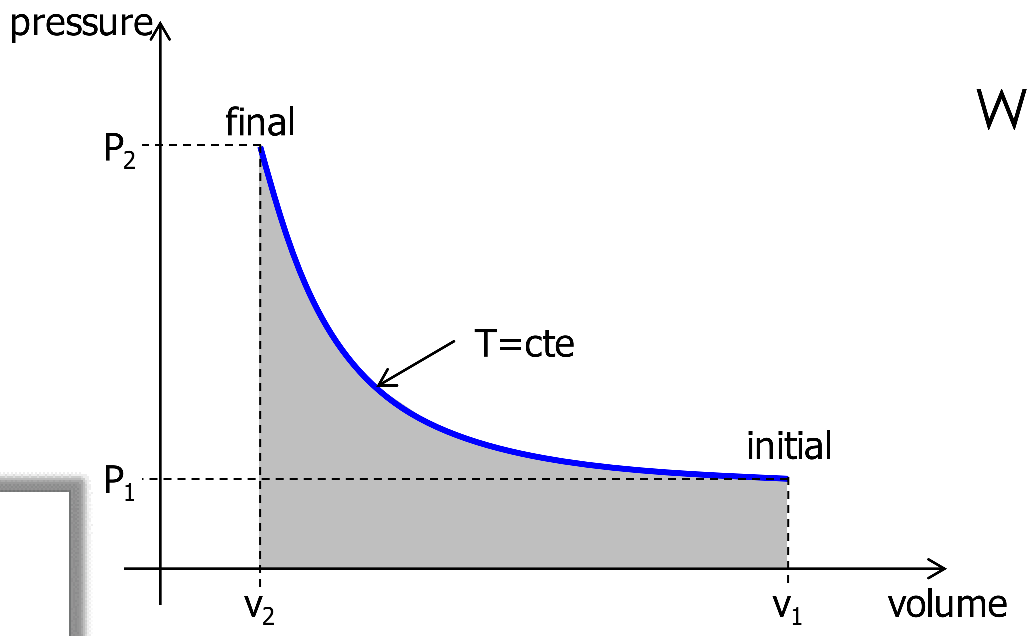


Obs: perfecto gases

$$T = cte \Rightarrow U = cte$$

Trabalho de Compressão Isotérmica





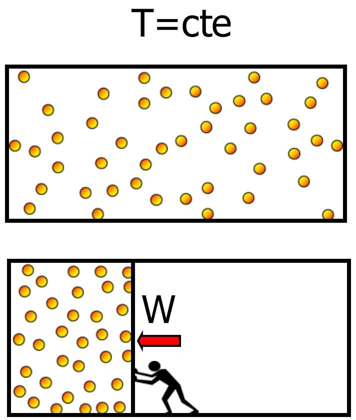
$$W=\int_1^2 P\cdot dV=\int_1^2 \frac{nRT}{V}\cdot dv$$

$$W=nRT\cdot\ln(V_2/V_1)$$

$$W=nRT\cdot\ln(P_1/P_2)$$

$$W=nRT\cdot\ln(y)$$

[y] = mol/mol



T=cte

$$Q - W = \cancel{\Delta U}$$

$$\Delta S = \frac{Q}{T} = \frac{W}{T} \qquad \leftarrow W = nRT \cdot \ln(y)$$

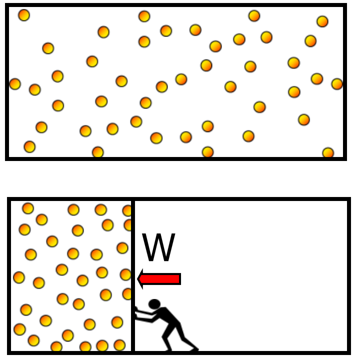
$$\Rightarrow \Delta S = nR \cdot \ln(y)$$

$[\Delta S]$ = kJ/K

Total entropy reduction associated with the separation of an ideal gases mixture

$$\Rightarrow \Delta S = R \cdot \sum_k n_k \cdot \ln(y_k)$$

T=cte



$$Q - W = \overset{T=cte}{\cancel{\Delta U}}$$

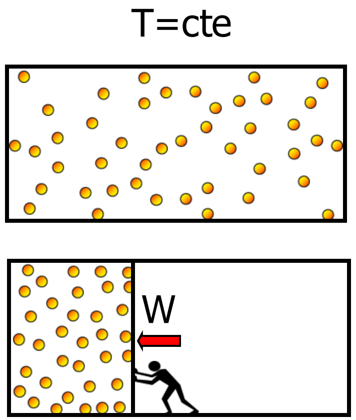
$$\Delta S = \frac{Q}{T} = \frac{W}{T} \qquad \leftarrow W = nRT \cdot \ln(y)$$

$$\Rightarrow \Delta S = nR \cdot \ln(y)$$

[ΔS] = kJ/K

Total entropy reduction associated with the separation of an ideal gases mixture

$$\Rightarrow \Delta S = R \cdot \sum_k n_k \cdot \ln(y_k) \times \frac{\sum n_k}{\sum n_k}$$



T=cte

$$Q - W = \cancel{\Delta U}$$

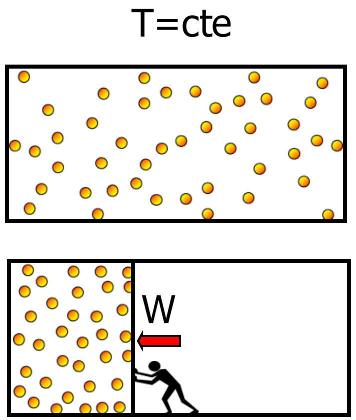
$$\Delta S = \frac{Q}{T} = \frac{W}{T} \qquad \leftarrow W = nRT \cdot \ln(y)$$

$$\Rightarrow \Delta S = nR \cdot \ln(y)$$

[ΔS] = kJ/K

Total entropy reduction associated with the separation of an ideal gases mixture

$$\Rightarrow \frac{\Delta S}{\sum n_k} = R \cdot \sum_k \frac{n_k}{\sum n_k} \cdot \ln(y_k)$$



$$Q - W = \overset{T=cte}{\cancel{\Delta U}}$$

$$\Delta S = \frac{Q}{T} = \frac{W}{T} \qquad \leftarrow W = nRT \cdot \ln(y)$$

$$\Rightarrow \Delta S = nR \cdot \ln(y)$$

[ΔS] = kJ/K

Total entropy reduction associated with the separation of an ideal gases mixture

$$\Rightarrow \Delta s = R \cdot \sum_k y_k \cdot \ln(y_k)$$

[ΔS] = kJ/K/mol

$$\Delta s = R \cdot \sum_k y_k \cdot \ln\left(y_k\right)$$

$$w = T_0 \cdot \left[y_{O_2} \cdot \Delta s_{O_2} + y_{N_2} \cdot \Delta s_{N_2} \right]$$

$$w = \underbrace{RT_0 \cdot \sum_k y_k \cdot \ln\left(y_k\right)}_{\text{MINIMUM SEPARATION WORK @ CONSTANT TEMPERATURE AND PRESSURE !}}$$

[w] = kJ/mol

MINIMUM SEPARATION WORK @
CONSTANT TEMPERATURE AND PRESSURE !

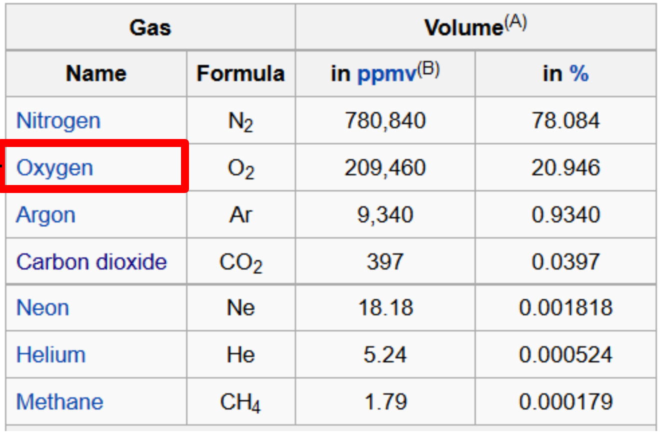
$$w = RT_0 \cdot \sum_k y_k \cdot \ln(y_k)$$

$$w = 8{,}314\,\frac{10^{-3}\,\mathrm{kJ}}{\mathrm{mol}\cdot\mathrm{K}}(25 + 273{,}15)\mathrm{K} \cdot \left[0{,}21 \cdot \ln(0{,}21) + 0{,}79 \cdot \ln(0{,}79)\right]$$

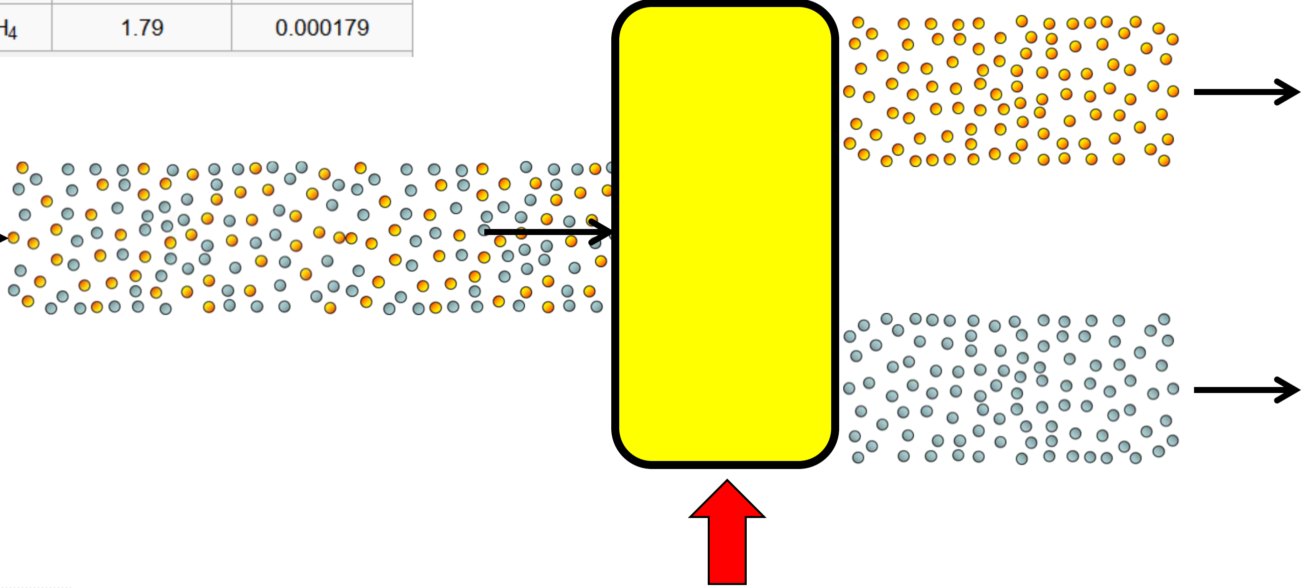
$$w = -1.274\,\frac{\mathrm{kJ}}{\mathrm{mol}}$$

← entering the cv

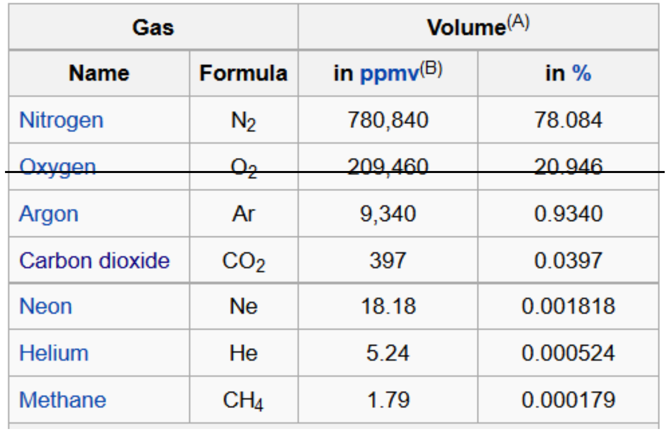
$$w = -1.274\,\frac{\mathrm{kJ}}{\mathrm{mol}}\,\frac{1000}{29{,}97\mathrm{kg/mol}} = -42.51\,\frac{\mathrm{kJ}}{\mathrm{kg}}$$



Gas		Volume[A]	
Name	**Formula**	**in ppmv**[B]	**in %**
Nitrogen	N_2	780,840	78.084
Oxygen	O_2	209,460	20.946
Argon	Ar	9,340	0.9340
Carbon dioxide	CO_2	397	0.0397
Neon	Ne	18.18	0.001818
Helium	He	5.24	0.000524
Methane	CH_4	1.79	0.000179



O_2 @ 100%



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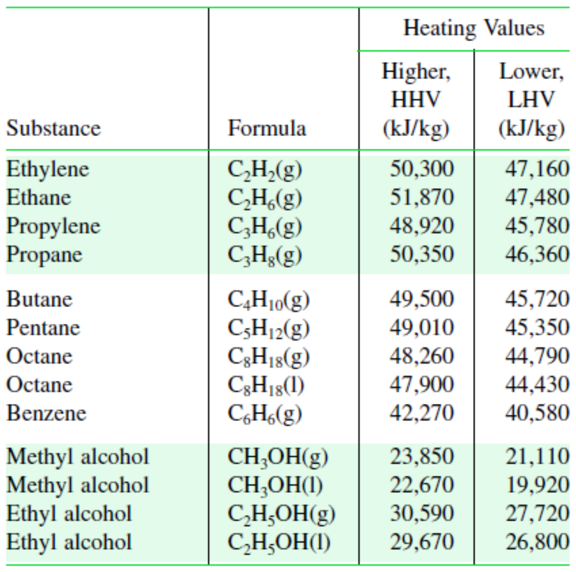
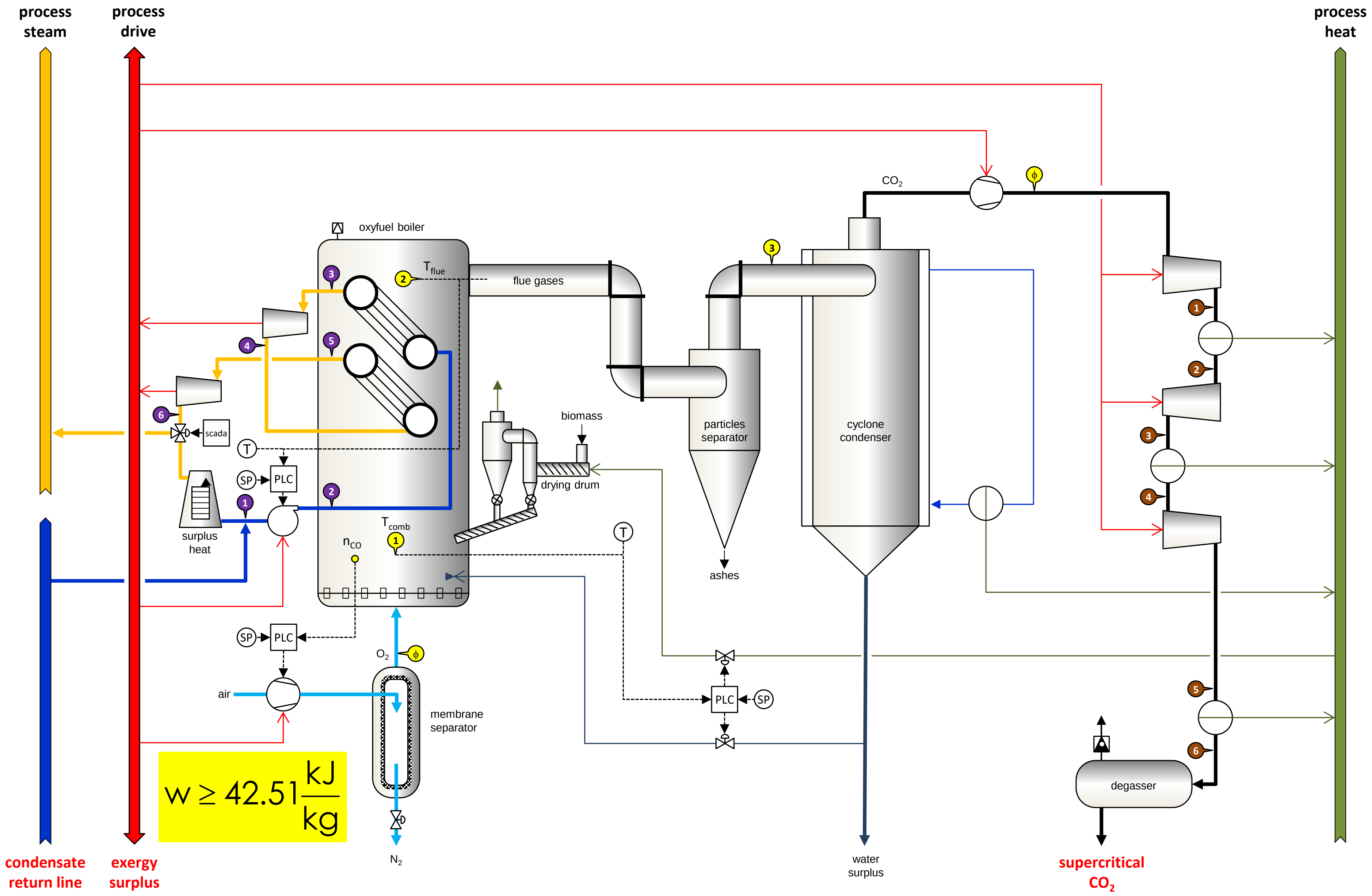
$$w \geq 42.51 \frac{kJ}{kg}$$

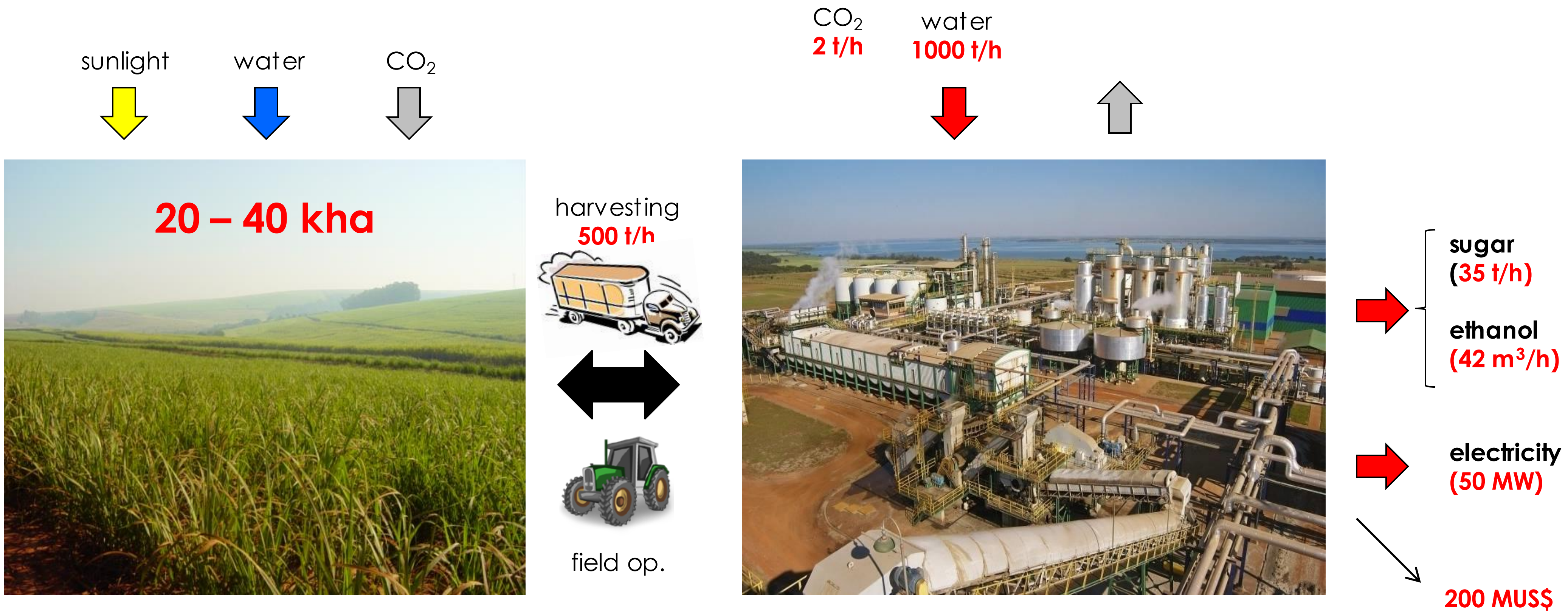


Substance	Formula	Heating Values	
		Higher, HHV (kJ/kg)	Lower, LHV (kJ/kg)
Ethylene	$C_2H_2(g)$	50,300	47,160
Ethane	$C_2H_6(g)$	51,870	47,480
Propylene	$C_3H_6(g)$	48,920	45,780
Propane	$C_3H_8(g)$	50,350	46,360
Butane	$C_4H_{10}(g)$	49,500	45,720
Pentane	$C_5H_{12}(g)$	49,010	45,350
Octane	$C_8H_{18}(g)$	48,260	44,790
Octane	$C_8H_{18}(l)$	47,900	44,430
Benzene	$C_6H_6(g)$	42,270	40,580
Methyl alcohol	$CH_3OH(g)$	23,850	21,110
Methyl alcohol	$CH_3OH(l)$	22,670	19,920
Ethyl alcohol	$C_2H_5OH(g)$	30,590	27,720
Ethyl alcohol	$C_2H_5OH(l)$	29,670	26,800



$$w \geq 42.51 \frac{kJ}{kg}$$

Reference Sugarcane Production and Processing System



sunlight

water

CO_2

20 – 40 kha

harvesting
500 t/h

field op.

CO_2
2 t/h

water
1000 t/h

sugar
(35 t/h)

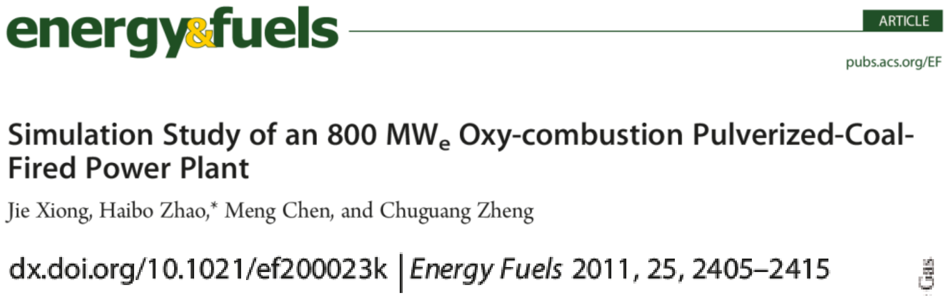
ethanol
($42\ m^3/h$)

electricity
(50 MW)

200 MUS$

$$W_{ref} = \frac{50 \cdot 10^3 kW}{500 \frac{10^3 kg}{3600\, s}} = 360 \frac{kW \cdot s}{kg} = 360 \frac{kJ}{kg}$$

… of which 42.5 kJ/kg would be used to separate O_2 from the atmosphere (~15%).



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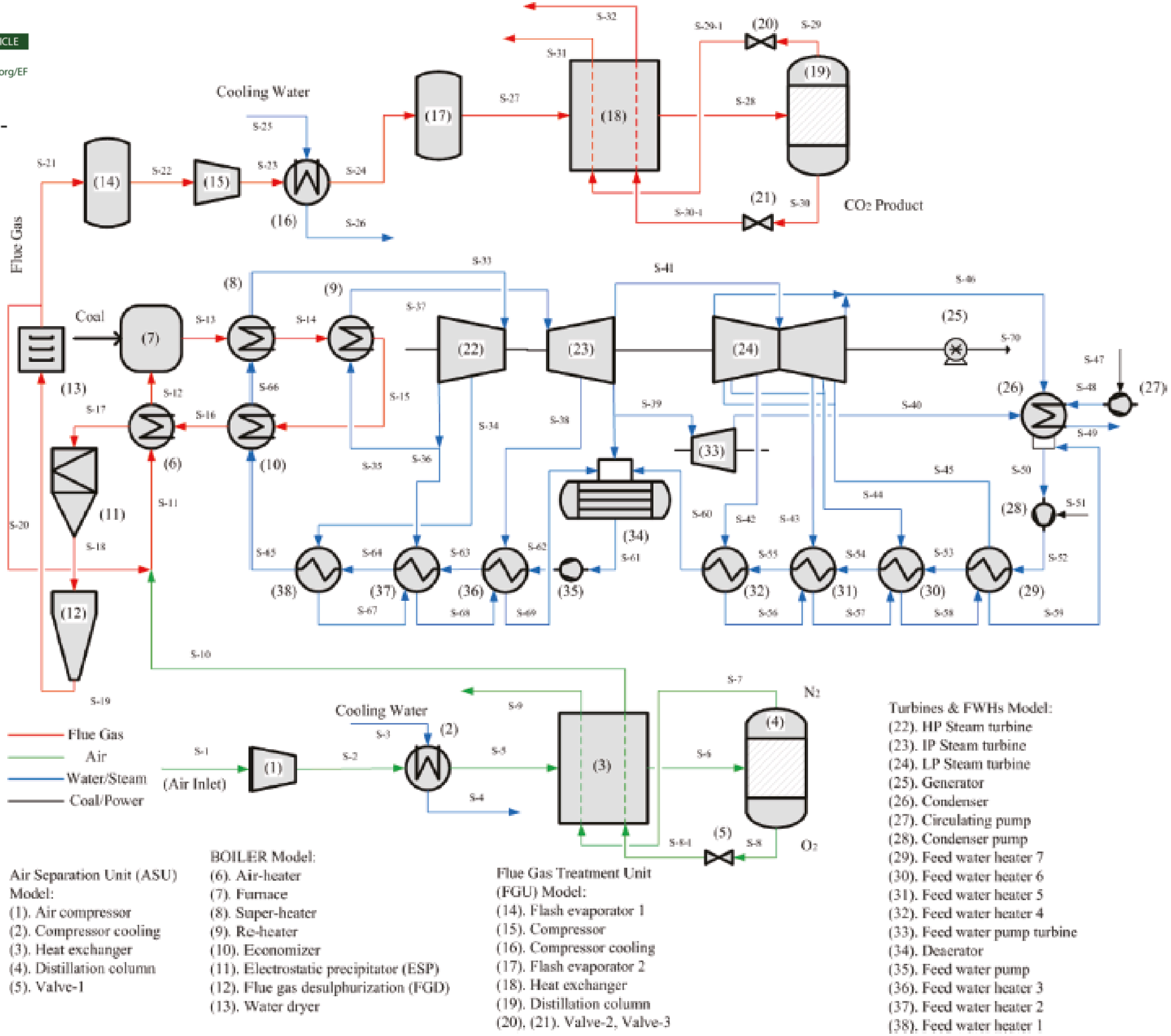
Simulation Study of an 800 MW_e Oxy-combustion Pulverized-Coal-Fired Power Plant

Jie Xiong, Haibo Zhao,* Meng Chen, and Chuguang Zheng

dx.doi.org/10.1021/ef200023k | *Energy Fuels* 2011, 25, 2405–2415

$$w \geq 42.51 kJ/kg$$

$$p/100\% O_2$$



Air Separation Unit (ASU) Model:
(1). Air compressor
(2). Compressor cooling
(3). Heat exchanger
(4). Distillation column
(5). Valve-1

BOILER Model:
(6). Air-heater
(7). Furnace
(8). Super-heater
(9). Re-heater
(10). Economizer
(11). Electrostatic precipitator (ESP)
(12). Flue gas desulphurization (FGD)
(13). Water dryer

Flue Gas Treatment Unit (FGU) Model:
(14). Flash evaporator 1
(15). Compressor
(16). Compressor cooling
(17). Flash evaporator 2
(18). Heat exchanger
(19). Distillation column
(20). (21). Valve-2, Valve-3

Turbines & FWHs Model:
(22). HP Steam turbine
(23). IP Steam turbine
(24). LP Steam turbine
(25). Generator
(26). Condenser
(27). Circulating pump
(28). Condenser pump
(29). Feed water heater 7
(30). Feed water heater 6
(31). Feed water heater 5
(32). Feed water heater 4
(33). Feed water pump turbine
(34). Deaerator
(35). Feed water pump
(36). Feed water heater 3
(37). Feed water heater 2
(38). Feed water heater 1

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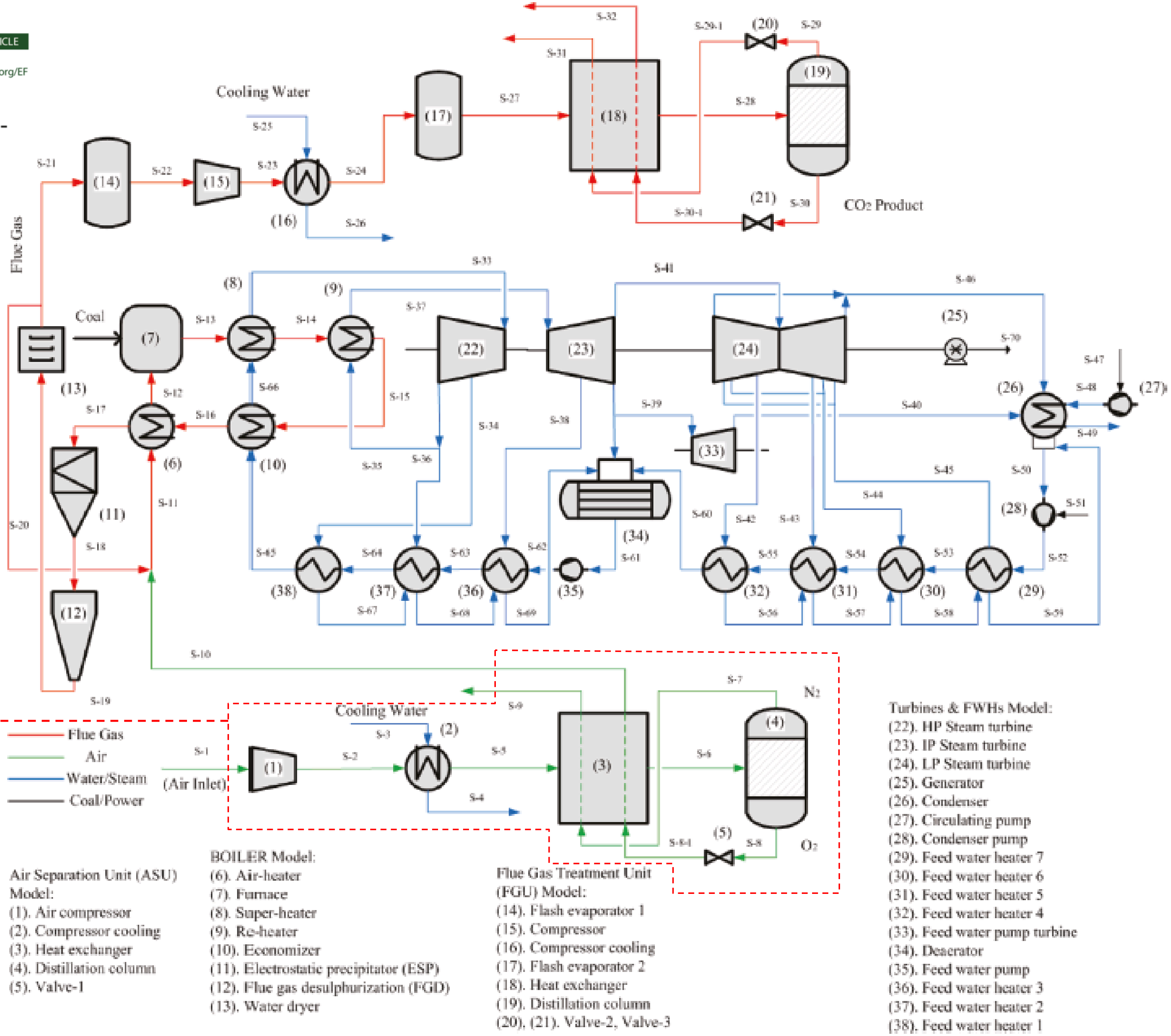
separação criogênica

$$w = 889{,}2 kJ/kg$$

$$w \geq 42.51 kJ/kg$$

$$p/100\% O_2$$



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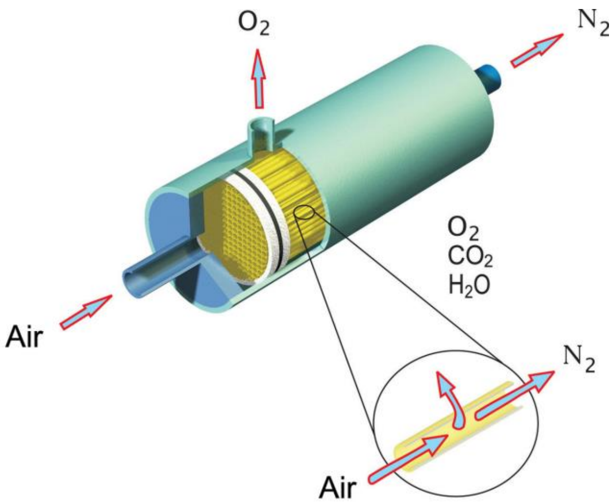
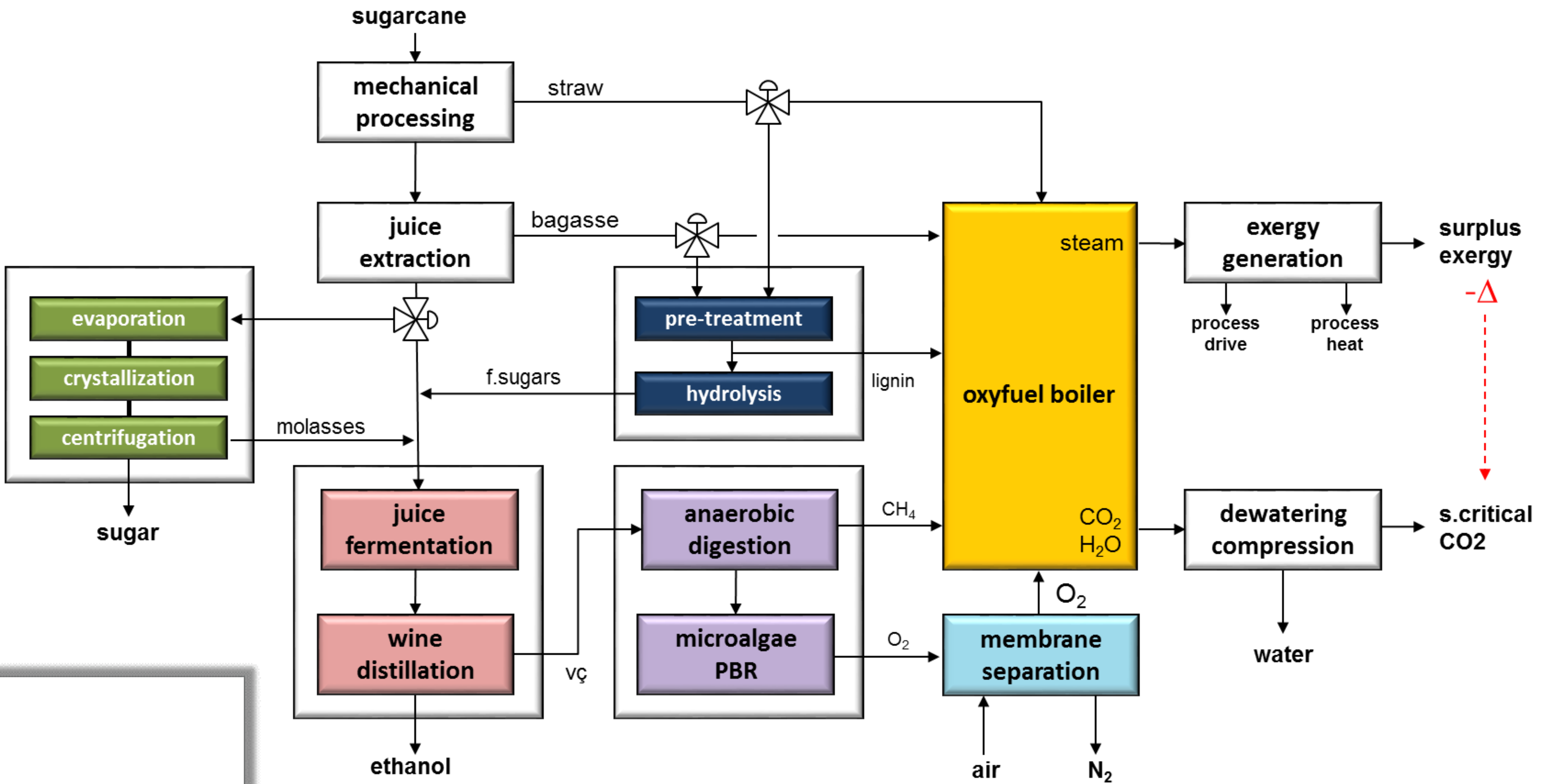
Membrane Gas Separation





sugarcane

mechanical processing

straw

juice extraction

bagasse

evaporation

crystallization

centrifugation

sugar

molasses

pre-treatment

hydrolysis

f.sugars

lignin

juice fermentation

wine distillation

ethanol

vç

anaerobic digestion

microalgae PBR

CH_4

O_2

oxyfuel boiler

steam

CO_2

H_2O

O_2

membrane separation

air

N_2

exergy generation

process drive

process heat

surplus exergy

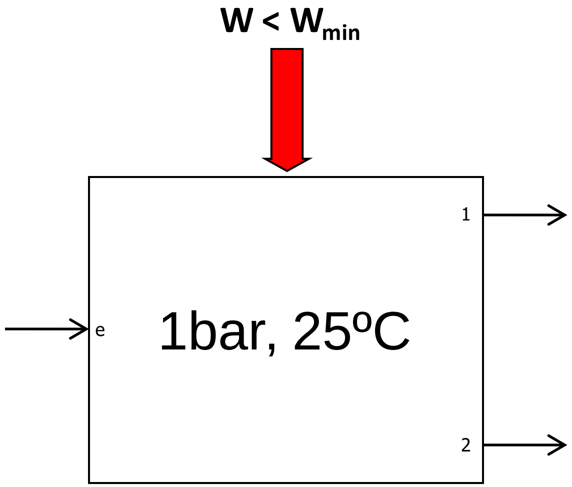
-Δ

dewatering compression

water

s.critical CO2

Example: specific demand of energy necessary to **partially** separate oxygen from the atmosphere



1bar, 25ºC

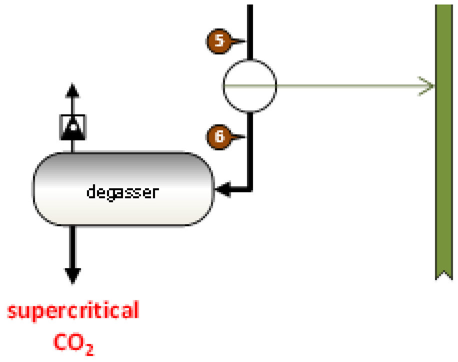
product of interest (O_2) **entering** at a specified input flow rate and concentration

product of interest (O_2) **exiting** at a specified output flow rate and concentration

other constituents

$$w_{min} = -42.51 kJ/kg$$

$$p/100\% O_2$$



Obs.: W_{min} = for complete separation

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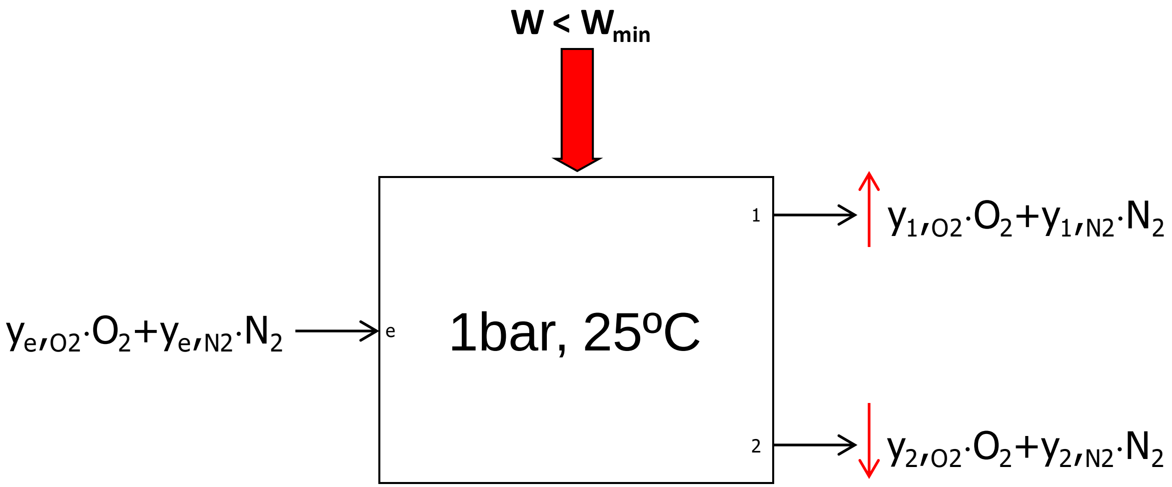

$W < W_{min}$

$y_{e,O2} \cdot O_2 + y_{e,N2} \cdot N_2$ → e

1bar, 25ºC

1 → $y_{1,O2} \cdot O_2 + y_{1,N2} \cdot N_2$

2 → $y_{2,O2} \cdot O_2 + y_{2,N2} \cdot N_2$

$$w_{min} = -42.51 kJ/kg$$

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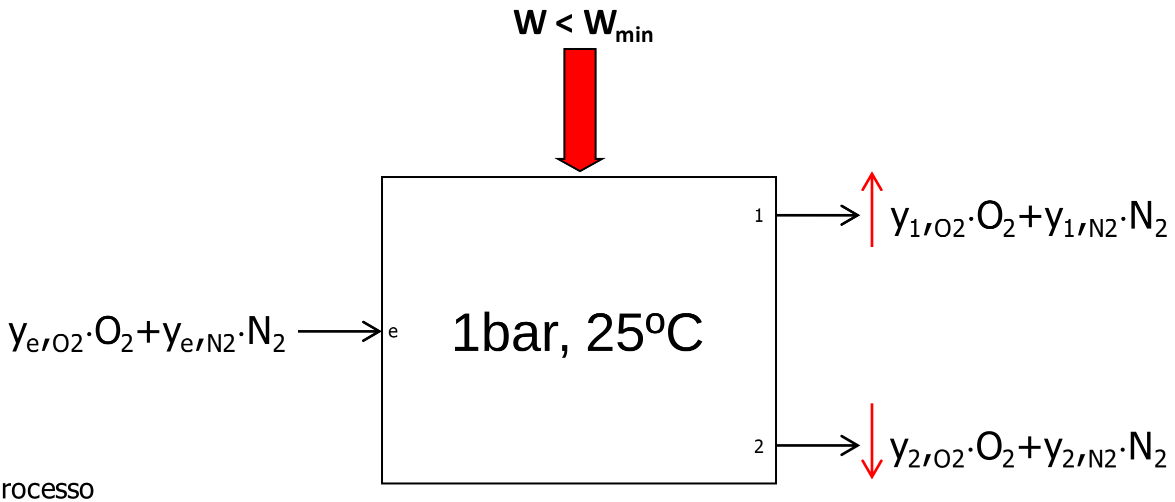
Example: specific demand of energy necessary to **partially** separate oxygen from the atmosphere



$$\overset{\text{processo adiabático}}{\cancel{\sum_k\left(1-\frac{T_0}{T_k}\right)\dot{Q}_k}} - \left(\dot{W} - \underset{\text{regime permanente}}{\cancel{P_0\frac{dV_{vc}}{dt}}}\right) + \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k - \dot{X}_{dest} = \underset{\text{regime permanente}}{\cancel{\frac{dX_{vc}}{dt}}}$$

Obs.: W_{min} = for complete separation

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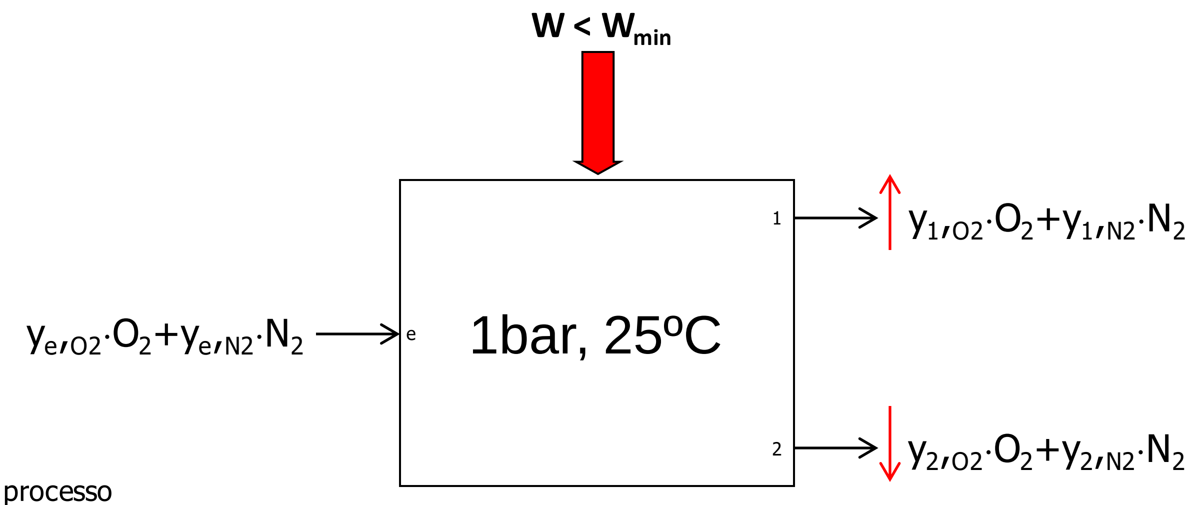


processo adiabático

$$\cancel{\sum_k\left(1-\frac{T_0}{T_k}\right)\dot{Q}_k} - \left(\dot{W} - \cancel{P_0\frac{dV_{vc}}{dt}}\right) + \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k - \cancel{\dot{X}_{dest}} = \cancel{\frac{dX_{vc}}{dt}}$$

mínimo trabalho de separação

regime permanente

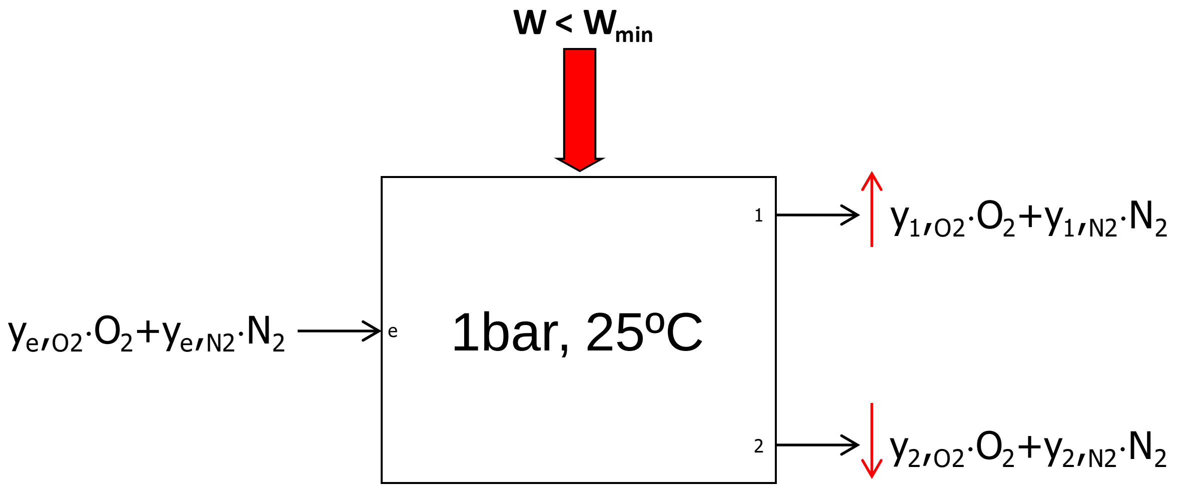
ausência de irreversibilidades

regime permanente

$$\dot{W} = \sum_{entra}\dot{m}_k x_k - \sum_{saída}\dot{m}_k x_k$$

Obs.: W_{min} = for complete separation

Example: specific demand of energy necessary to **partially** separate oxygen from the atmosphere



$$\dot{W} = \sum_{entra} \dot{m}_k x_k - \sum_{saída} \dot{m}_k x_k$$

$$\dot{W} = \left(\dot{m}_{O_2,e} x_{O_2,e} + \dot{m}_{N_2,e} x_{N_2,e}\right) - \left(\dot{m}_{O_2,1} x_{O_2,1} + \dot{m}_{N_2,1} x_{N_2,1}\right) + \ldots$$

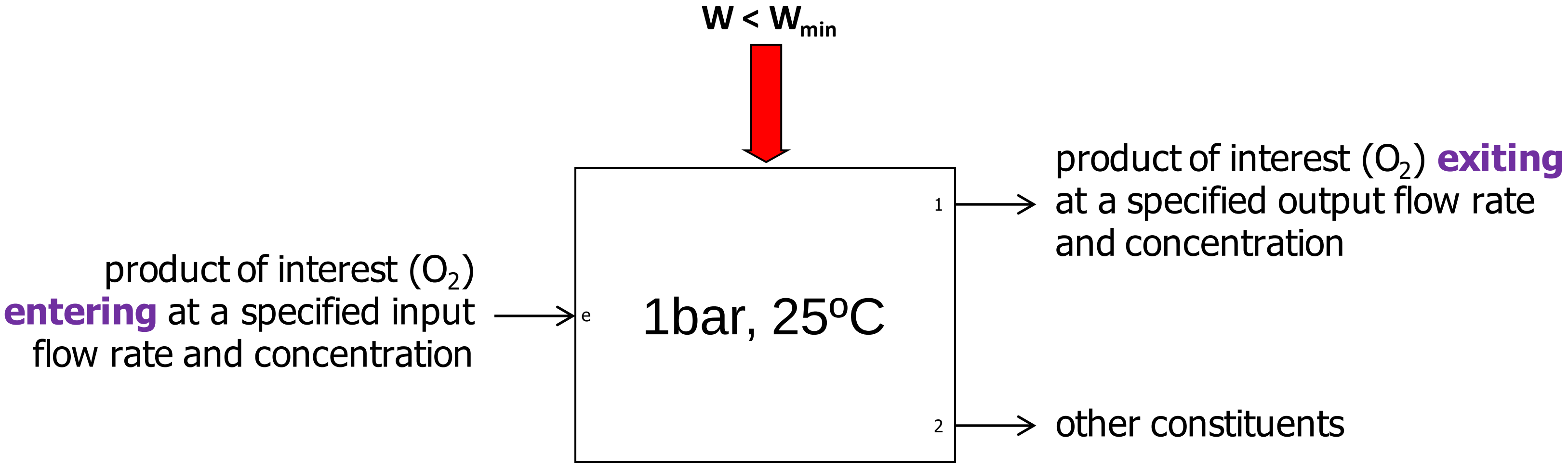
$$\ldots - \left(\dot{m}_{O_2,2} x_{O_2,2} + \dot{m}_{N_2,2} x_{N_2,2}\right)$$

Obs.: W_{min} = for complete separation

$$\frac{\dot{W}}{\dot{n}_e R T_0} = \left[y_{O_2,e} \ln(y_{O_2,e}) + y_{N_2,e} \ln(y_{N_2,e}) \right] + \ldots$$

$$\ldots - \frac{n_1}{n_e} \left[y_{O_2,1} \ln(y_{O_2,1}) + y_{N_2,1} \ln(y_{N_2,1}) \right] + \ldots$$

$$\ldots - \frac{n_2}{n_e} \left[y_{O_2,2} \ln(y_{O_2,2}) + y_{N_2,2} \ln(y_{N_2,2}) \right]$$



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1bar, 25ºC

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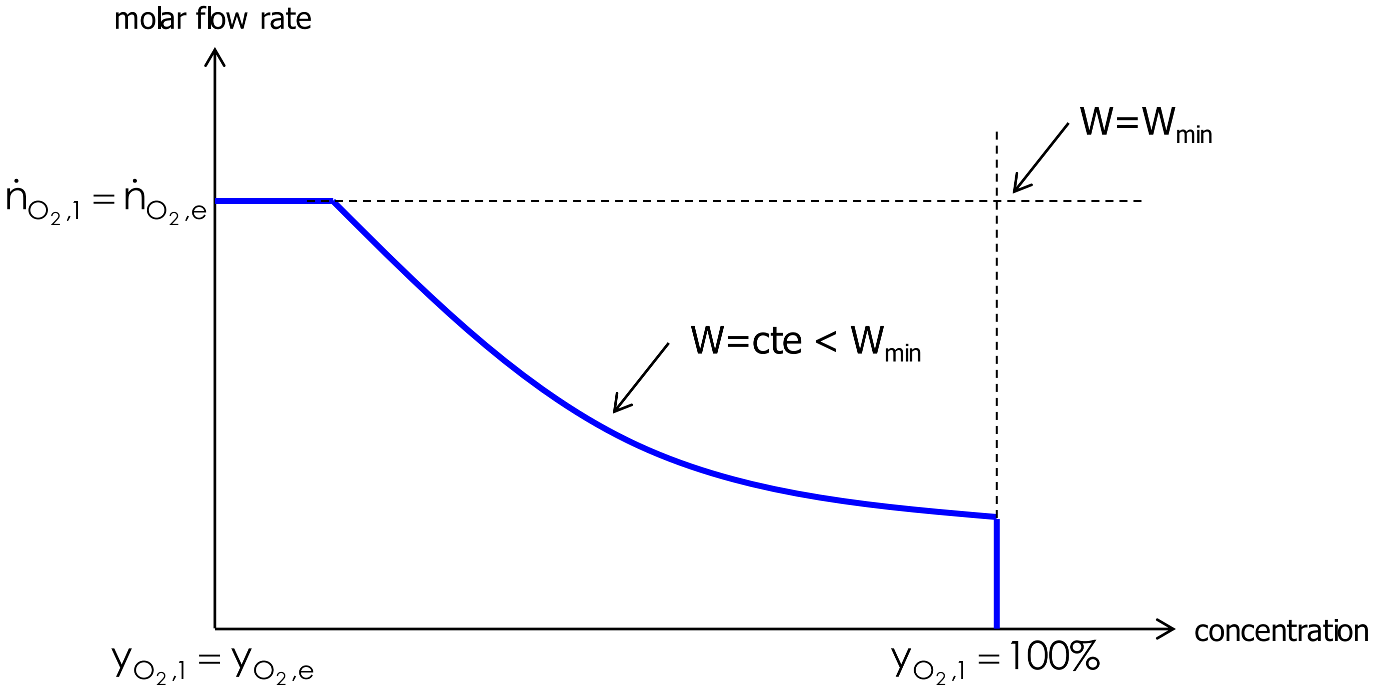
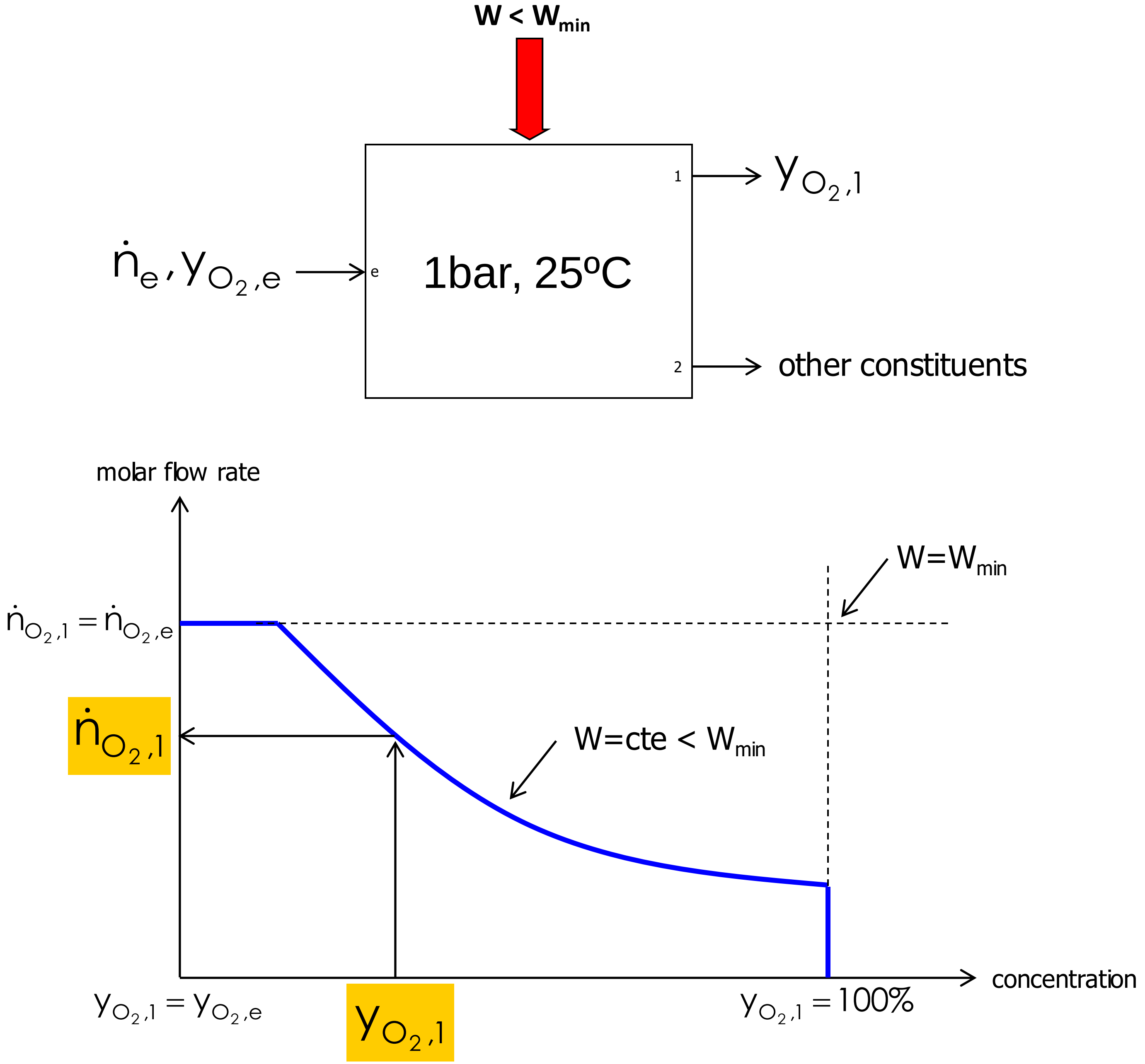


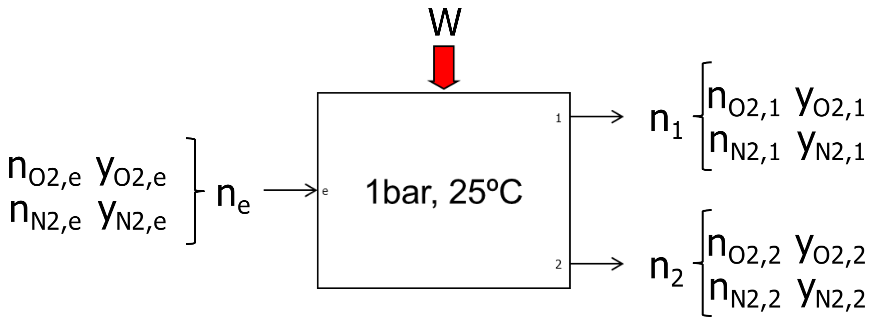
Obs.: W_{min} for complete separation



Obs.: W_{min} for complete separation

Construction of the theoretical operational envelope…

variables/parameters describing the problem = 15 →



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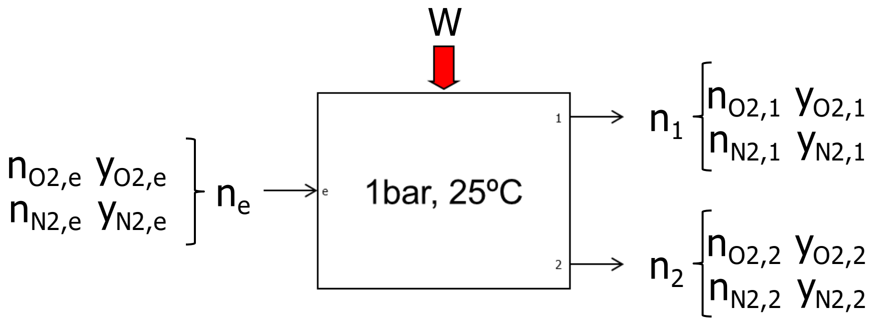
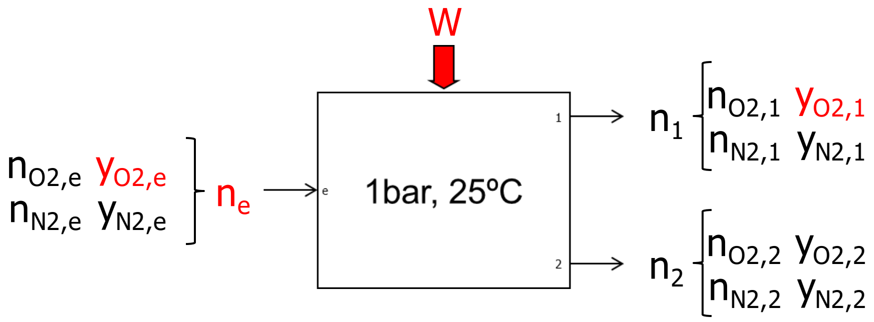


parameters known a priori = 5 →



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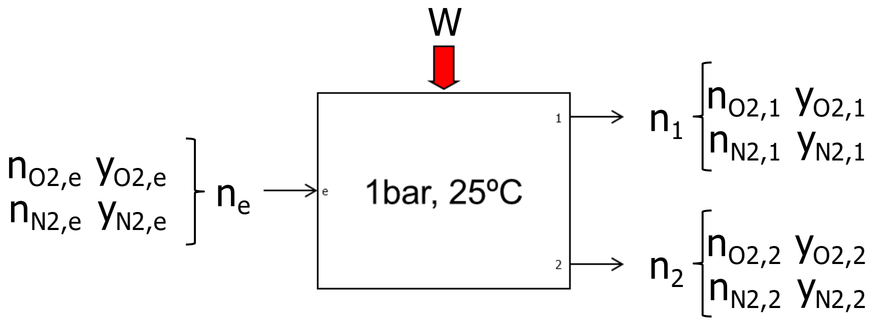
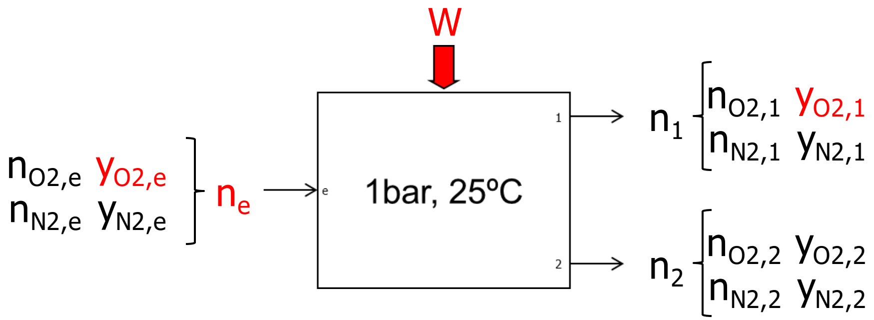


parameters known a priori = 5 →

parameters calculated = 3

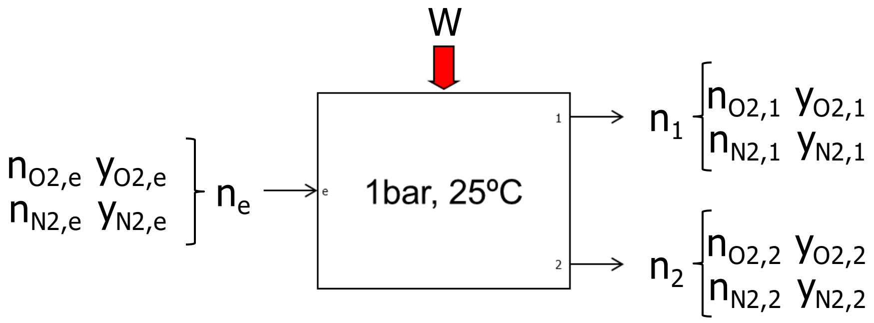


$$y_{N_2,1} = 1 - y_{O_2,1} \qquad y_{N_2,e} = 1 - y_{O_2,e}$$

$$n_{O2,e} = y_{O_2,e} \cdot n_e$$

$$n_{N2,e} = y_{N_2,e} \cdot n_e$$

variables/parameters describing the problem = 15 →



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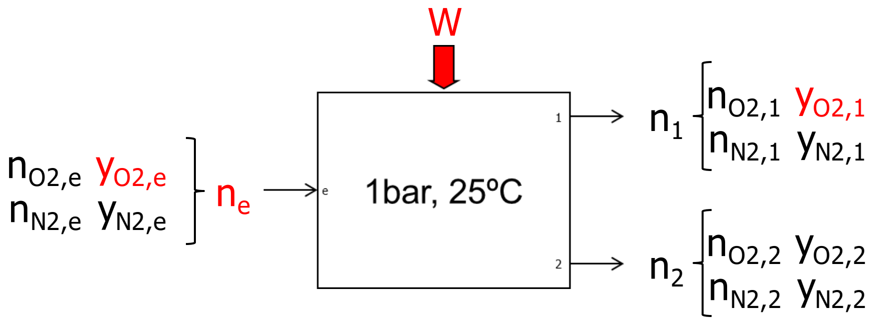

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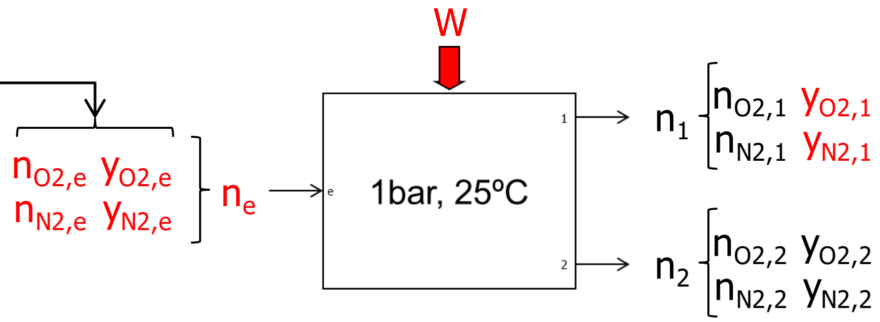
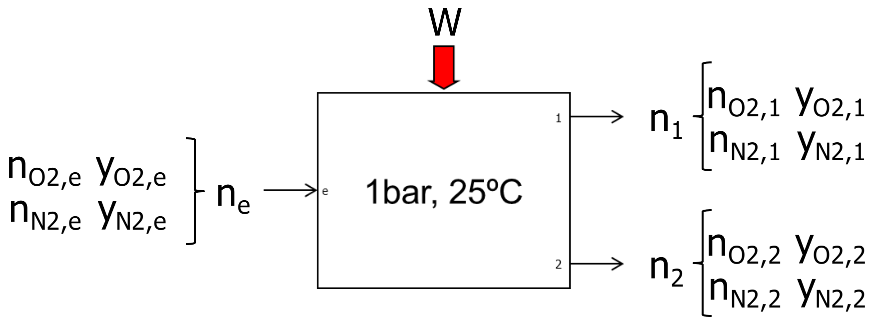


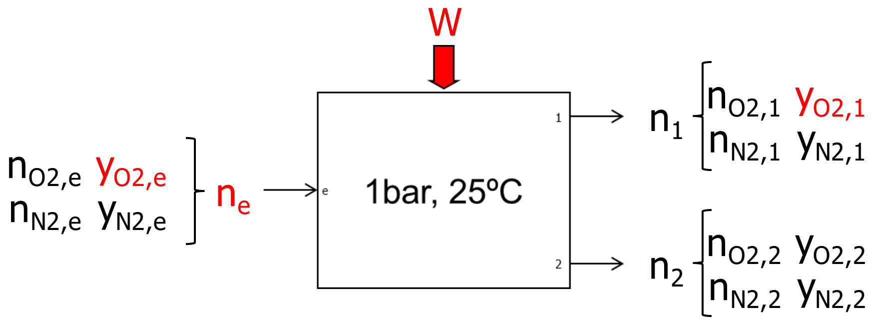
$$\longleftarrow y_{N_2,1} = 1 - y_{O_2,1}$$

variables/parameters describing the problem = 15



parameters known a priori = 5

parameters calculated = 3



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$$n_{O2,e} = y_{O_2,e} \cdot n_e$$

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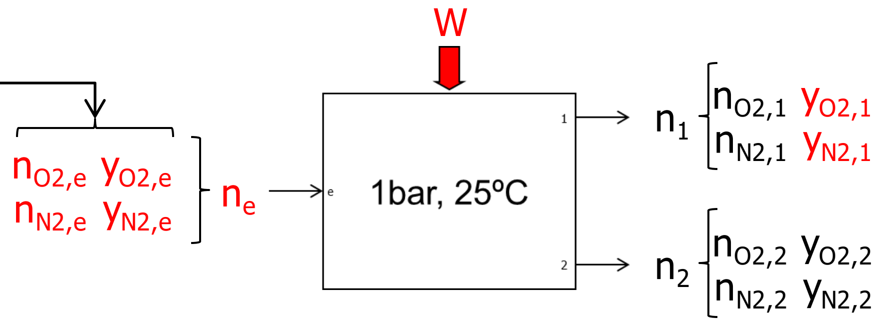
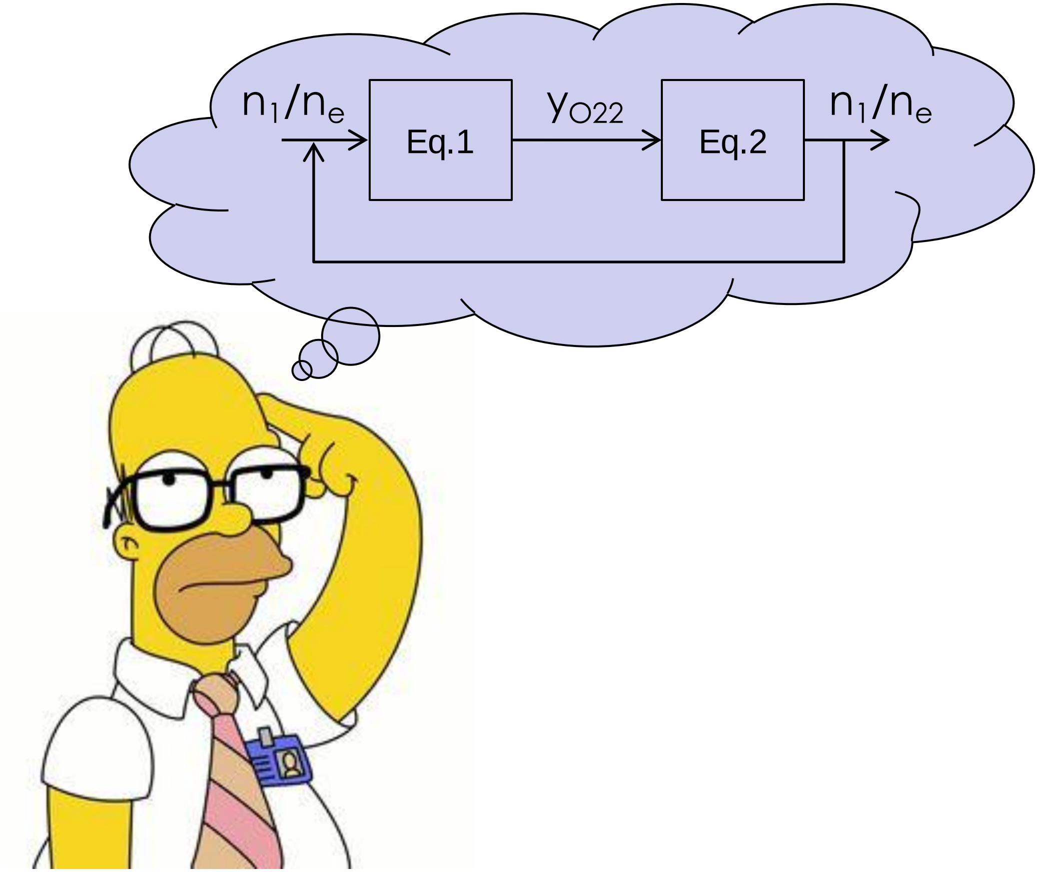


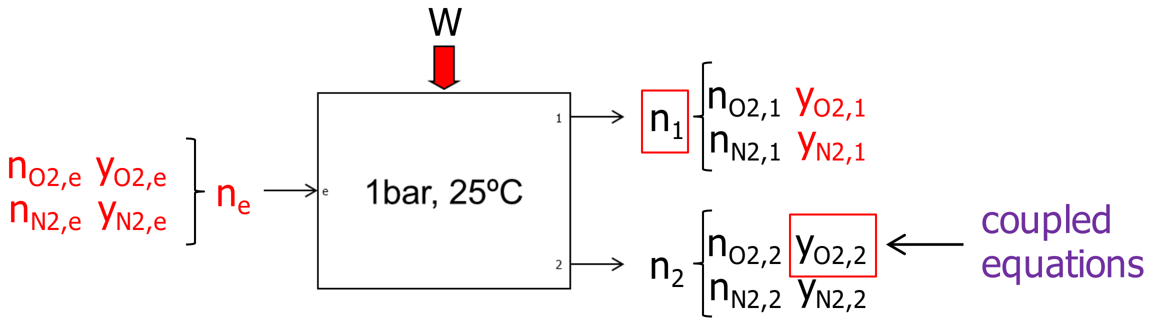
$$y_{N_2,1} = 1 - y_{O_2,1}$$

coupled equations

Functional iteration method



n_1/n_e → Eq.1 → y_{O22} → Eq.2 → n_1/n_e



$n_{O2,e}$ $y_{O2,e}$

$n_{N2,e}$ $y_{N2,e}$

n_e

W

1bar, 25ºC

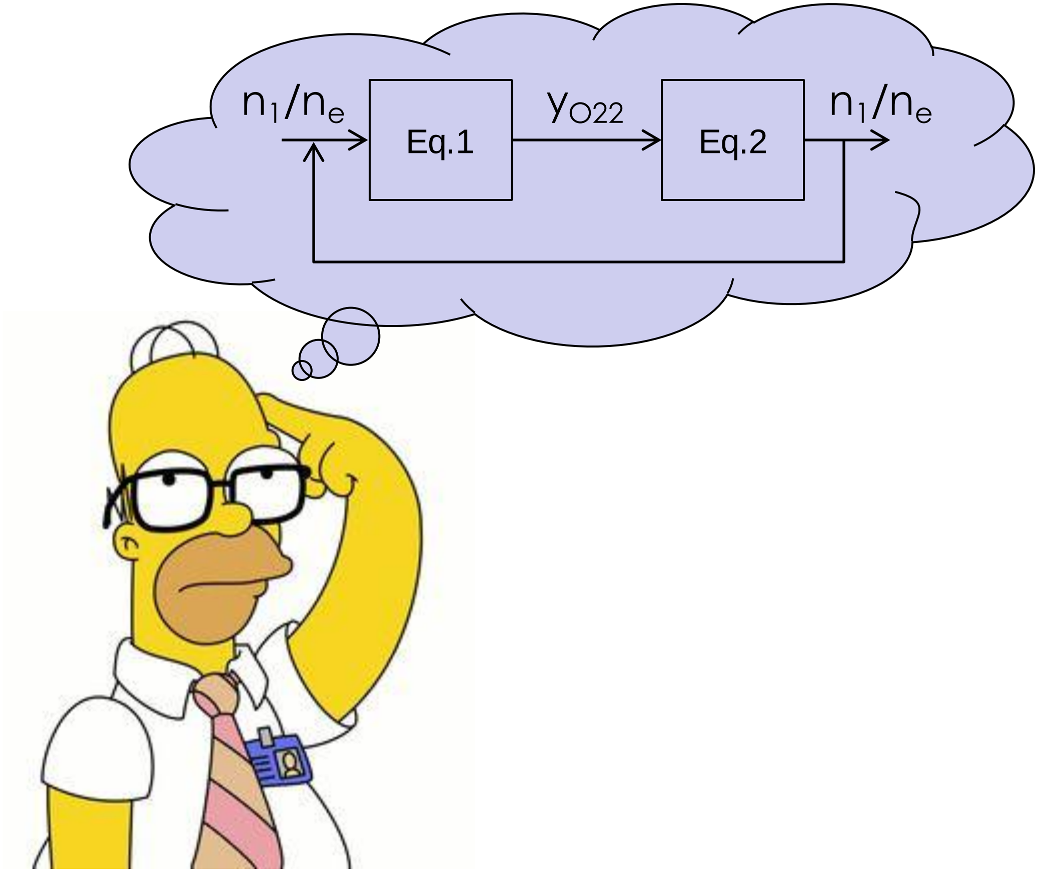
$\boxed{n_1}$ $n_{O2,1}$ $y_{O2,1}$

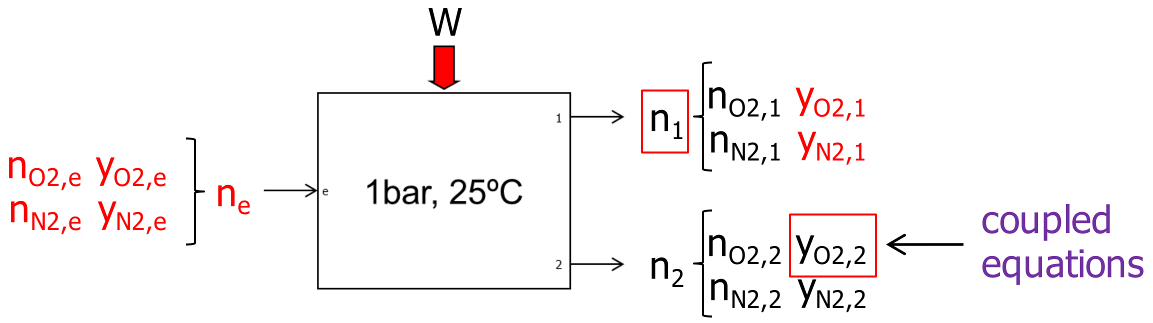
$n_{N2,1}$ $y_{N2,1}$

n_2 $n_{O2,2}$ $\boxed{y_{O2,2}}$ ← coupled equations

$n_{N2,2}$ $y_{N2,2}$

Functional iteration method





Mass balances:

$$n_{O2e} = n_{O21} + n_{O22}$$

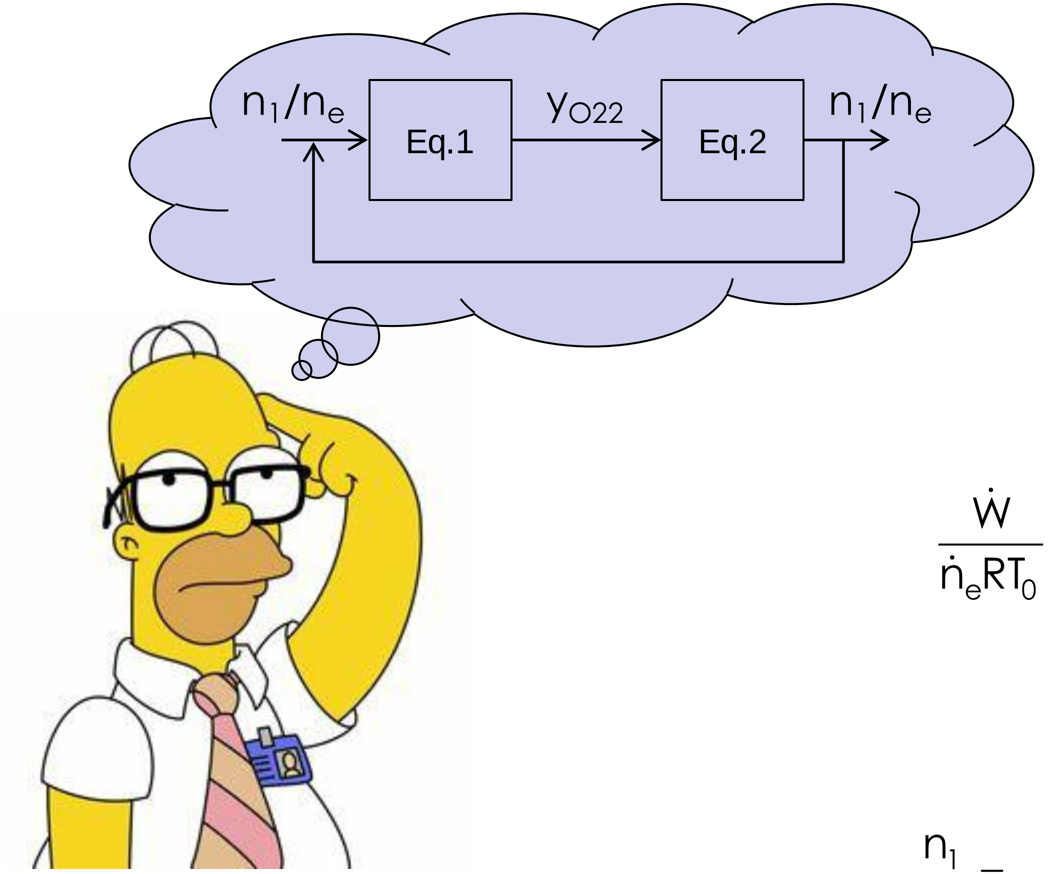
$$y_{O2e} \cdot n_e = y_{O21} \cdot n_1 + y_{O22} \cdot n_2$$

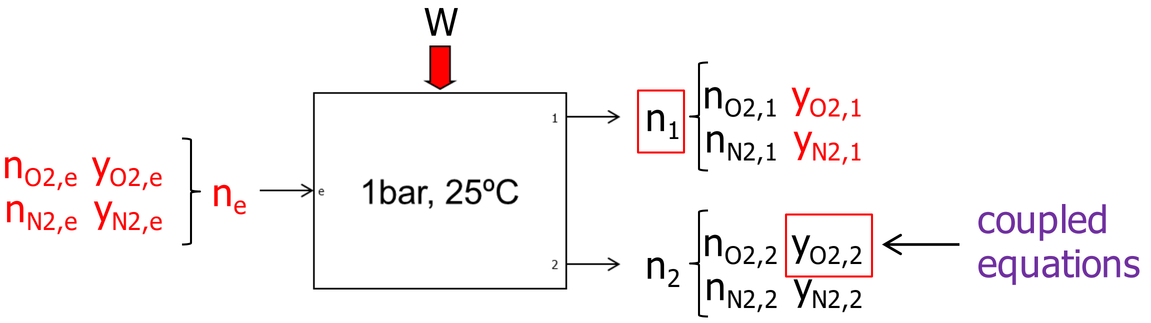
$$\Big\Downarrow \; n_e = n_1 + n_2$$

$$y_{O2e} \cdot n_e = y_{O21} \cdot n_1 + y_{O22} \cdot (n_e - n_1)$$

$$y_{O22} = \frac{y_{O2e} \cdot n_e - y_{O21} \cdot n_1}{n_e - n_1} \rightarrow \underset{\text{Eq.1}\,\uparrow}{y_{O22}} = \frac{y_{O2e} - y_{O21} \cdot n_1 / n_e}{1 - n_1 / n_e}$$

Functional iteration method





Exergy balance:

$$\frac{\dot{W}}{\dot{n}_e RT_0} = \left[y_{O_2,e}\ln(y_{O_2,e}) + y_{N_2,e}\ln(y_{N_2,e})\right] - \frac{n_1}{n_e}\left[y_{O_2,1}\ln(y_{O_2,1}) + y_{N_2,1}\ln(y_{N_2,1})\right] + \ldots$$

$$\ldots - \frac{n_2}{n_e}\left[y_{O_2,2}\ln(y_{O_2,2}) + y_{N_2,2}\ln(y_{N_2,2})\right]$$

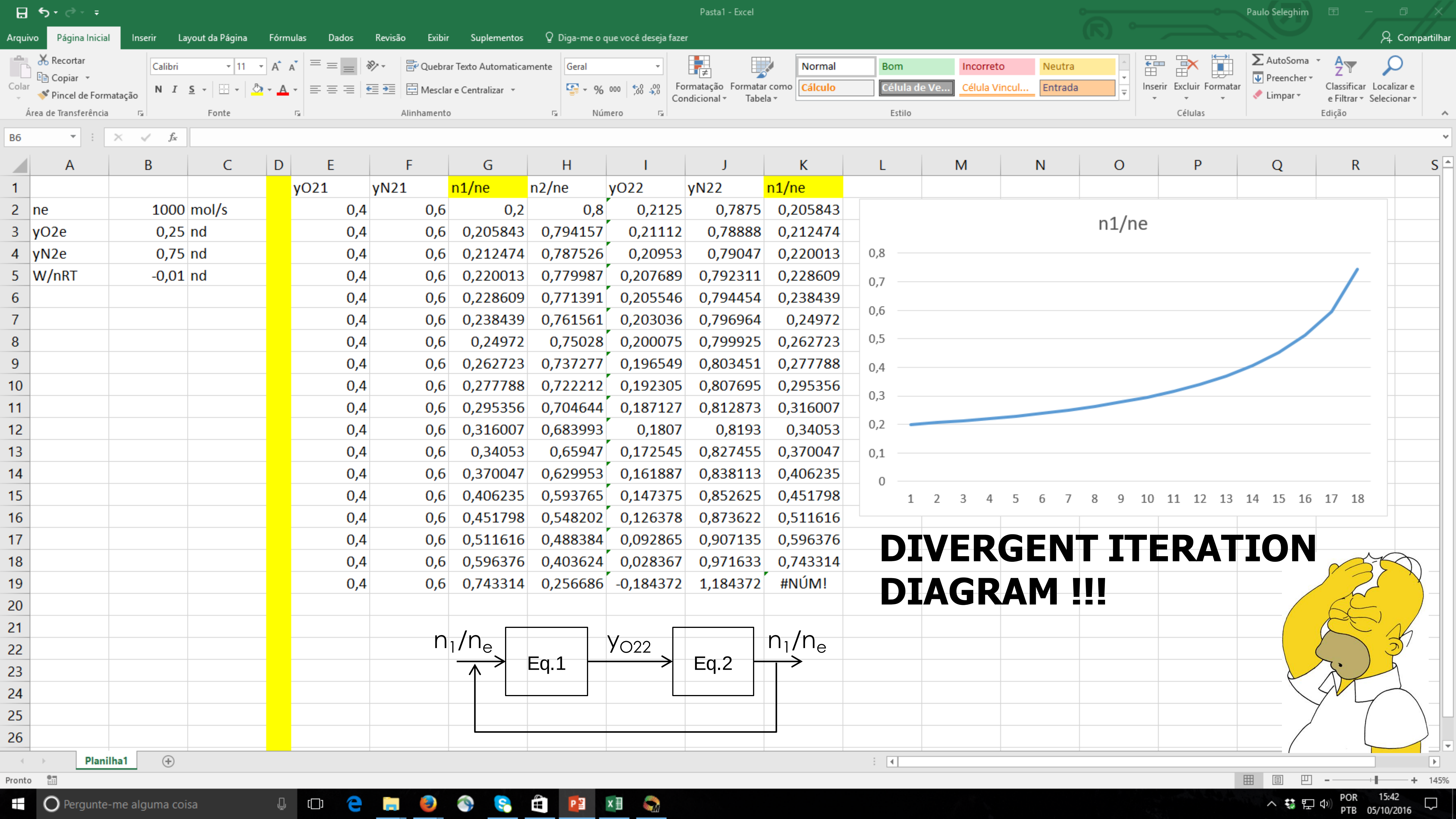
$$\frac{n_1}{n_e} = \frac{1}{\left[y_{O_2,1}\ln(y_{O_2,1}) + y_{N_2,1}\ln(y_{N_2,1})\right]} \cdot \left(\left[y_{O_2,e}\ln(y_{O_2,e}) + y_{N_2,e}\ln(y_{N_2,e})\right] - \frac{\dot{W}}{\dot{n}_e RT_0} \ldots\right.$$

$$\left.\ldots - \frac{n_2}{n_e}\left[y_{O_2,2}\ln(y_{O_2,2}) + y_{N_2,2}\ln(y_{N_2,2})\right]\right)$$

Eq.2

$n_2 / n_e = 1 - n_1 / n_e$

$y_{N22} = 1 - y_{O22}$

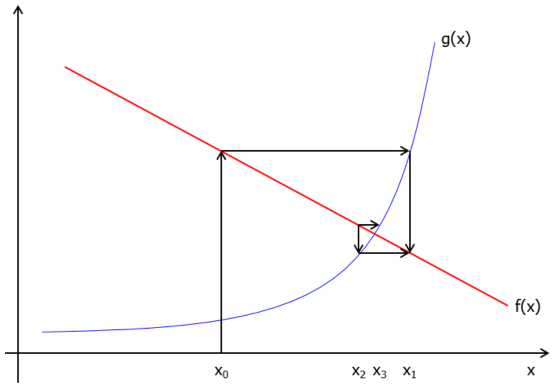


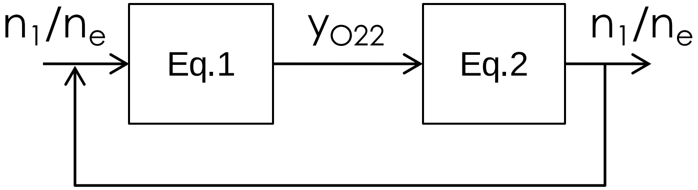
	A	B	C	D	E	F	G	H	I	J	K
1					yO21	yN21	n1/ne	n2/ne	yO22	yN22	n1/ne
2	ne	1000	mol/s		0,4	0,6	0,2	0,8	0,2125	0,7875	0,205843
3	yO2e	0,25	nd		0,4	0,6	0,205843	0,794157	0,21112	0,78888	0,212474
4	yN2e	0,75	nd		0,4	0,6	0,212474	0,787526	0,20953	0,79047	0,220013
5	W/nRT	-0,01	nd		0,4	0,6	0,220013	0,779987	0,207689	0,792311	0,228609
6					0,4	0,6	0,228609	0,771391	0,205546	0,794454	0,238439
7					0,4	0,6	0,238439	0,761561	0,203036	0,796964	0,24972
8					0,4	0,6	0,24972	0,75028	0,200075	0,799925	0,262723
9					0,4	0,6	0,262723	0,737277	0,196549	0,803451	0,277788
10					0,4	0,6	0,277788	0,722212	0,192305	0,807695	0,295356
11					0,4	0,6	0,295356	0,704644	0,187127	0,812873	0,316007
12					0,4	0,6	0,316007	0,683993	0,1807	0,8193	0,34053
13					0,4	0,6	0,34053	0,65947	0,172545	0,827455	0,370047
14					0,4	0,6	0,370047	0,629953	0,161887	0,838113	0,406235
15					0,4	0,6	0,406235	0,593765	0,147375	0,852625	0,451798
16					0,4	0,6	0,451798	0,548202	0,126378	0,873622	0,511616
17					0,4	0,6	0,511616	0,488384	0,092865	0,907135	0,596376
18					0,4	0,6	0,596376	0,403624	0,028367	0,971633	0,743314
19					0,4	0,6	0,743314	0,256686	-0,184372	1,184372	#NÚM!

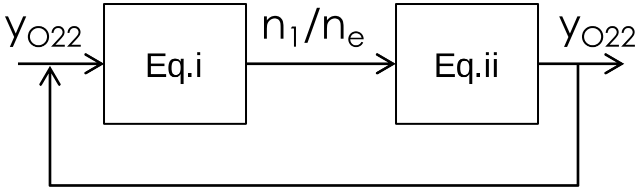
DIVERGENT ITERATION DIAGRAM !!!

MODIFICATION OF THE ITERATION DIAGRAM...

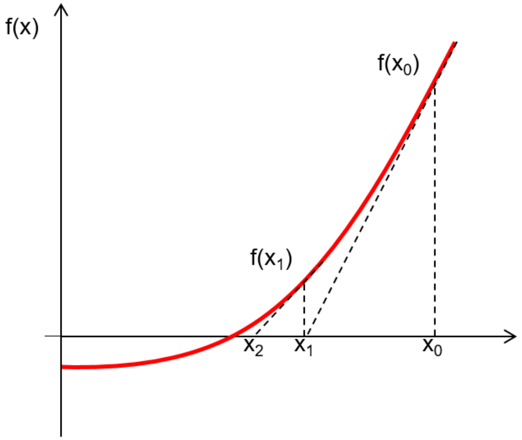
$x_{k+1} = g^{-1}(f(x_k))$




n_1/n_e → Eq.1 → y_{O22} → Eq.2 → n_1/n_e


y_{O22} → Eq.i → n_1/n_e → Eq.ii → y_{O22}

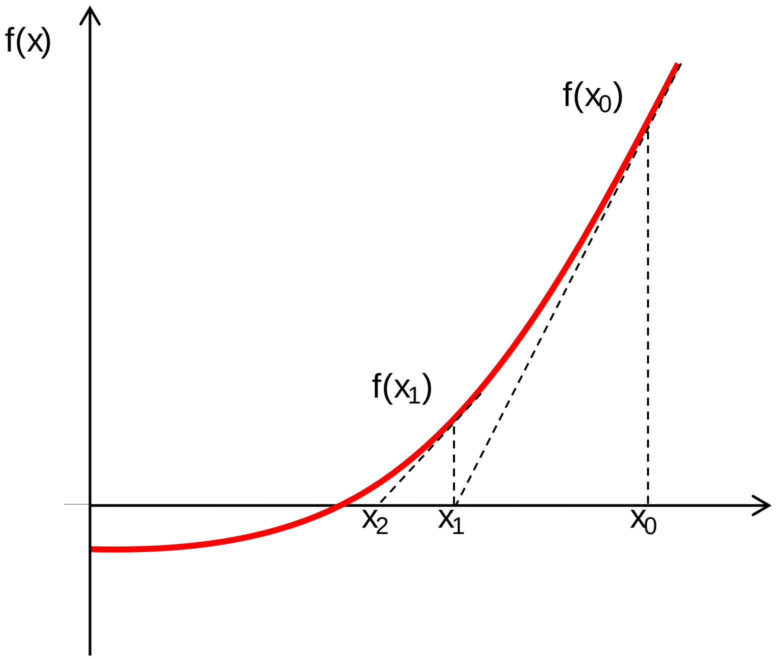
SOLUTION BY THE NEWTON-RAPHSON METHOD...



$$x_{k+1} = x_k - \frac{1}{f'(x_k)} \times f(x_k)$$

$$[x_{k+1}] = [x_k] - [Jac]^{-1}[f(x_k)]$$

Solution by the Newton-Raphson method: 1D



Equation of tangent line:

$$y = a \cdot x + b$$

$$a = f'(x_0)$$

$$f(x_0) = f'(x_0) \cdot x_0 + b$$

$$b = f(x_0) - f'(x_0) \cdot x_0$$

Root of tangent line:

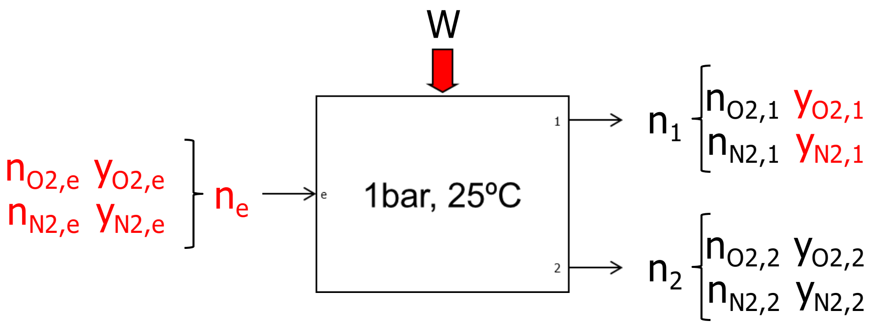
$$x = -b / a$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

⇒

Recurrence formula:

$$x_{k+1} = x_k - \frac{1}{f'(x_k)} \times f(x_k)$$



W

$n_{O2,e}$ $y_{O2,e}$
$n_{N2,e}$ $y_{N2,e}$
n_e

e

1bar, 25ºC

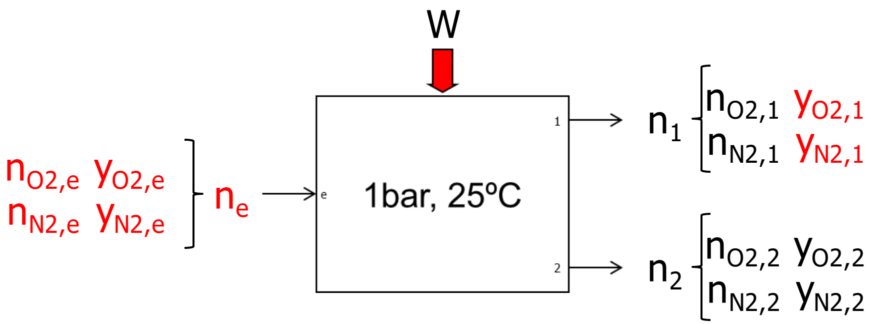
1

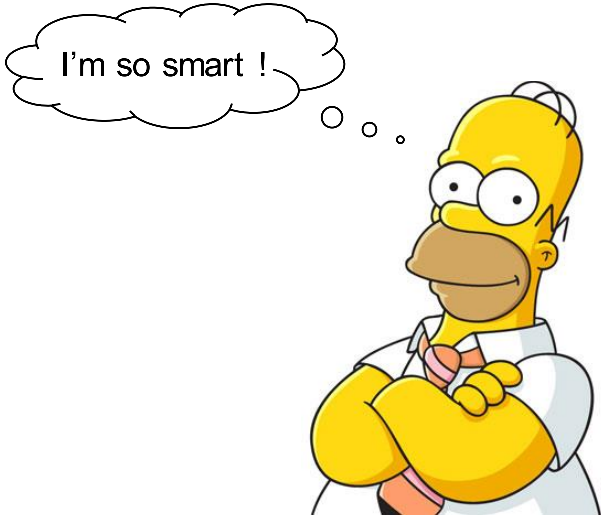
2

n_1 $n_{O2,1}$ $y_{O2,1}$
$n_{N2,1}$ $y_{N2,1}$

n_2 $n_{O2,2}$ $y_{O2,2}$
$n_{N2,2}$ $y_{N2,2}$

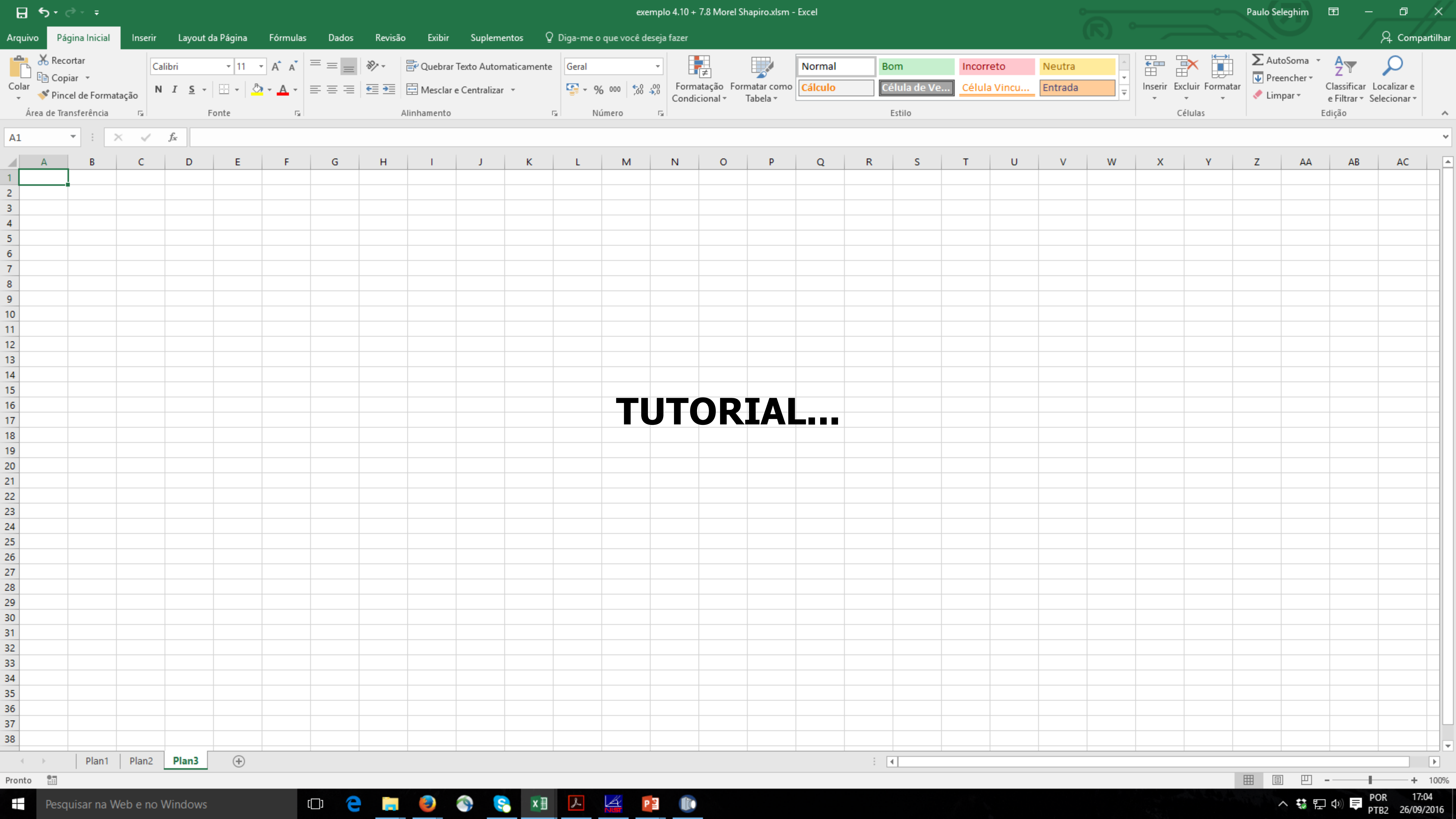
$$\frac{n_1}{n_e} = \frac{1}{\left[y_{O_2,1}\ln(y_{O_2,1}) + y_{N_2,1}\ln(y_{N_2,1})\right]} \cdot \left(\left[y_{O_2,e}\ln(y_{O_2,e}) + y_{N_2,e}\ln(y_{N_2,e})\right] - \frac{\dot{W}}{\dot{n}_e R T_0} - \frac{n_2}{n_e}\left[y_{O_2,2}\ln(y_{O_2,2}) + y_{N_2,2}\ln(y_{N_2,2})\right]\right)$$





$$\frac{n_1}{n_e}=\frac{1}{\left[y_{O_2,1}\ln(y_{O_2,1})+y_{N_2,1}\ln(y_{N_2,1})\right]}\cdot\left(\left[y_{O_2,e}\ln(y_{O_2,e})+y_{N_2,e}\ln(y_{N_2,e})\right]-\frac{\dot{W}}{\dot{n}_eRT_0}-\underbrace{\frac{n_2}{n_e}}_{\frac{n_2}{n_e}=1-\frac{n_1}{n_e}}\left[\underbrace{y_{O_2,2}\ln(y_{O_2,2})}_{y_{O22}=\frac{y_{O2e}-y_{O21}\cdot n_1/n_e}{1-n_1/n_e}}+\underbrace{y_{N_2,2}\ln(y_{N_2,2})}_{y_{N22}=1-y_{O22}}\right]\right)$$

$$\boxed{f(n_1/n_e)=0\ \rightarrow\qquad x_{k+1}=x_k-\frac{1}{f'(x_k)}\cdot f(x_k)}$$


exemplo 4.10 + 7.8 Morel Shapiro.xlsm - Excel
Paulo Seleghim
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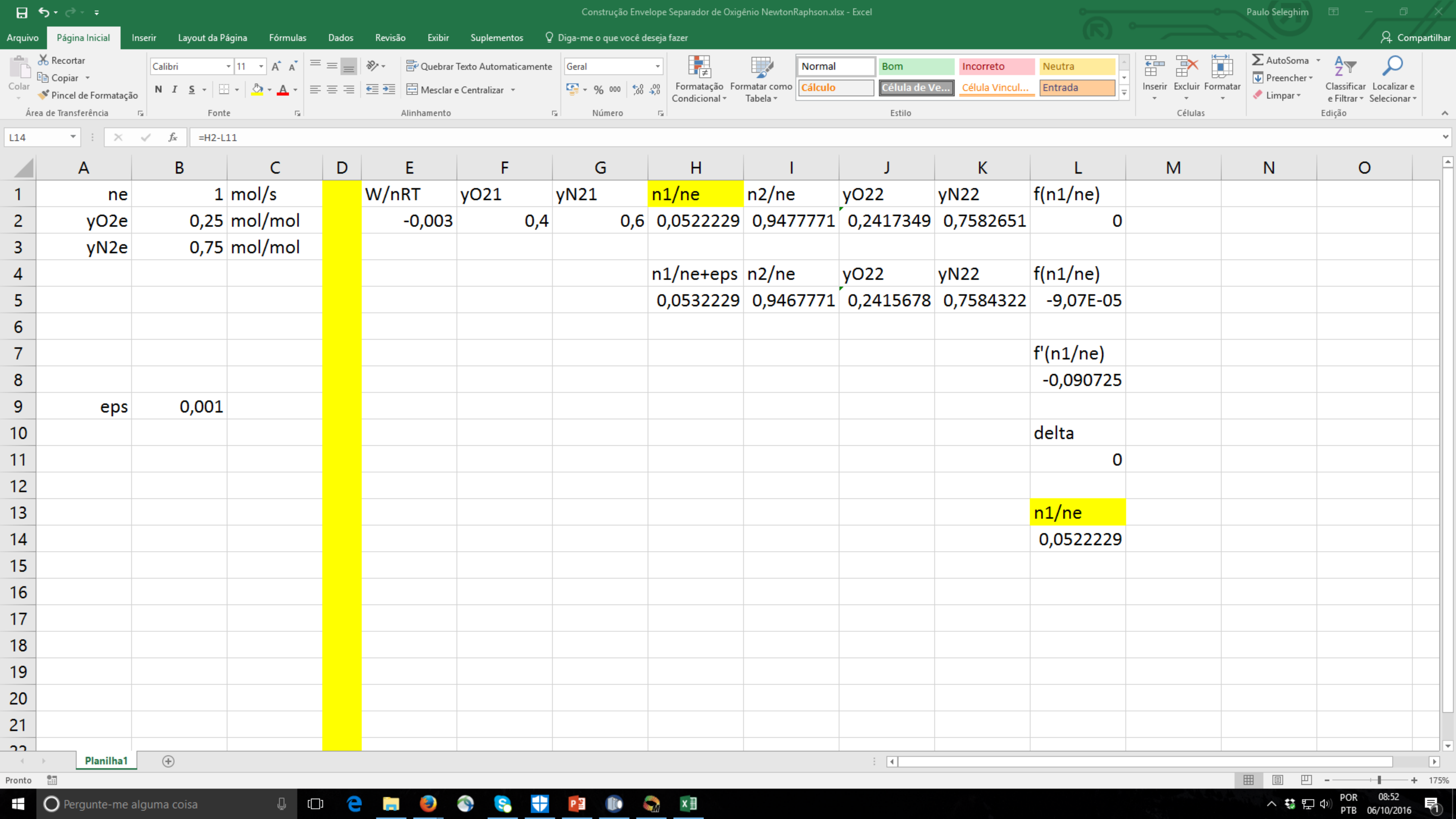
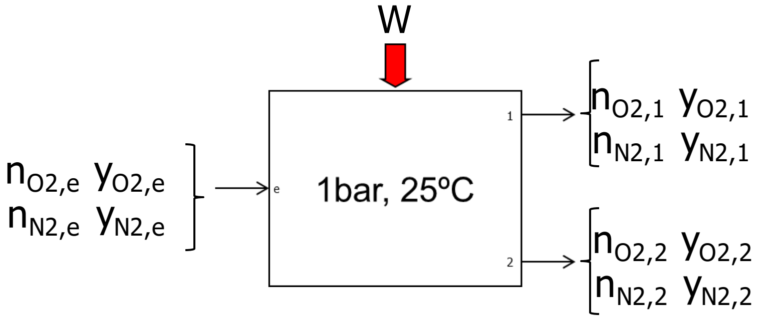
TUTORIAL...



L14 =H2-L11

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	ne	1	mol/s		W/nRT	yO21	yN21	n1/ne	n2/ne	yO22	yN22	f(n1/ne)			
2	yO2e	0,25	mol/mol		-0,003	0,4	0,6	0,0522229	0,9477771	0,2417349	0,7582651	0			
3	yN2e	0,75	mol/mol												
4								n1/ne+eps	n2/ne	yO22	yN22	f(n1/ne)			
5								0,0532229	0,9467771	0,2415678	0,7584322	-9,07E-05			
6															
7												f'(n1/ne)			
8												-0,090725			
9	eps	0,001													
10												delta			
11												0			
12															
13												n1/ne			
14												0,0522229			
15															
16															
17															
18															
19															
20															
21															

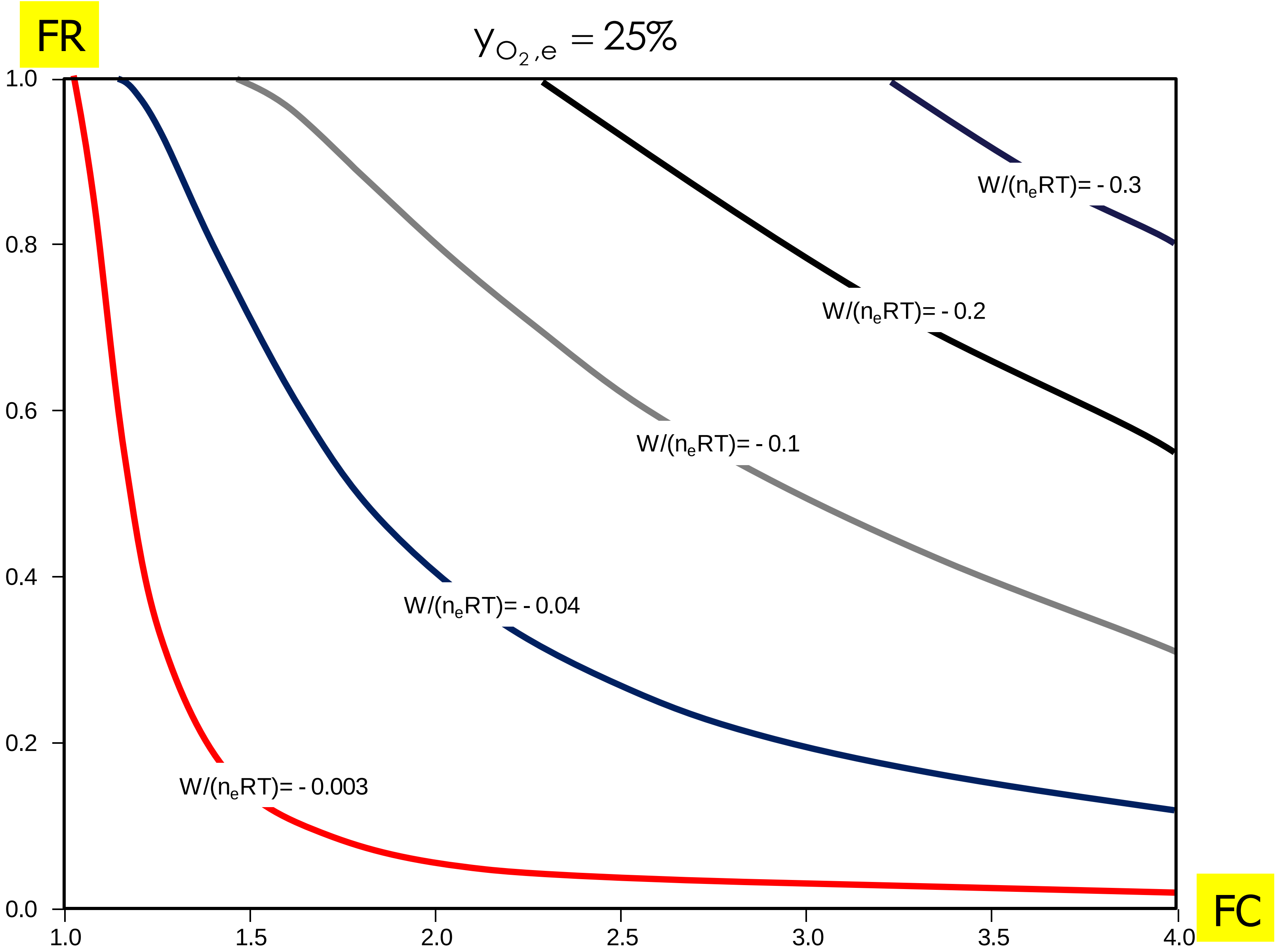


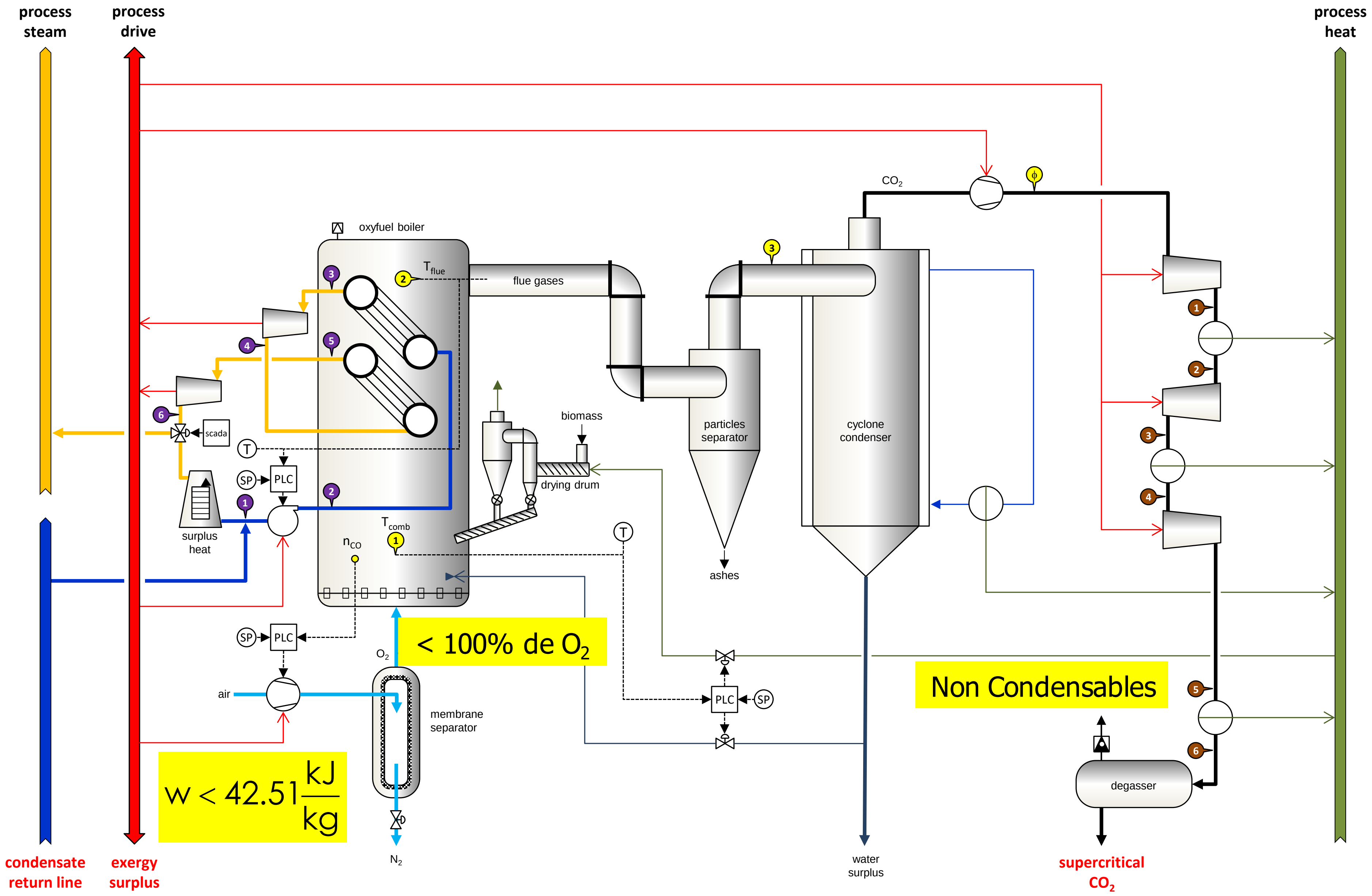
Recovery Factor

$$FR = \frac{\dot{n}_{O_2,1}}{\dot{n}_{O_2,e}}$$

Concentration Factor

$$FC = y_{O_2,1} / y_{O_2,e}$$





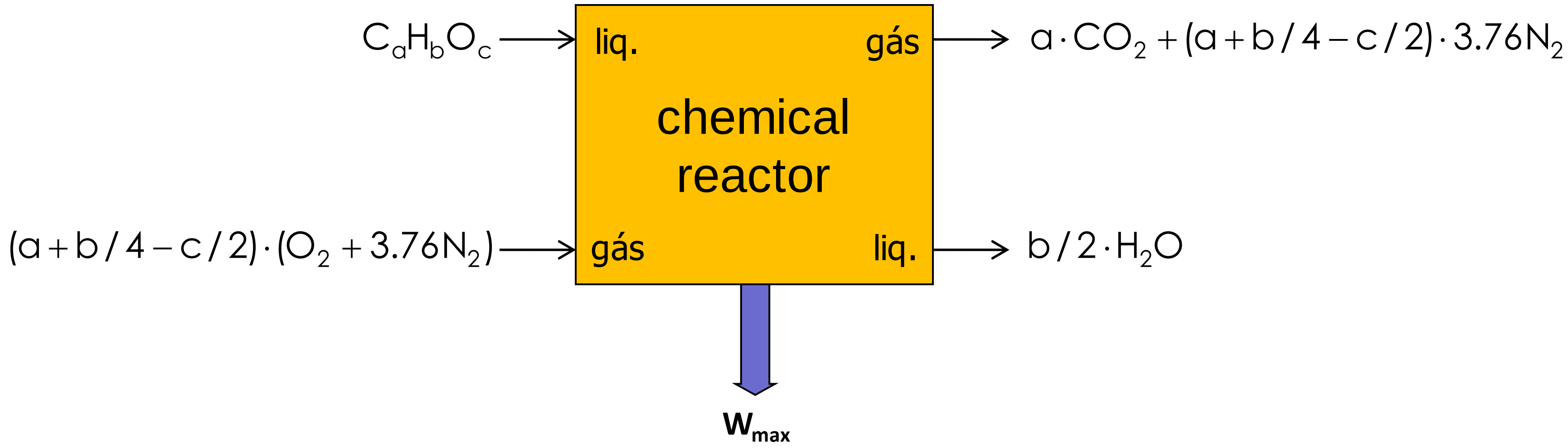
$< 100\%$ de O_2

Non Condensables

$$w < 42.51 \frac{kJ}{kg}$$

Next class: CHEMICAL EXERGY

$$C_aH_bO_c + (a + b/4 - c/2)\cdot(O_2 + 3.76N_2) \xrightarrow{P_0,T_0} a\cdot CO_2 + b/2\cdot H_2O$$



$C_aH_bO_c$ → liq.

$(a + b/4 - c/2)\cdot(O_2 + 3.76N_2)$ → gás

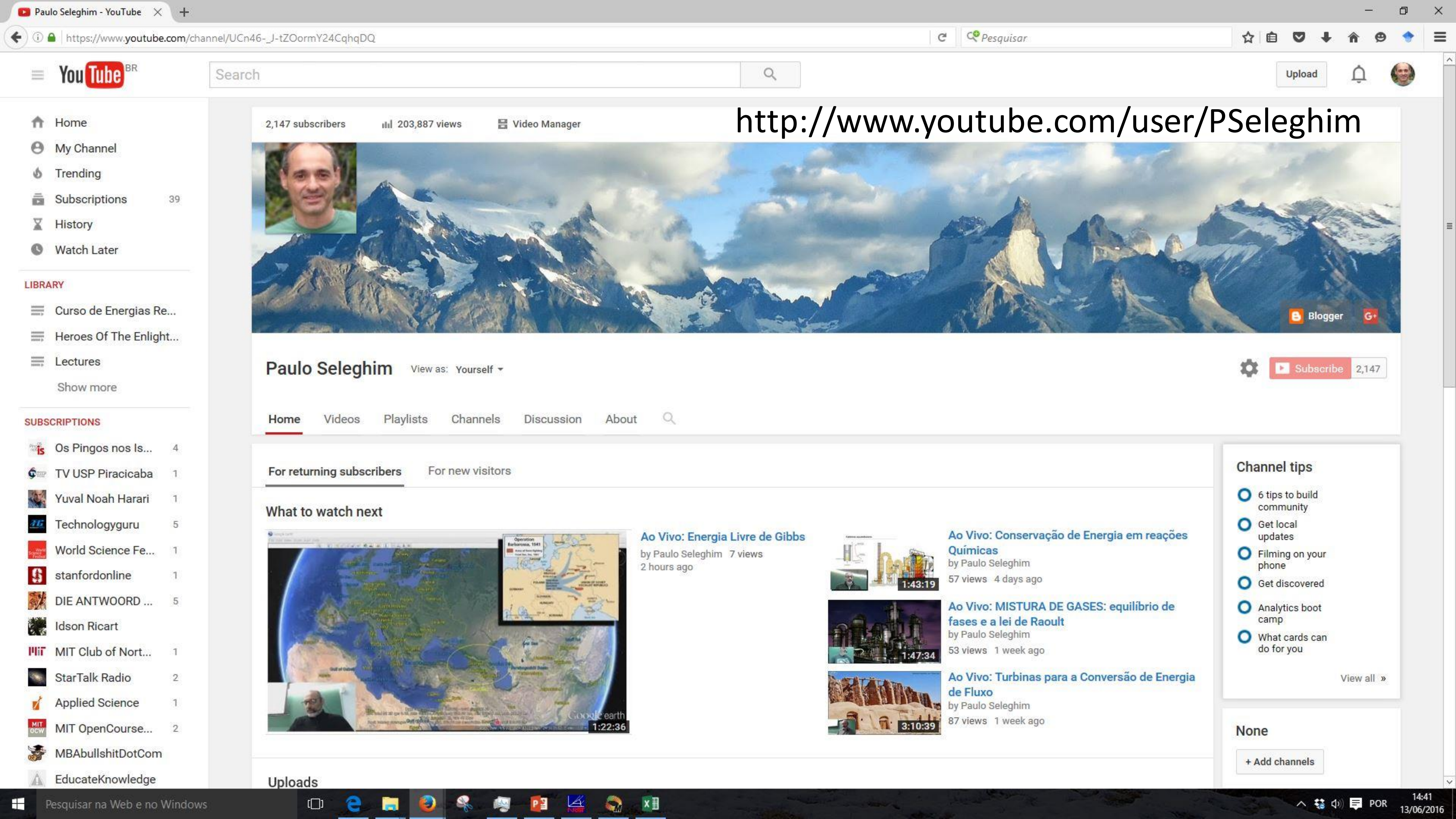
chemical reactor

gás → $a\cdot CO_2 + (a + b/4 - c/2)\cdot 3.76N_2$

liq. → $b/2\cdot H_2O$

$\mathbf{W_{max}}$

The maximum amount of mechanical work (organized energy) that can be obtained from a chemical compound in a specific environment…



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