



UNIVERSIDAD DE LAS PALMAS
DE GRAN CANARIA



Università degli Studi di Firenze

ADVANCED THERMODYNAMICS AND THERMOECONOMICS

Seminar:

***Advanced exergetic analysis of a steam methane
reforming process for hydrogen production***

27th May, 2010

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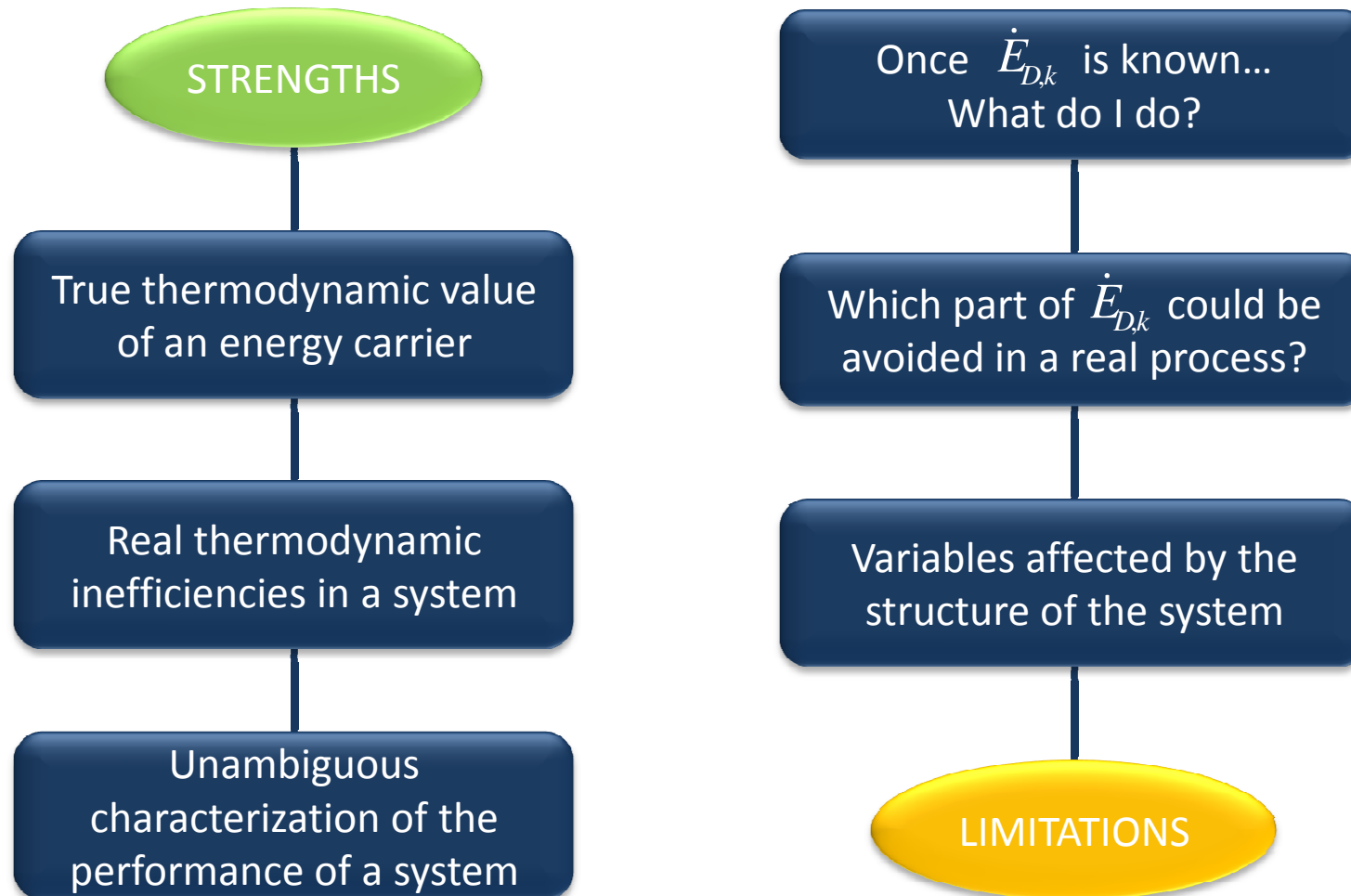
- Introduction
- Conventional Exergetic Analysis
- Advanced Exergetic Analysis
- Application to a SMR process for H₂ production
- Conclusions

- ❑ *Introduction*
- ❑ Conventional Exergetic Analysis
- ❑ Advanced Exergetic Analysis
- ❑ Application to a SMR process for H₂ production
- ❑ Conclusions

Exergy analysis $\xrightarrow{\text{What?}}$ Location
Magnitude
Sources \longrightarrow Thermodynamic
inefficiencies

Exergy analysis $\xrightarrow{\text{Exclusive}}$ Not provided by other means

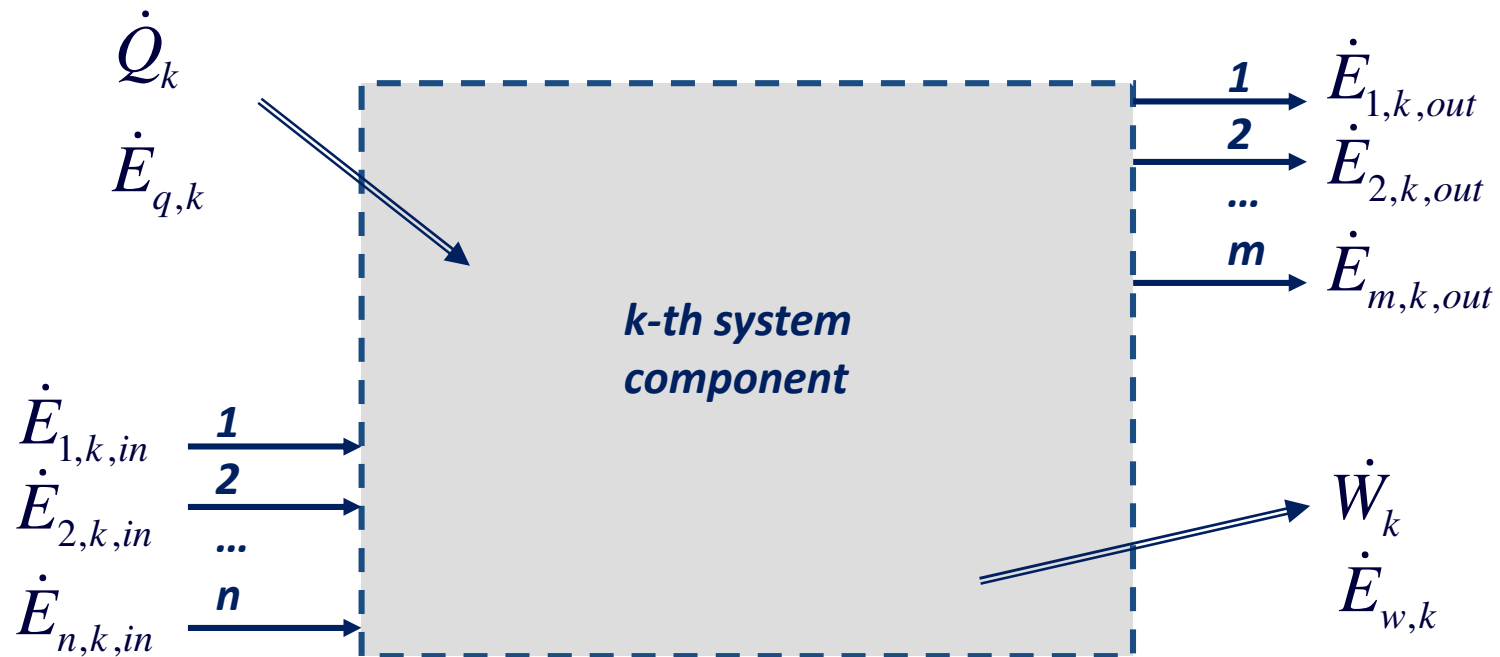
Exergy analysis $\xrightarrow{\text{Why?}}$ Improving:
• overall efficiency
• cost effectiveness
Performance comparison



- Introduction
- *Conventional Exergetic Analysis*
 - Exergy analysis
 - Exergoeconomic analysis
 - Exergoenvironmental analysis
- Advanced Exergetic Analysis
- Application to a SMR process for H₂ production
- Conclusions

Exergy analysis

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$$\sum_{i=1}^n \dot{E}_{i,k,in} + \dot{E}_{q,k} = \sum_{i=1}^m \dot{E}_{i,k,out} + \dot{E}_{w,k} + \dot{E}_{D,k} + \dot{E}_{L,k}$$

Exergy analysis

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Exergy destruction rate

$$\dot{E}_{D,k} = T_0 \cdot \dot{S}_{gen,k}$$

Exergy loss rate

$$\dot{E}_{L,k}$$

Exergetic efficiency

$$\varepsilon_k = \frac{\dot{E}_{P,k}}{\dot{E}_{F,k}}$$

Exergy balance *k*th: $\dot{E}_{F,k} = \dot{E}_{P,k} + \dot{E}_{D,k} + \dot{E}_{L,k}$

Total exergy balance : $\dot{E}_{F,tot} = \dot{E}_{P,tot} + \sum_k \dot{E}_{D,k} + \dot{E}_{L,tot}$

Exergy destruction ratio

$$y_{D,k} = \frac{\dot{E}_{D,k}}{\dot{E}_{F,tot}}$$

Percentage of Exergy destruction

$$y_{D,k}^* = \frac{\dot{E}_{D,k}}{\sum_i \dot{E}_{D,i}}$$

Exergy loss ratio

$$y_{L,k} = \frac{\dot{E}_{L,k}}{\dot{E}_{F,tot}}$$



Fuel ➡ resources expended

- ❑ Regarding **material streams: exergy decreases** between inlet and outlet **minus exergy increases** that are not in accord with the purpose of the component..
- ❑ Due to **other flows: exergy values** to be considered at the **inlet**.

Product ➡ results generated

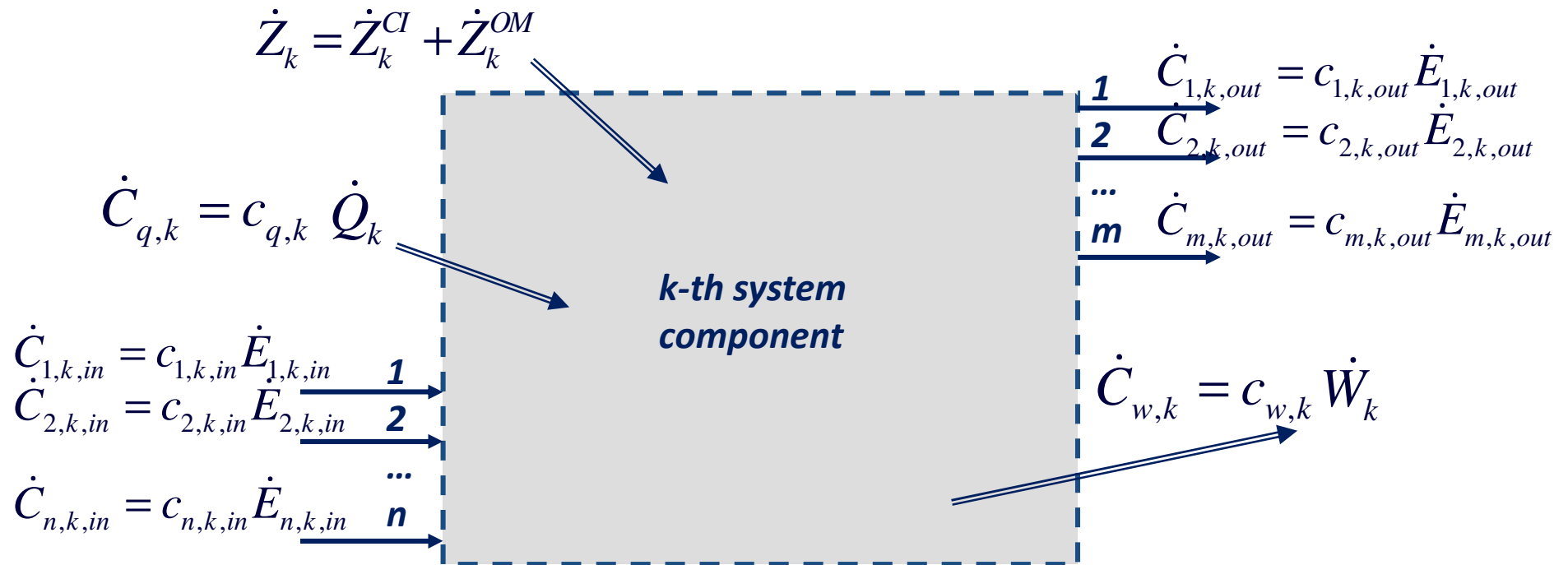
- ❑ Regarding **material streams: exergy increases** between inlet and outlet that are in accord with the purpose of the component.
- ❑ Due to **other flows: exergy values** to be considered at the **outlet**.



1. $\downarrow \dot{E}_{D,k}$
 - \downarrow Thermodynamic inefficiencies
 - \downarrow Investment cost
2. Exergy assign monetary values
 - Interactions system - surroundings
 - Sources thermodynamic inefficiencies
3. Cost of exergy destruction
 - Different for each component
 - Depends on its relative position

Conducted at the component level

Identifies the relative cost importance



$$\sum_{i=1}^n \dot{C}_{i,k,in} + \dot{C}_{q,k} + \dot{Z}_k = \sum_{i=1}^m \dot{C}_{i,k,out} + \dot{C}_{w,k}$$

Exergy costing

$$\dot{C}_j = c_j \dot{E}_j$$

Cost balances:

$$\dot{C}_{P,k} = \dot{C}_{F,k} + \dot{Z}_k$$

$$c_{P,k} \dot{E}_{P,k} = c_{F,k} \dot{E}_{F,k} + \dot{Z}_k$$

$$\dot{Z}_k = \dot{Z}_k^{CI} + \dot{Z}_k^{OM}$$

Auxiliary costing equations

(Lazzaretto and Tsatsaronis, 2006)

Cost exergy destruction

$$\dot{C}_{D,k} = c_{F,k} \dot{E}_{D,k}$$

Relative cost difference

$$r = \frac{c_{P,k} - c_{F,k}}{c_{F,k}} = \frac{1 - \varepsilon_k}{\varepsilon_k} + \frac{\dot{Z}_k}{\dot{C}_{D,k}}$$

Exergoeconomic factor

$$f_k = \frac{\dot{Z}_k}{\dot{Z}_k + \dot{C}_{D,k}}$$



F Equations

The specific cost (cost per exergy unit) associated with the removal of exergy from a fuel stream in a component *is equal to* the average specific cost at which the removed exergy was supplied to the same stream in upstream components

The exergy difference of this stream between inlet and outlet is considered in the definition of *fuel* for the component.

P Equations

Each exergy unit is supplied to any stream associated with the product of a component at the same average cost $c_{P,k}$




This cost can be calculated directly from the cost balance and the *F* equations.

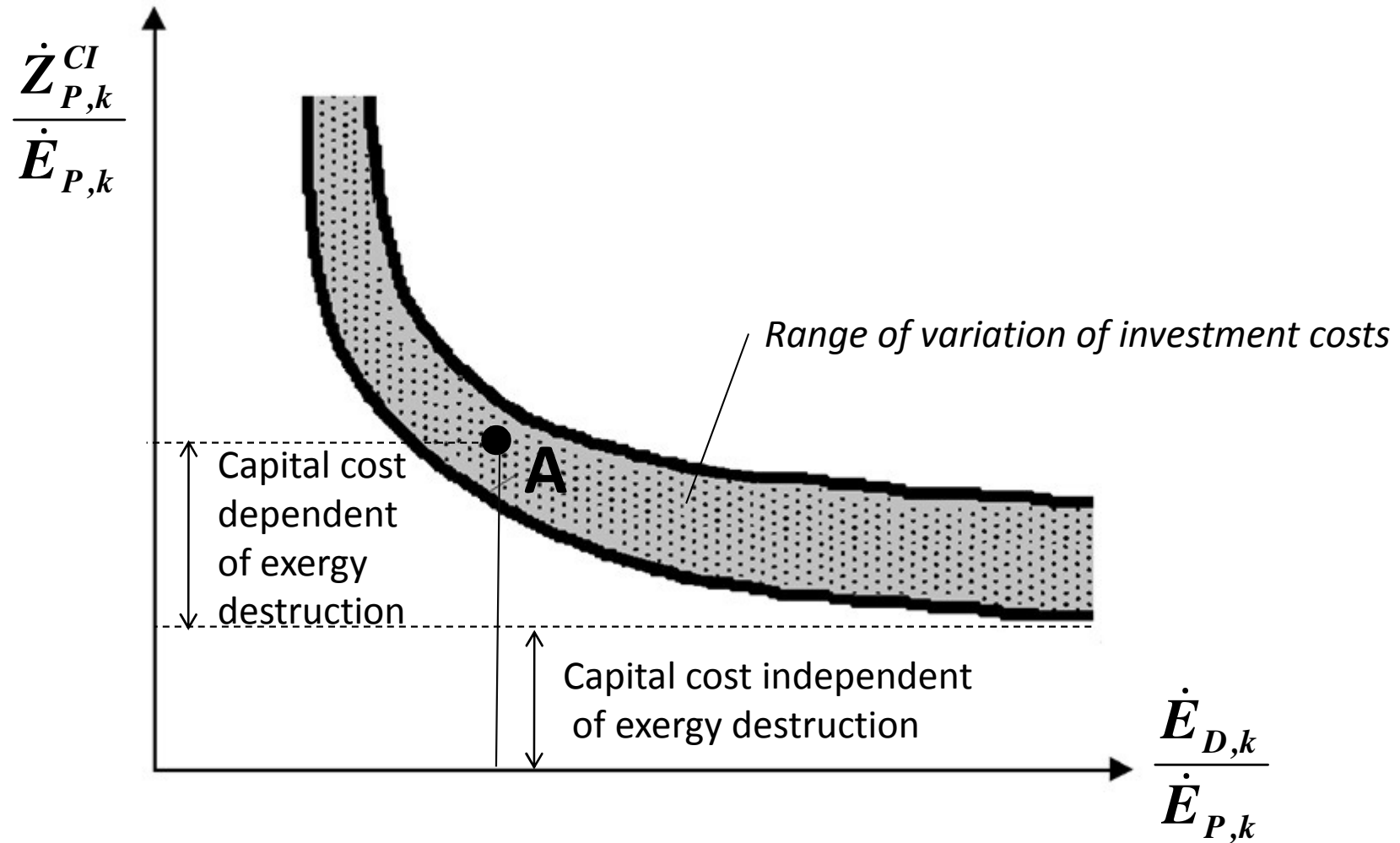


The rules for improving the cost effectiveness of the overall energy conversion system:

1. Identify the cost relevant system components: $\uparrow \dot{C}_{TOT,k} = \dot{Z}_k + \dot{C}_{D,k}$

2. Select the ones that have the highest improvement potential: r


3. f_k  $\uparrow f_k \Rightarrow \uparrow \dot{Z}_k$  Try to reduce the capital investment
 $\downarrow f_k \Rightarrow \uparrow \dot{C}_{D,k}$  Try to improve the component efficiency

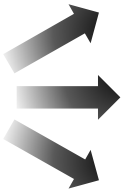


Exergoenvironmental costing

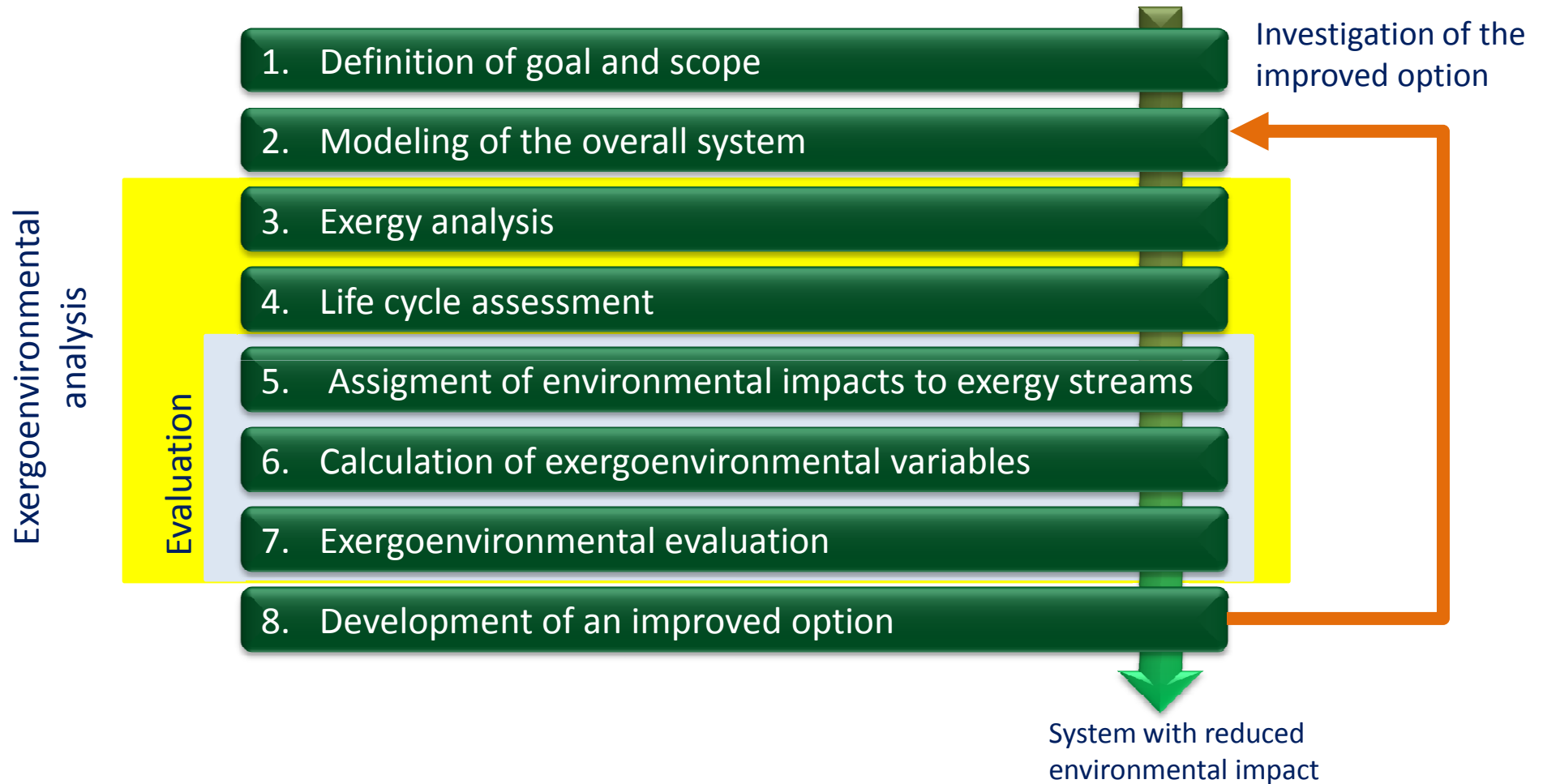
Steps:

1. Exergy analysis

2. LCA  Each relevant system component
All relevant input streams to the overall system

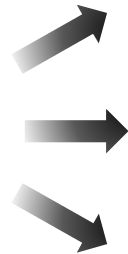
3.  Assigning environmental impacts to exergy systems
Calculation of exergoenvironmental variables
Exergoenvironmental evaluation

Structure of the exergoenvironmental analysis of an energy conversion system:





1. Goal definition and scoping
2. Inventory analysis (consumption and release)
3. Interpretation of results



- Generic data, standard modules (transportation, energy production,...)
- Simplified assessment (most important environmental aspects, potential environmental impacts, stages)
- Thorough assessment of the reliability of the results

Eco-indicator 99

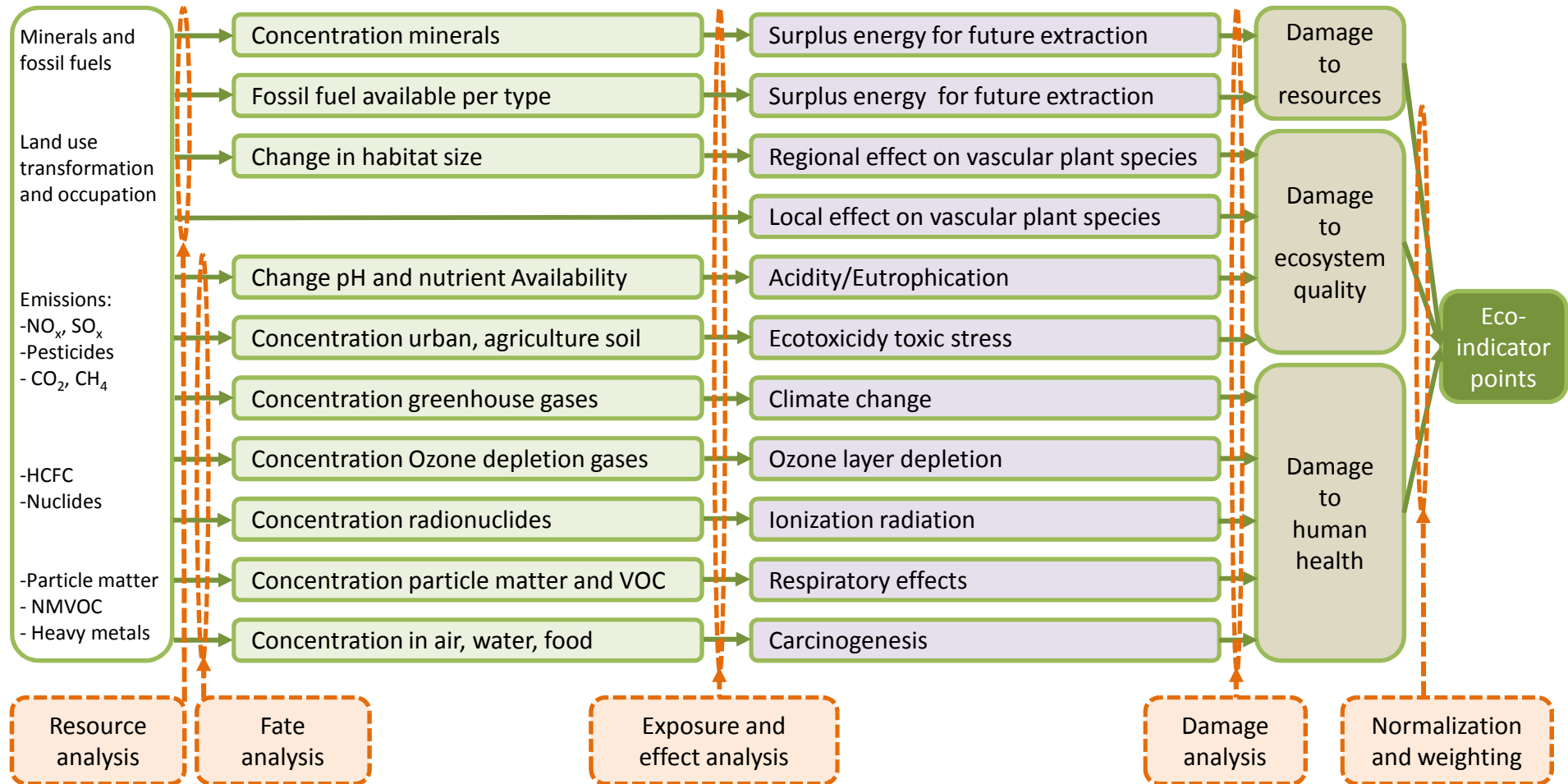


- Human health
- Ecosystem
- Resources depletion



Eco-Indicator 99 LCA method

General structure and model of the Eco-Indicator 99 LCA method.



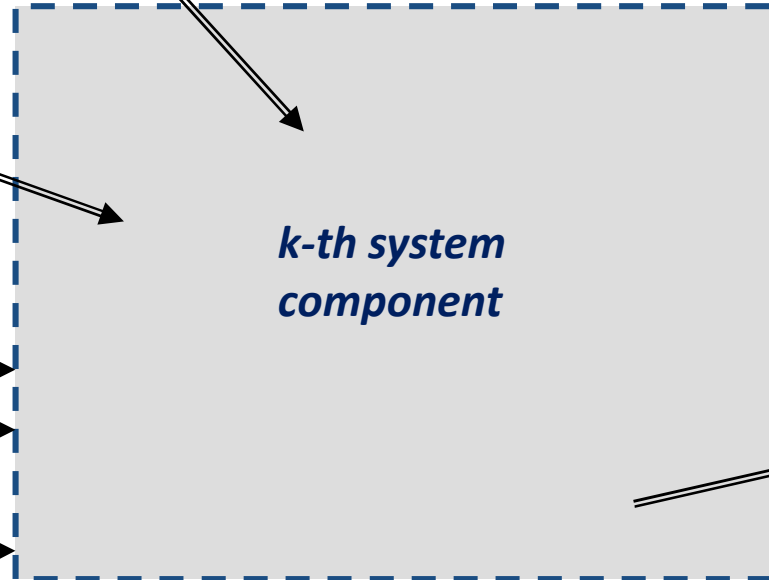
$$\dot{Y}_k = \dot{Y}_k^{CO} + \dot{Y}_k^{OM} + \dot{Y}_k^{DI}$$

$$\dot{B}_{q,k} = b_{q,k} \dot{Q}_k$$

$$\dot{B}_{1,k,in} = b_{1,k,in} \dot{E}_{1,k,in} \quad \mathbf{1}$$

$$\dot{B}_{2,k,in} = b_{2,k,in} \dot{E}_{2,k,in} \quad \mathbf{2}$$

$$\dot{B}_{n,k,in} = b_{n,k,in} \dot{E}_{n,k,in} \quad \mathbf{n}$$



$$\mathbf{1} \quad \dot{B}_{1,k,out} = b_{1,k,out} \dot{E}_{1,k,out}$$

$$\mathbf{2} \quad \dot{B}_{2,k,out} = b_{2,k,out} \dot{E}_{2,k,out}$$

$$\mathbf{m} \quad \dot{B}_{m,k,out} = b_{m,k,out} \dot{E}_{m,k,out}$$

$$\dot{B}_{w,k} = b_{w,k} \dot{W}_k$$

$$\sum_{i=1}^n \dot{B}_{i,k,in} + \dot{B}_{q,k} + \dot{Y}_k = \sum_{i=1}^m \dot{B}_{i,k,out} + \dot{B}_{w,k}$$

Environmental impact

$$\dot{B}_j = b_j \dot{E}_j$$

$$\dot{B}_j \text{ (Pts / s)}$$

$$b_j \text{ (Pts / GJ exergy)}$$

Environmental
Impact
balances

$$\dot{B}_{P,k} = \dot{B}_{F,k} + \dot{Y}_k$$

$$b_{P,k} \dot{E}_{P,k} = b_{F,k} \dot{E}_{F,k} + \dot{Y}_k$$

$$\dot{Y}_k = \dot{Y}_k^{CO} + \dot{Y}_k^{OM} + \dot{Y}_k^{DI}$$

Auxiliary environmental
impact equations
(Meyer et al, 2008)

Environmental impact
of exergy destruction

$$\dot{B}_{D,k} = b_{F,k} \dot{E}_{D,k}$$

$$\dot{B}_{TOT,k} = \dot{Y}_k + \dot{B}_{D,k}$$

Relative difference

$$r_{b,k} = \frac{b_{P,k} - b_{F,k}}{b_{F,k}}$$

Exergoenvironmental factor

$$f_{b,k} = \frac{\dot{Y}_k}{\dot{Y}_k + \dot{B}_{D,k}} = \frac{\dot{Y}_k}{\dot{B}_{TOT,k}}$$



F Equations

The specific environmental impact of each exergy stream associated with fuel remains constant between inlet and outlet.

P Equations

Each exergy unit is supplied to all exergy streams associated with the product at the same average specific environmental impact: b_{pk}

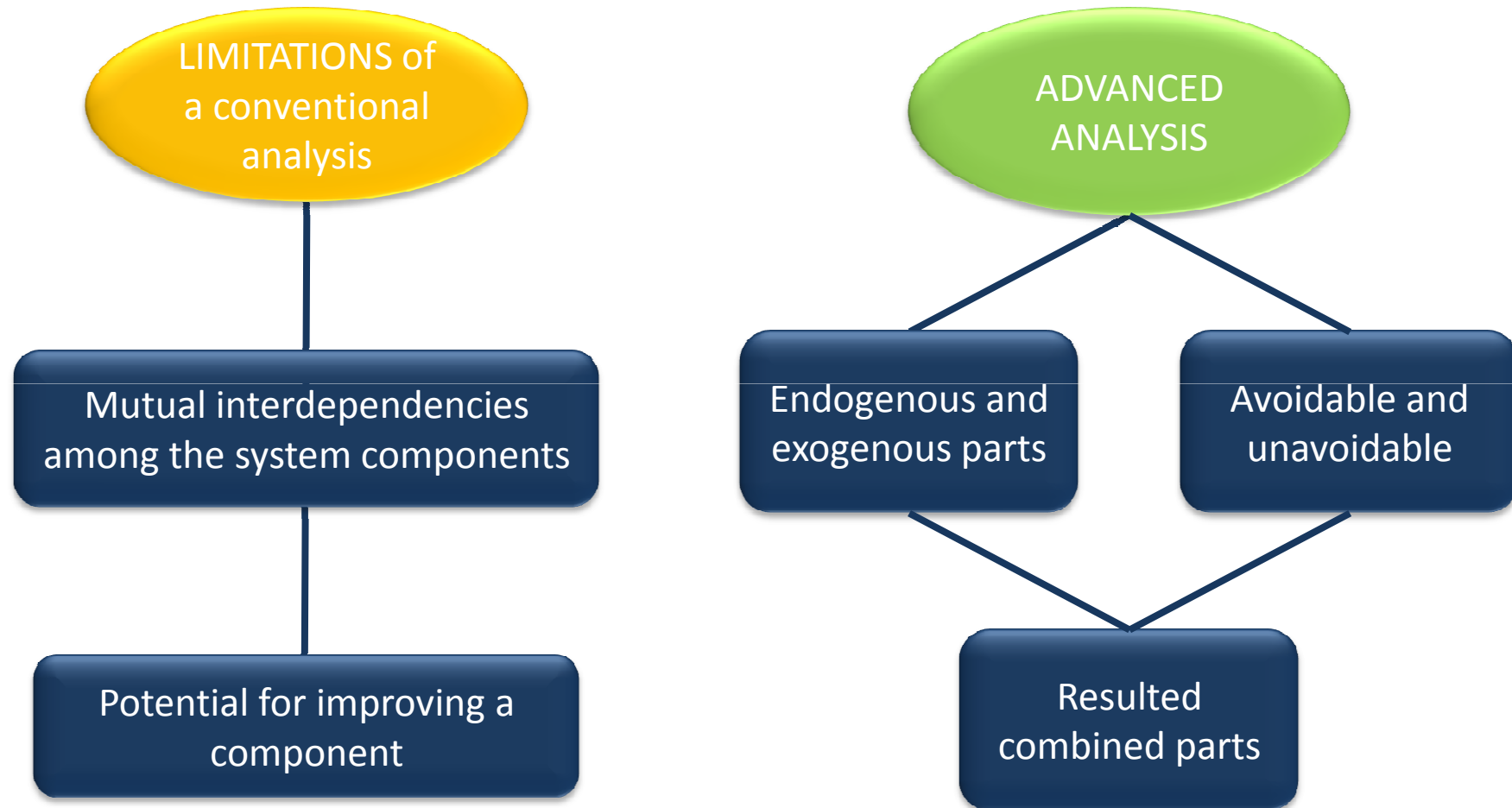


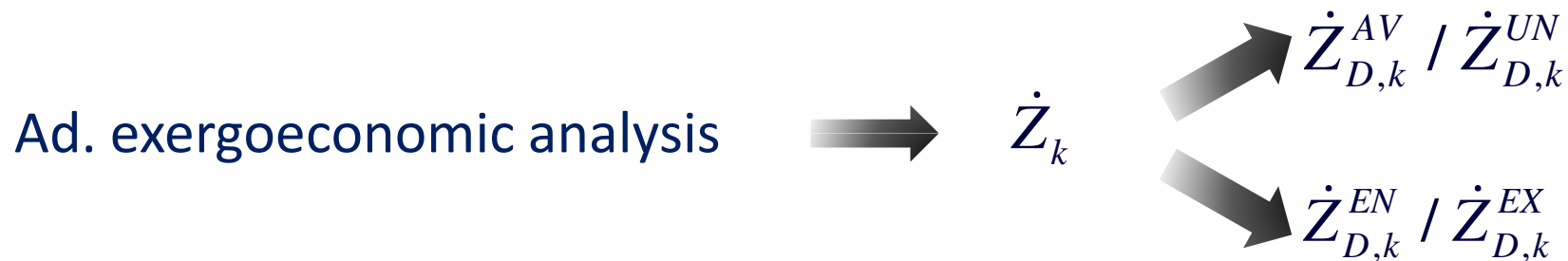
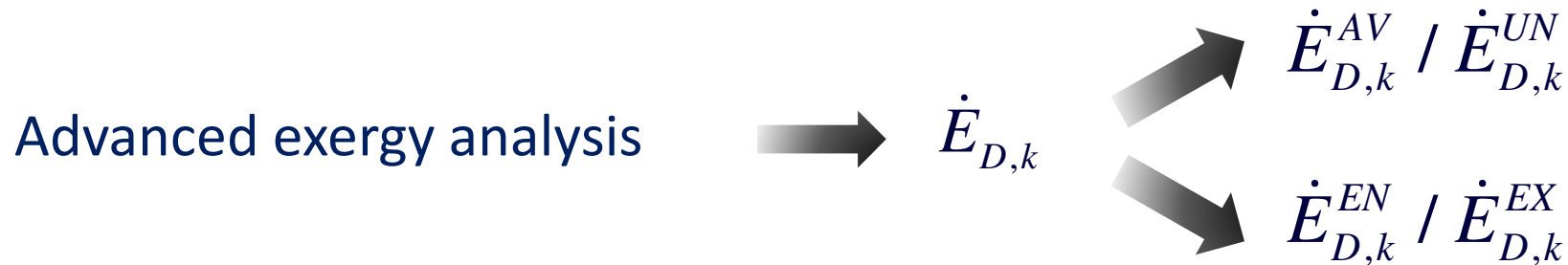
Steps:

1. Identify the environmentally relevant system components: $\uparrow \dot{B}_{TOT,k}$
2. Select the ones that have the highest improvement potential: $r_{b,k}$

3. $f_{b,k}$
 - $\uparrow f_{b,k} \Rightarrow \uparrow \dot{Y}_k \Rightarrow$ The component related impact dominates the overall impact
 - $\downarrow f_{b,k} \Rightarrow \uparrow \dot{B}_{D,k} \Rightarrow$ The thermodynamic inefficiencies are the dominant source of environmental impact

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$\dot{E}_{D,k}^{UN}$ \longrightarrow $\dot{E}_{D,k,\min}$ with best available technology

$$\dot{E}_{D,k}^{AV} = \dot{E}_{D,k} - \dot{E}_{D,k}^{UN}$$

$$\dot{E}_{D,k} = \dot{E}_{D,k}^{AV} + \dot{E}_{D,k}^{UN}$$

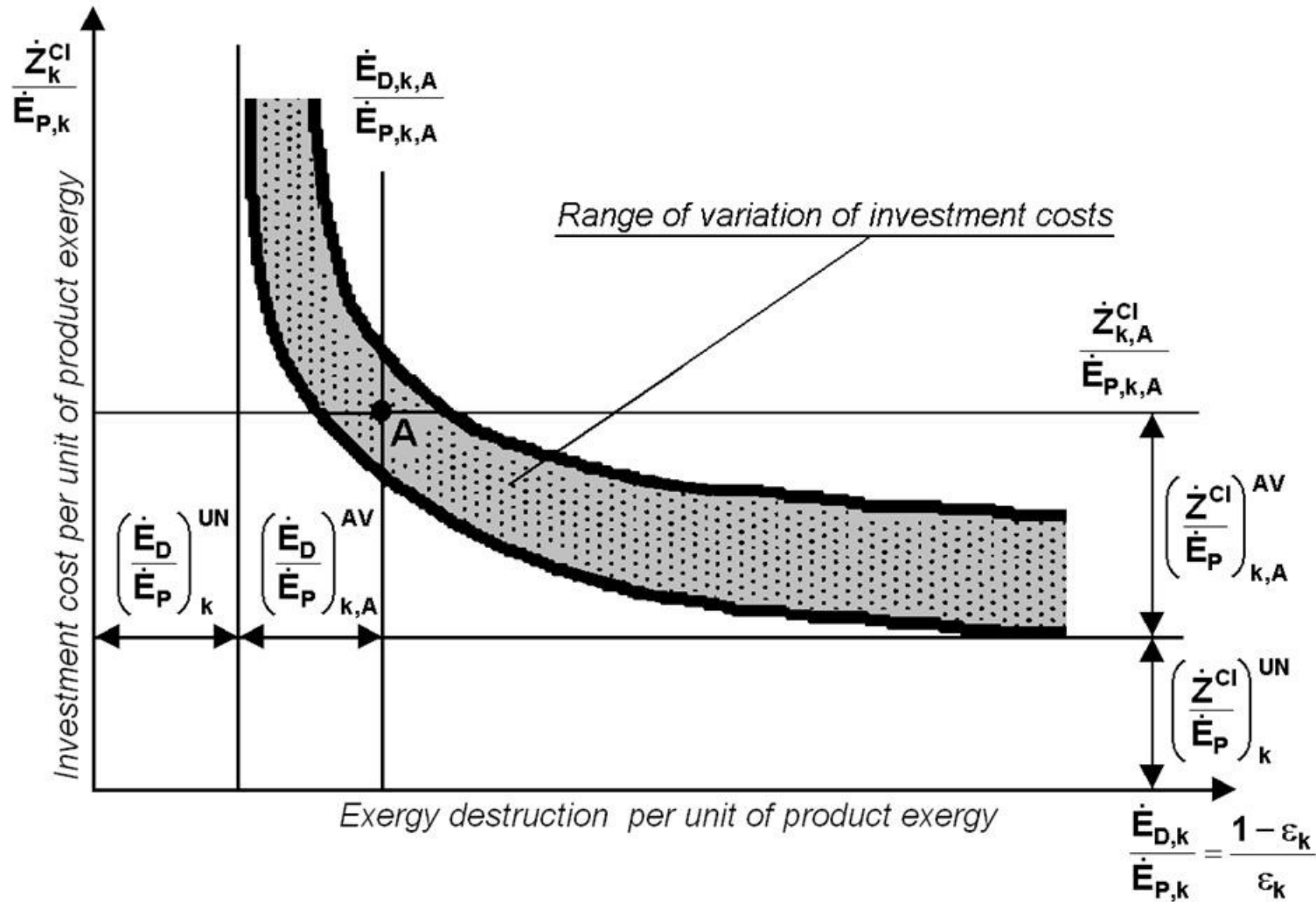
$$\left(\frac{\dot{E}_{D,k}}{\dot{E}_{P,k}} \right)^{UN} \longrightarrow \dot{E}_{D,k}^{UN} = \dot{E}_{P,k}^{real} \left(\frac{\dot{E}_{D,k}}{\dot{E}_{P,k}} \right)^{UN}$$

$\dot{Z}_k^{UN} \longrightarrow \dot{Z}_{k,\min}$ extremely inefficient version (low cost)

$$\dot{Z}_k^{AV} = \dot{Z}_k - \dot{Z}_k^{UN}$$

$$\dot{Z}_k = \dot{Z}_k^{AV} + \dot{Z}_k^{UN}$$

$$\left(\frac{\dot{Z}_k}{\dot{E}_{P,k}} \right)^{UN} \longrightarrow \dot{Z}_k^{UN} = \dot{E}_{P,k}^{real} \left(\frac{\dot{Z}_k}{\dot{E}_{P,k}} \right)^{UN}$$



Avoidable/Unavoidable \dot{Y}_k

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$\dot{Y}_k^{UN} \longrightarrow \dot{Y}_{k,\min}$ min environmental impact

$$\dot{Y}_k^{AV} = \dot{Y}_k - \dot{Y}_k^{UN}$$

$$\dot{Y}_k = \dot{Y}_k^{AV} + \dot{Y}_k^{UN}$$

$$\left(\frac{\dot{Y}_k}{\dot{E}_{P,k}} \right)^{UN} \longrightarrow \dot{Y}_k^{UN} = \dot{E}_{P,k}^{real} \left(\frac{\dot{Y}_k}{\dot{E}_{P,k}} \right)^{UN}$$

$$\dot{E}_{D,k}^{EN} \longrightarrow \dot{E}_{D,k} \text{ when } \varepsilon_k = \varepsilon_{real} \text{ and } \varepsilon_{j \neq k} = 1$$

$$\dot{E}_{D,k}^{EX} = \dot{E}_{D,k} - \dot{E}_{D,k}^{EN}$$

$$\dot{E}_{D,k} = \dot{E}_{D,k}^{EN} + \dot{E}_{D,k}^{EX}$$

$$\dot{Z}_k = \dot{Z}_k^{EN} + \dot{Z}_k^{EX}$$

$$\dot{Z}_k^{EN} = \dot{E}_{P,k}^{EN} \left(\frac{\dot{Z}_k}{\dot{E}_{P,k}} \right)^{real}$$

$$\dot{Y}_k = \dot{Y}_k^{EN} + \dot{Y}_k^{EX}$$

$$\dot{Y}_k^{EN} = \dot{E}_{P,k}^{EN} \left(\frac{\dot{Y}_k}{\dot{E}_{P,k}} \right)^{real}$$



$$\dot{E}_{D,k} = \dot{E}_{F,k} - \dot{E}_{P,k} = \frac{\dot{E}_{P,k}}{\epsilon_k} - \dot{E}_{P,k} = \dot{E}_{P,k} \left(\frac{1}{\epsilon_k} - 1 \right)$$

$$\dot{E}_{D,C} = \dot{E}_{P,C} \left(\frac{1}{\epsilon_C} - 1 \right) = \dot{E}_{P,TOT} \left(\frac{1}{\epsilon_C} - 1 \right)$$

$$\dot{E}_{D,B} = \dot{E}_{P,B} \left(\frac{1}{\epsilon_B} - 1 \right) = \dot{E}_{F,C} \left(\frac{1}{\epsilon_B} - 1 \right) = \frac{\dot{E}_{P,TOT}}{\epsilon_C} \left(\frac{1}{\epsilon_B} - 1 \right)$$

$$\dot{E}_{D,A} = \dot{E}_{P,A} \left(\frac{1}{\epsilon_A} - 1 \right) = \dot{E}_{F,B} \left(\frac{1}{\epsilon_A} - 1 \right) = \frac{\dot{E}_{P,B}}{\epsilon_B} \left(\frac{1}{\epsilon_A} - 1 \right) = \frac{\dot{E}_{P,TOT}}{\epsilon_B \cdot \epsilon_C} \left(\frac{1}{\epsilon_A} - 1 \right)$$

Endogenous/Exogenous

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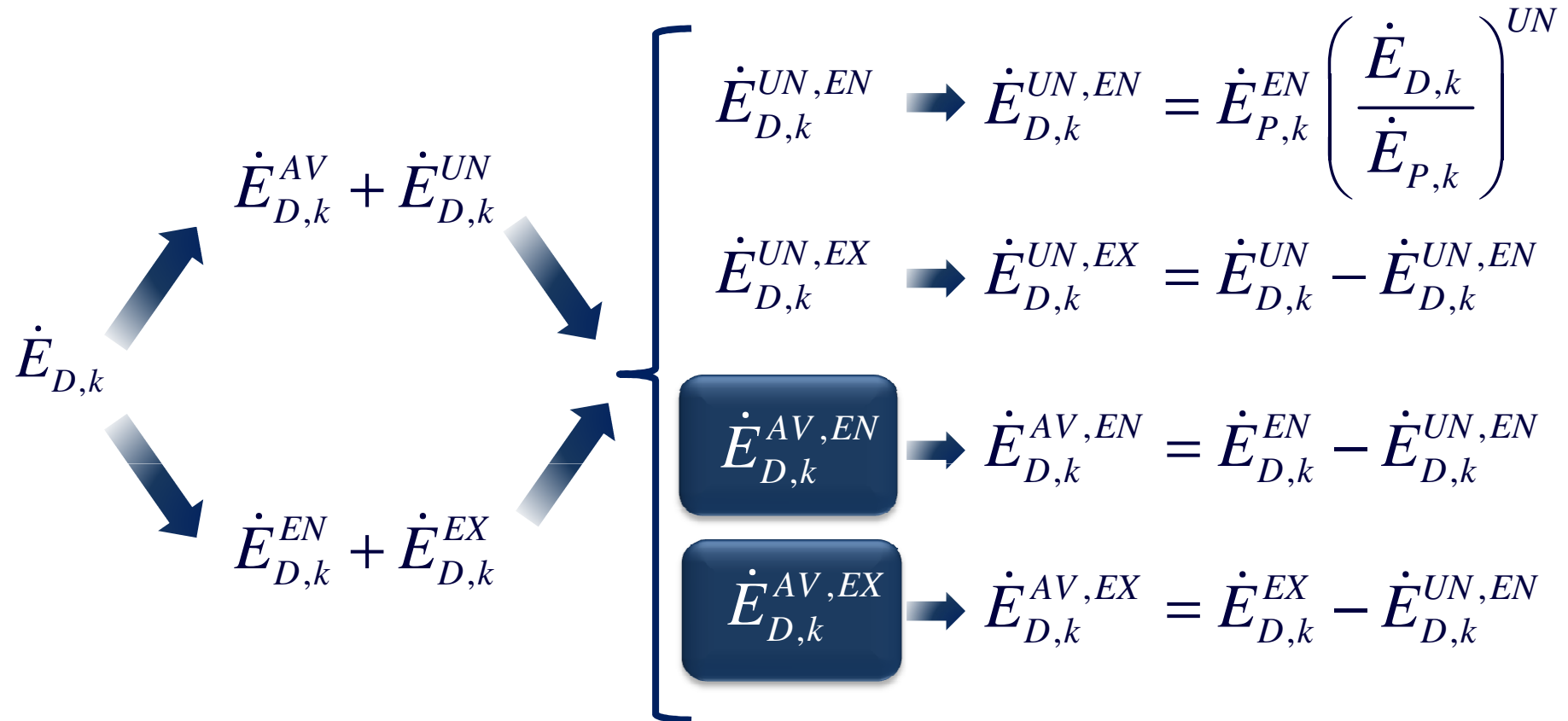


$$\dot{E}_{D,B} = \frac{\dot{E}_{P,TOT}}{\varepsilon_C} \left(\frac{1}{\varepsilon_B} - 1 \right) \xrightarrow[\varepsilon_C = 1]{\varepsilon_B \neq 1} \dot{E}_{D,B}^{EN} = \dot{E}_{P,TOT} \left(\frac{1}{\varepsilon_B} - 1 \right)$$

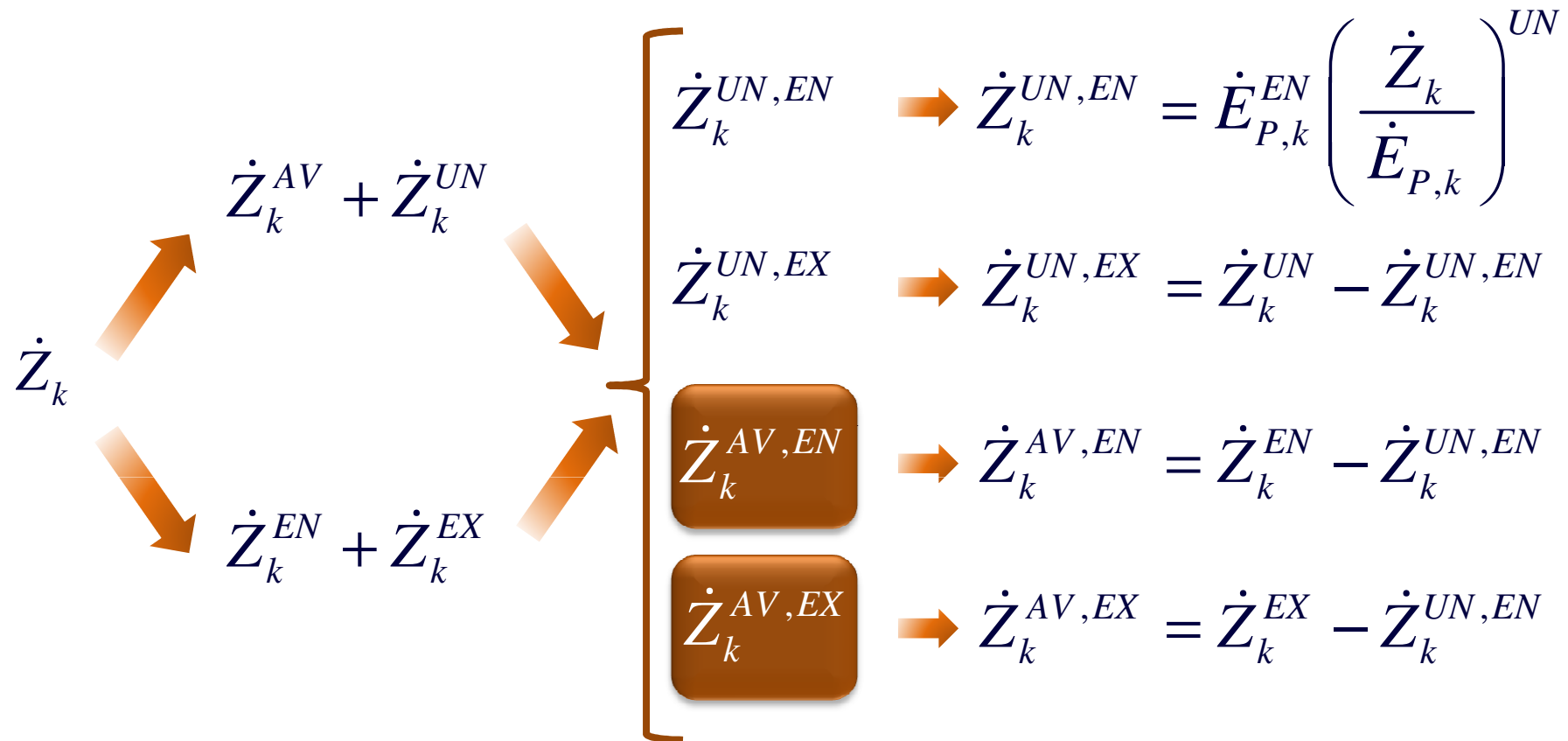
$$\dot{E}_{D,B}^{EX} = \dot{E}_{D,B} - \dot{E}_{D,B}^{EN} = \dot{E}_{P,TOT} \left(\frac{1}{\varepsilon_C} - 1 \right) \left(\frac{1}{\varepsilon_B} - 1 \right)$$

$$\dot{E}_{D,A} = \frac{\dot{E}_{P,TOT}}{\varepsilon_B \cdot \varepsilon_C} \left(\frac{1}{\varepsilon_A} - 1 \right) \xrightarrow[\varepsilon_C = 1, \varepsilon_B = 1]{\varepsilon_A \neq 1} \dot{E}_{D,A}^{EN} = \dot{E}_{P,TOT} \left(\frac{1}{\varepsilon_A} - 1 \right)$$

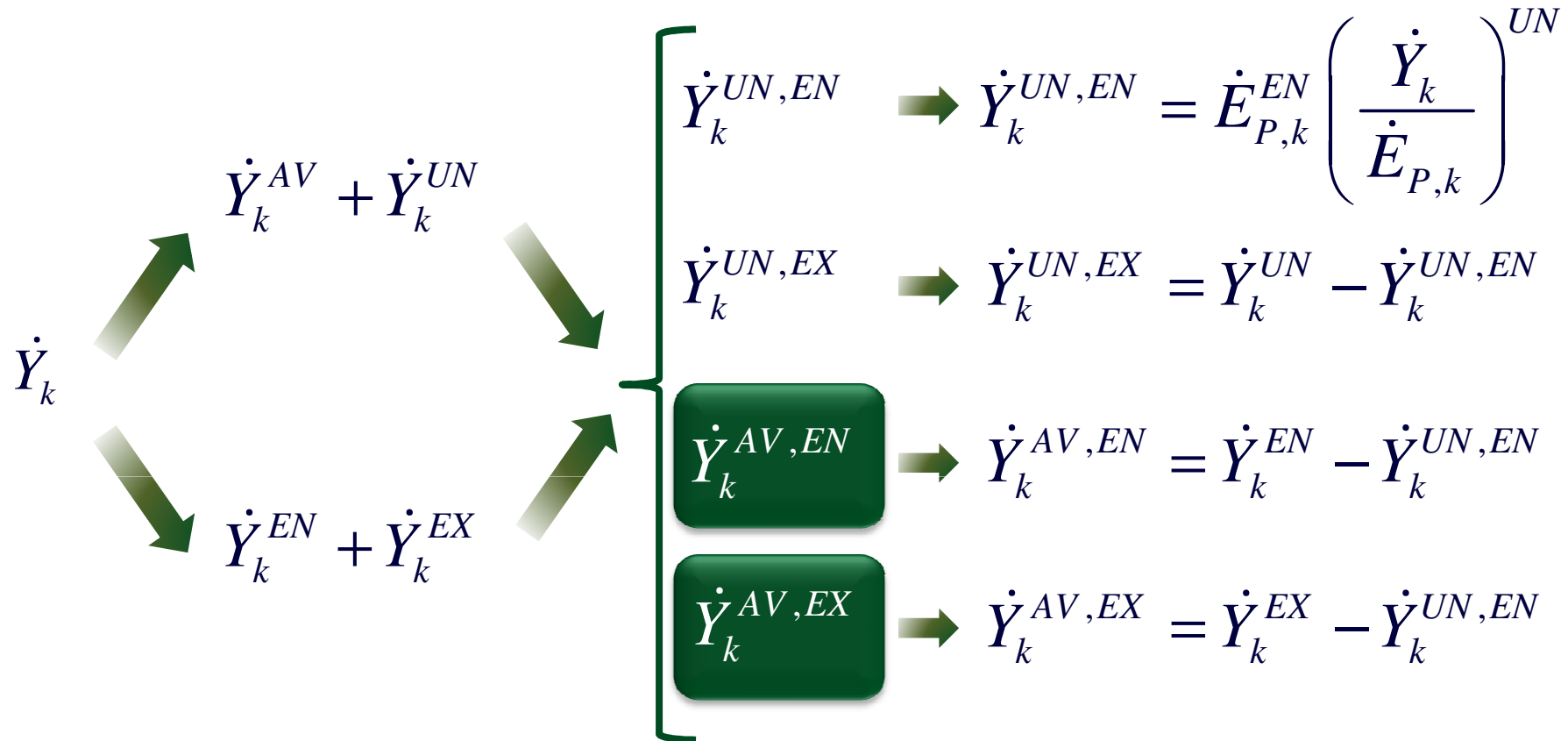
$$\dot{E}_{D,A}^{EX} = \dot{E}_{D,A} - \dot{E}_{D,A}^{EN} = \dot{E}_{P,TOT} \left(\frac{1}{\varepsilon_B \varepsilon_C} - 1 \right) \left(\frac{1}{\varepsilon_A} - 1 \right)$$



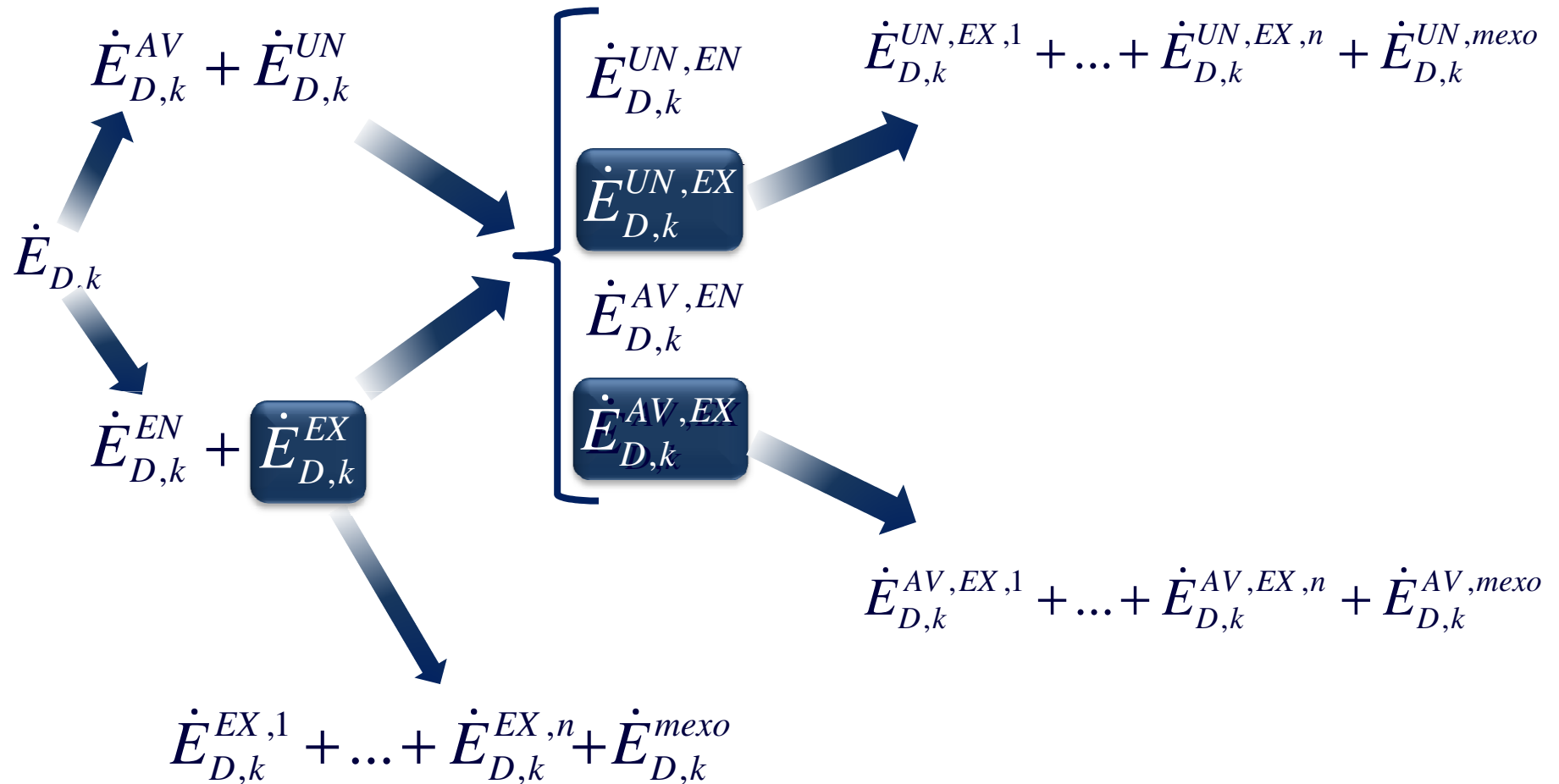
$$\dot{E}_{D,k} = \dot{E}_{D,k}^{UN,EN} + \dot{E}_{D,k}^{UN,EX} + \dot{E}_{D,k}^{AV,EN} + \dot{E}_{D,k}^{AV,EX}$$



$$\dot{Z}_k = \dot{Z}_k^{UN,EN} + \dot{Z}_k^{UN,EX} + \dot{Z}_k^{AV,EN} + \dot{Z}_k^{AV,EX}$$



$$\dot{Y}_k = \dot{Y}_k^{UN,EN} + \dot{Y}_k^{UN,EX} + \dot{Y}_k^{AV,EN} + \dot{Y}_k^{AV,EX}$$



$$\dot{E}_{D,k}^{UN,EX} = \dot{E}_{D,k}^{UN,EX,1} + \dots + \dot{E}_{D,k}^{UN,EX,n} + \dot{E}_{D,k}^{UN,mexo}$$

$$\dot{E}_{D,k}^{UN,EX,n} = \dot{E}_{D,k}^{UN,EN,n+k} - \dot{E}_{D,k}^{UN,EN}$$

$$\dot{E}_{D,k}^{UN,EN,n+k} = \dot{E}_{P,k}^{UN,EN,n+k} \left(\frac{\dot{E}_{D,k}}{\dot{E}_{P,k}} \right)^{UN}$$

$$1. \quad \dot{E}_{D,k}^{AV,EN} \longrightarrow \dot{C}_{D,k}^{AV,EN} = c_{F,k} \dot{E}_{D,k}^{AV,EN}$$

$$\dot{E}_{D,k}^{AV,EX} \longrightarrow \dot{C}_{D,k}^{AV,EX} = c_{F,k} \dot{E}_{D,k}^{AV,EX}$$

$$2. \quad \dot{Z}_k^{AV,EN}$$

$$\varepsilon_k^{AV,EN} = \frac{\dot{E}_{P,k}}{\dot{E}_{F,k} - \dot{E}_{D,k}^{UN} - \dot{E}_{D,k}^{AV,EX}} = 1 - \frac{\dot{E}_{D,k}^{AV,EN}}{\dot{E}_{F,k} - \dot{E}_{D,k}^{UN} - \dot{E}_{D,k}^{AV,EX}}$$

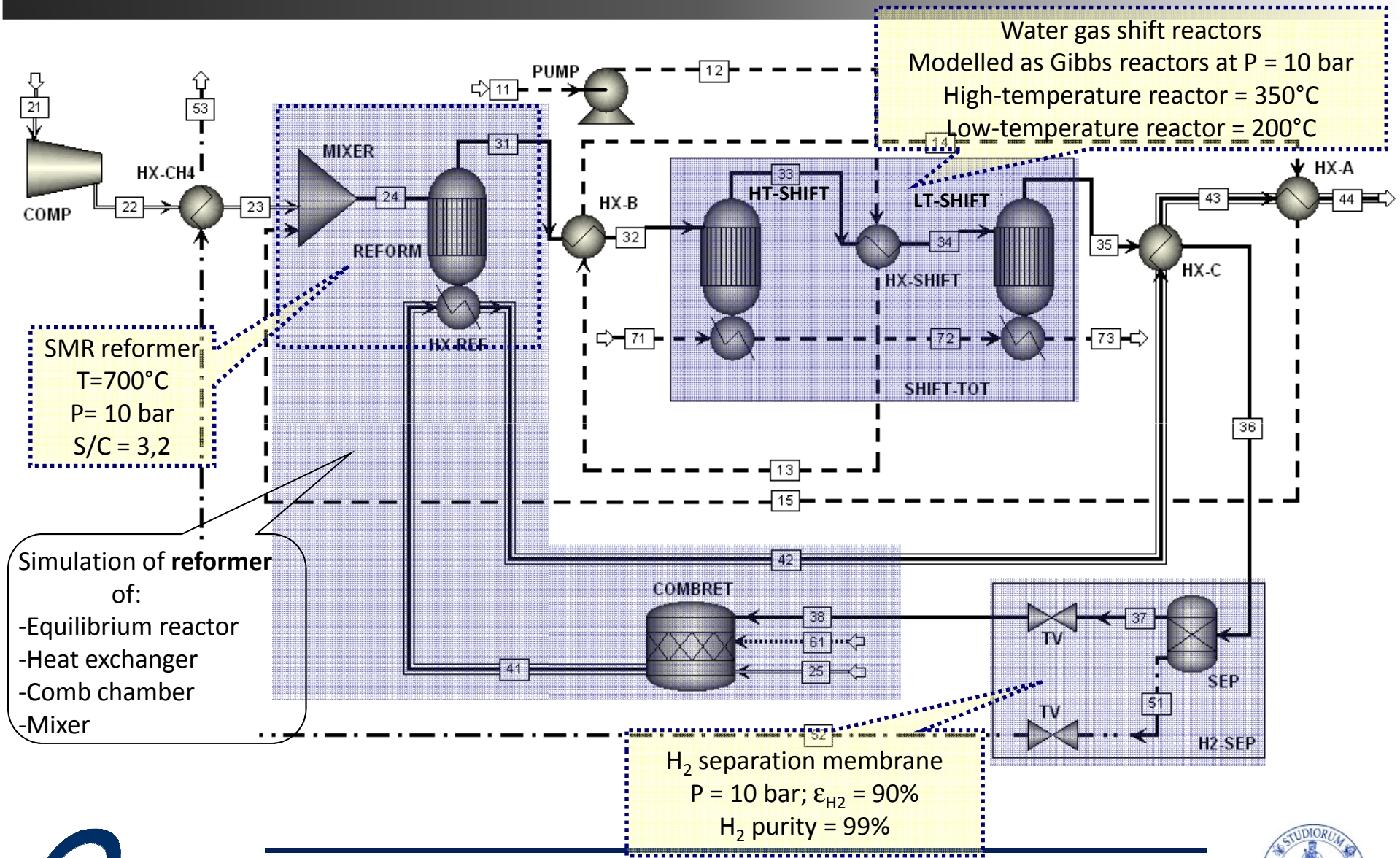
$$f_k^{AV,EN} = \frac{\dot{Z}_k^{AV,EN}}{\dot{Z}_k^{AV,EN} + \dot{C}_{D,k}^{AV,EN}} = \frac{\dot{Z}_k^{AV,EN}}{\dot{Z}_k^{AV,EN} + c_{F,k} \dot{E}_{D,k}^{AV,EN}}$$

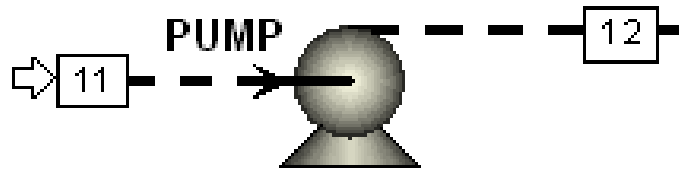
$$f_{b,k}^{AV,EN} = \frac{\dot{Y}_k^{AV,EN}}{\dot{Y}_k^{AV,EN} + \dot{B}_{D,k}^{AV,EN}} = \frac{\dot{Y}_k^{AV,EN}}{\dot{Y}_k^{AV,EN} + b_{F,k} \dot{E}_{D,k}^{AV,EN}}$$

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Application to a SMR process for H₂ production

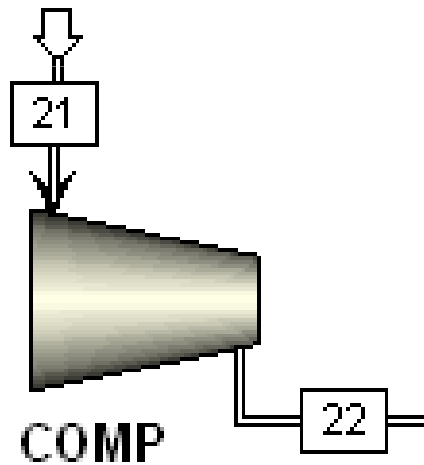
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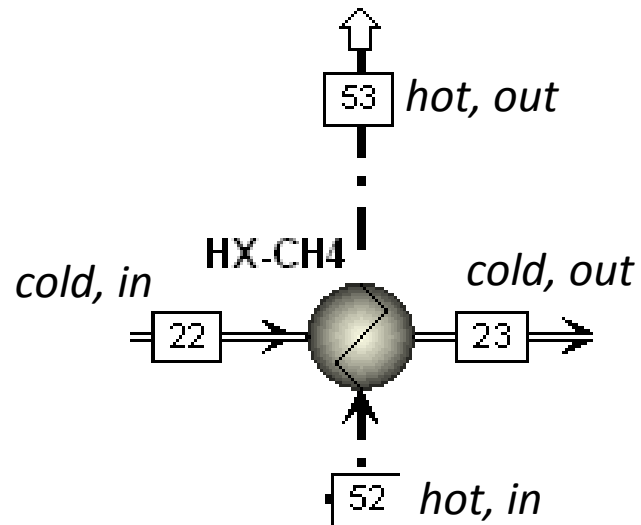
$$\dot{E}_{F,PUMP} = \dot{W}_{PUMP}$$

$$\dot{E}_{P,PUMP} = \dot{E}_{12} - \dot{E}_{11}$$



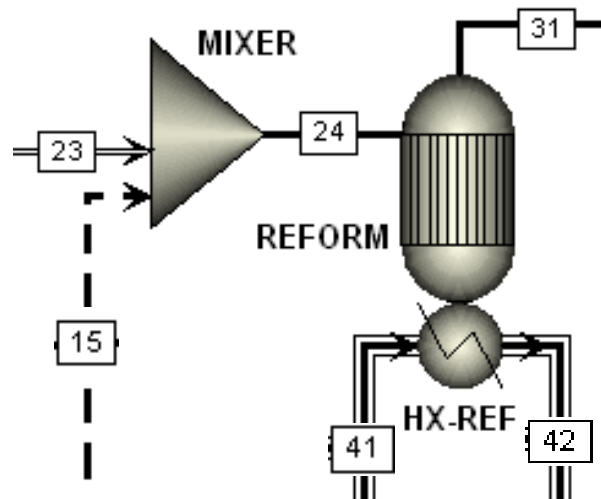
$$\dot{E}_{F,COMP} = \dot{W}_{COMP}$$

$$\dot{E}_{P,COMP} = \dot{E}_{22} - \dot{E}_{21}$$



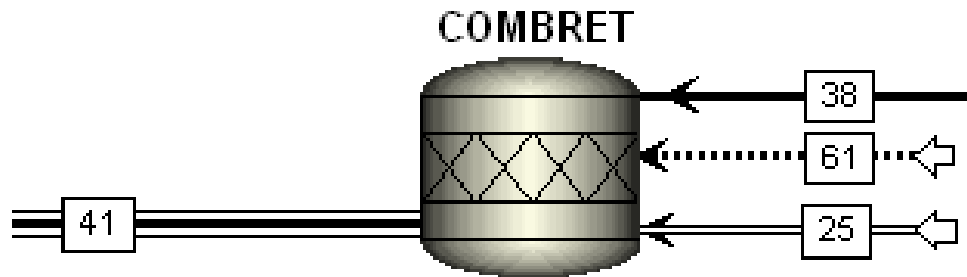
$$\dot{E}_{F,HX} = \dot{E}_{hot,in} - \dot{E}_{hot,out}$$

$$\dot{E}_{P,HX} = \dot{E}_{cold,out} - \dot{E}_{cold,in}$$



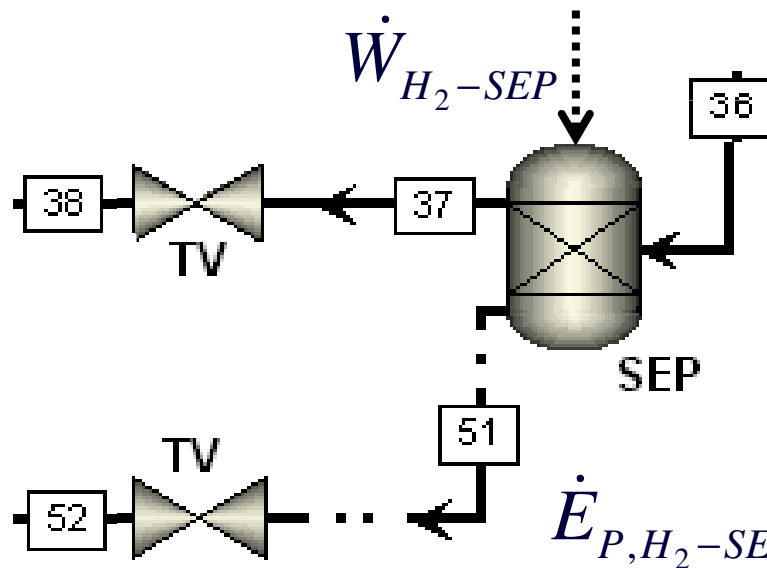
$$\dot{E}_{F,REFORM} = \dot{E}_{41} - \dot{E}_{42}$$

$$\dot{E}_{P,REFORM} = \dot{E}_{31} - (\dot{E}_{23} + \dot{E}_{15})$$



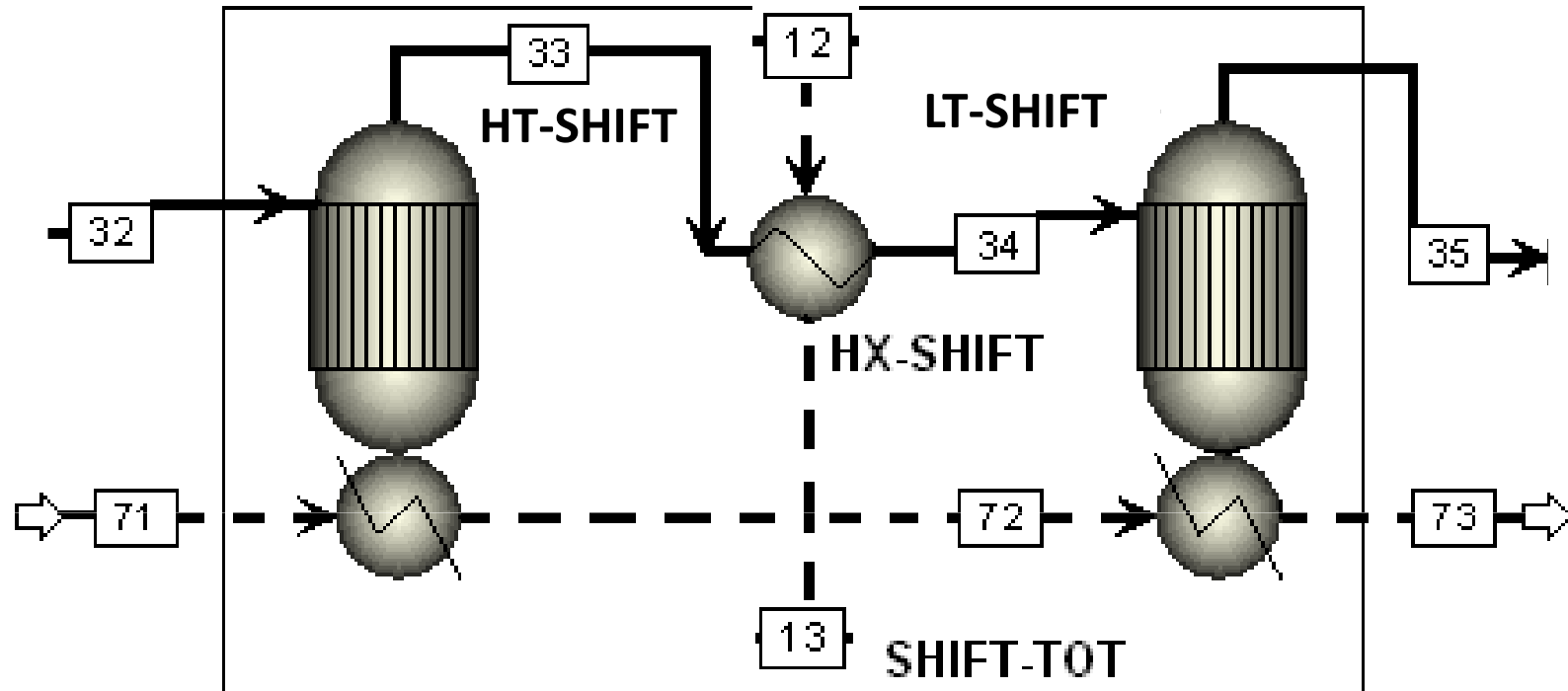
$$\dot{E}_{F,COMBRET} = \dot{E}_{25} + \dot{E}_{38}$$

$$\dot{E}_{P,COMBRET} = \dot{E}_{41} - \dot{E}_{61}$$



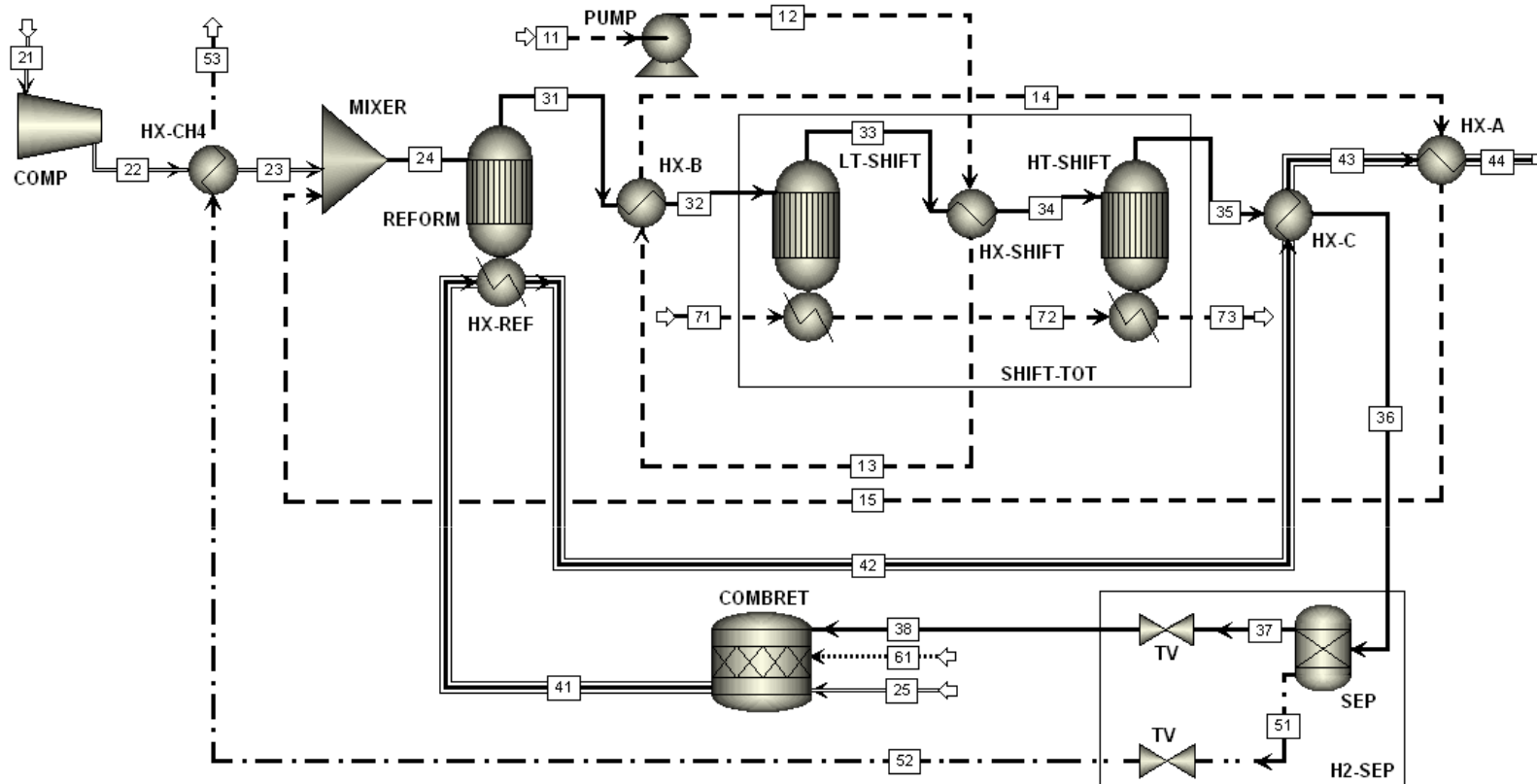
$$\dot{E}_{F,H_2-SEP} = \dot{W}_{H_2-SEP} + \dot{m}_{38} (e_{36}^{PH} - e_{38}^{PH})$$

$$\dot{E}_{P,H_2-SEP} = \dot{E}_{52}^{CH} + \dot{E}_{38}^{CH} - \dot{E}_{36}^{CH} + \dot{m}_{52} (e_{52}^{PH} - e_{36}^{PH})$$



$$\dot{E}_{F,SHIFT} = \left[\begin{aligned} & \left(\dot{m}_{in}^{CO} e_{in}^{CO} - \dot{m}_{out}^{CO} e_{out}^{CO} \right) + \left(\dot{m}_{in}^{H_2O} e_{in}^{H_2O} - \dot{m}_{out}^{H_2O} e_{out}^{H_2O} \right) + \\ & \left(\dot{m}_{in}^{CH_4} e_{in}^{CH_4} - \dot{m}_{out}^{CH_4} e_{out}^{CH_4} \right) + \left(\dot{m}_{out}^{CO_2} e_{out}^{CO_2} - \dot{m}_{in}^{CO_2} e_{in}^{CO_2} \right) \end{aligned} \right]^{CH} + \left(\dot{E}_{out}^{PH} - \dot{E}_{in}^{PH} \right)$$

$$\dot{E}_{P,SHIFT} = \left(\dot{m}_{in}^{H_2} e_{in}^{CH,H_2} - \dot{m}_{out}^{H_2} e_{out}^{CH,H_2} \right) + \left(\dot{E}_{water,out} - \dot{E}_{water,in} \right)$$



$$\dot{E}_{F,TOT} = \dot{E}_{P,TOT} + \sum_k \dot{E}_{D,k} + \dot{E}_{L,TOT} \qquad \dot{E}_{L,TOT} = \dot{E}_{44} + (\dot{E}_{73} - \dot{E}_{71})$$

$$\varepsilon = \frac{\dot{E}_{P,TOT}}{\dot{E}_{F,TOT}} = \frac{\dot{E}_{53}}{(\dot{E}_{11} + \dot{E}_{21} + \dot{E}_{61} + \dot{E}_{25} + \dot{W}_{COMP} + \dot{W}_{PUMP} + \dot{W}_{H_2-SEP})}$$

SMR Process: Exergy analysis

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Component	$\dot{E}_{F,k}$ (MW)	$\dot{E}_{P,k}$ (MW)	$\dot{E}_{D,k}$ (MW)	y_k (%)	ϵ_k (%)
COMBRET	424.30	290.60	133.70	14.25	68.49
H2-SEP	41.56	11.42	30.14	3.21	27.48
REFORM	153.80	118.10	35.70	3.81	76.78
HT-SHIFT	9.39	8.67	0.72	0.08	92.33
HX-SHIFT	13.12	5.80	7.32	0.78	44.20
LT-SHIFT	63.43	59.69	3.73	0.40	94.11
HX-A	52.35	39.61	12.74	1.36	75.66
HX-B	44.69	26.19	18.50	1.97	58.60
HX-C	34.68	24.47	10.21	1.09	70.55
HX-CH4	4.66	4.54	0.12	0.01	97.43
COMP	8.70	7.95	0.75	0.08	91.31
PUMP	0.06	0.05	0.01	<0.01	90.78
Overall system	937.90	631.20	253.60	27.04	67.30

$$\dot{E}_{L,TOT} = 53.08 \text{ MW}$$

RAW MATERIAL COSTS AND FINANCIAL PARAMETERS

Beginning of the construction period	01.01.2010
Start of commercial operation	01.01.2012
Plant economic life	20 years (2012-2032)
Total purchased-equipment costs (2008)	119 Million €
Total capital investment	397 Million €
Unit cost of methane (2008)	0,2848 €/kg of CH ₄
Unit cost of water process (2008)	0,0002 €/kg of H ₂ O
Unit cost of electricity (2008)	0,00002 €/kJ
Average general inflation rate (2008-2032)	2,5 %
Average nominal escalation rate at all costs except fuels (2008-2032)	0,0 %
Average nominal escalation rate of fuel costs(2008-2032)	0,5 %
Required return on investment (2008-2032)	10,0 %

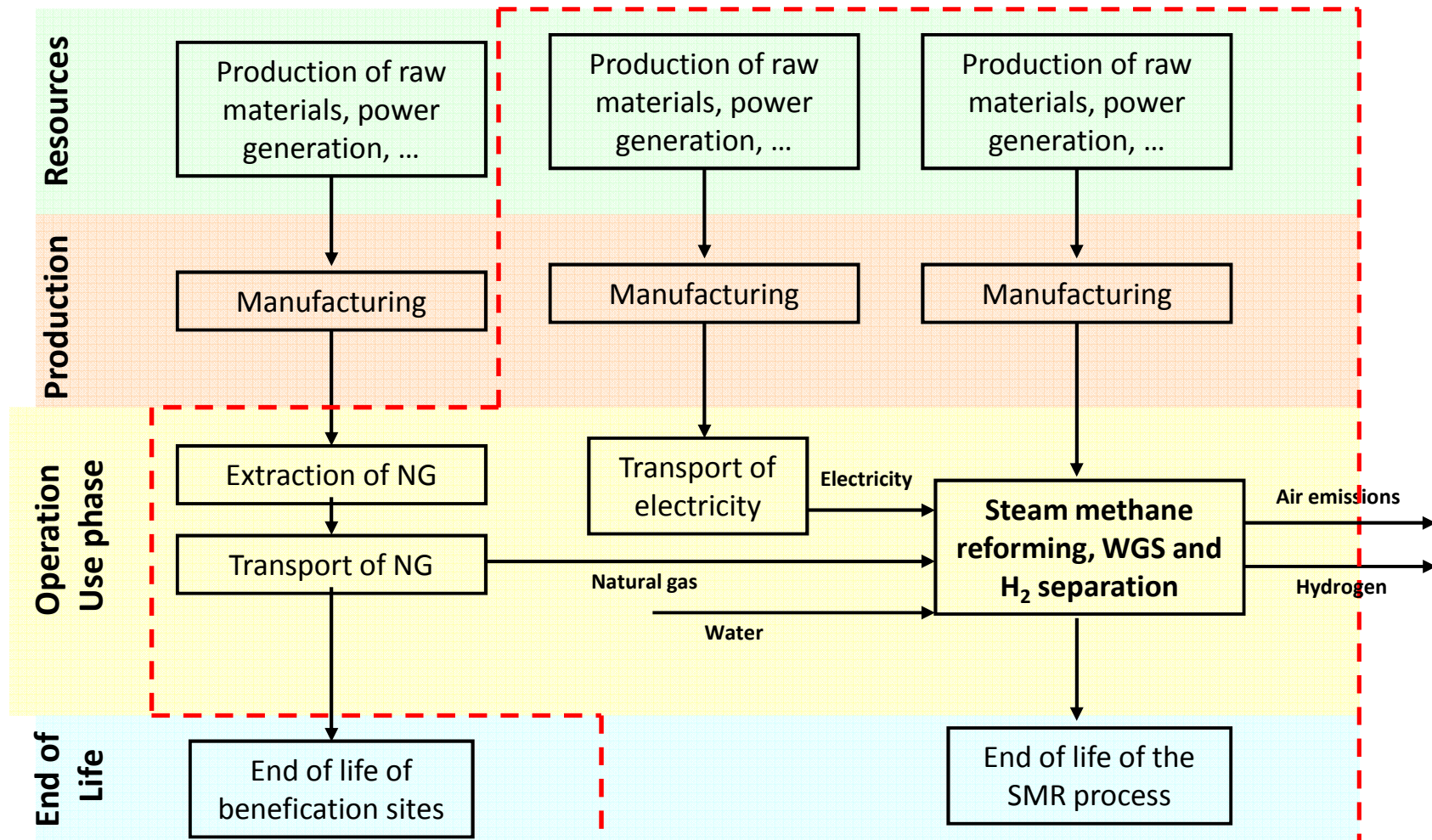
CONVENTIONAL EXERGOECONOMIC ANALYSIS

Capacity of the SRM plant	Cost of H ₂ (€ ₂₀₀₇ /kg of H ₂)	Energy efficiency	Exergy efficiency	Exergy loss Exergy destruction	Reference
22,4 Nm ³ /s	1,37 €/kg of H ₂	80 %	67 %	27%	This work, 2010
22,4 Nm ³ /s		67 %	63 %	30%	Simpson et al, IJHE 32 (2007)4811
		86 %	79%	--	Rosen MA. IJHE 1991;16(3):207–17
		--	77%	--	Lambert J et al. Energy 1997;22(8):817–25
		--	80%	--	Sorin M, Trans IChemE 1998;76(A).
		76%	--	--	Simbeck et al. GHGT-7 Vancouver, Sept 2004.
		81%	--	--	Lutz A et al. IJHE 2003;28:159–67
		77%	71%	--	Bargigli S et al Energy 2004;29:2145–59.
Small facility	1,58 €/kg of H ₂				Chen et al, Chem Eng Mag. New York March 2006
Large facility	0,43 €/kg of H ₂				Chen et al, Chem Eng Mag. New York March 2006
2,83 Nm ³ /day	2,13 €/kg of H ₂				Maribal et al 2003, PhD, University of Florida

CONVENTIONAL EXERGEOECONOMIC ANALYSIS

PLANT COMPONENT	C_D (€/h)	C_F (€/GJ)	C_P (€/GJ)	Z_k (€/h)	$Z_k + C_D$ (€/h)	r_k (%)	f_k (%)
TOTAL-shift	1977	24	41	2625	4603	71,95	82,70
Combustion chamber	1523	3	5	423	1946	52,73	49,98
Reformer	179	2	5	1463	1642	165,79	96,72
Hydrogen separation unit	709	7	66	751	1460	869,39	79,22
HXB	79	1	8	745	1127	516,44	97,13
HXA	1000	14	26	126	825	83,22	31,26
HXC	192	2	5	89	281	165,14	62,68
Compressor	67	24	30	89	155	23,71	82,80
HXCH ₄	17	9	17	76	93	86,23	94,12
Pump	1	18	42	4	4	126,32	94,13

SYSTEM BOUNDARIES AND STRUCTURE OF THE LCA STUDIES



System boundary

COMPONENT RELATED ENVIRONMENTAL IMPACT

Component	Material	ECO 99 (mPts/kg)	Quantity (kg)	Total (mPts)	Σ (mPts)
H ₂ separation unit	Alumina	1,000	43	43,000	19,216,250
	Steel high alloy	910	20,615	18,759,650	
	Aluminium	500	172	86,000	
	Iron	1,300	252	327,600	
Reformer	Steel high alloy	910	361,359	328,836,690	328,970,690
	Nickel	1,200	70	84,000	
	Alumina	1,000	50	50,000	
WGS reactor	Steel low alloy	110	10,765	1,184,150	452,525,682
	Steel	86	3,281,582	282,216,052	
	Cast iron	240	697,002	167,280,480	
	Alumina	1,000	1,677	1,677,000	
	Nickel	1,200	140	168,000	
Heat exchanger A	Steel low alloy	110	70,517	7,756,870	31,081,704
	Steel	86	271,219	23,324,834	
Heat exchanger c	Steel low alloy	110	24,089	2,649,790	10,617,862
	Steel	86	92,652	7,968,072	
Compressor	Steel	86	89,315	7,681,090	35,073,840
	Cast iron	240	59,543	14,290,320	
	Steel low alloy	110	119,113	13,102,430	

CONVENTIONAL EXERGOENVIRONMENTAL ANALYSIS

Component	\dot{Y}_k (mPts/h)	$\dot{B}_{D,k}$ (mPts/h)	$(\dot{Y}_k + \dot{B}_{D,k})$ (mPts/h)	$b_{F,k}$ (mPts/GJ)	$b_{P,k}$ (mPts/GJ)	$r_{b,k}$ (-)	$f_{b,k}$ (%)
Combustion chamber	353	10,273,539	10,273,892	59,070	89,610	0.52	0.001
H ₂ separation unit	120	1,743,185	1,743,305	42,660	302,440	6.01	0.001
Reformer	2,056	2,861,809	2,863,865	78,470	95,420	0.22	0.070
Water gas shift reactor	2,786	3,913,144	3,915,930	222,770	383,400	0.72	0.070
Heat Exchanger-A	194	998,952	999,146	52,050	70,550	0.36	0.020
Heat Exchanger-B	21	1,573,800	1,573,822	57,340	100,530	0.75	0.001
Heat Exchanger-C	66	1,513,398	1,513,464	120,360	163,210	0.36	0.002
Heat Exchanger-CH ₄	10	32,908	32,918	86,820	92,100	0.06	0.030
Compressor	219	33,893	34,112	3,620	4,810	0.33	0.642
Pump	0	100	100	3,620	4,150	0.15	0.193
Overall system	5,825	585,796	591,621	671	34825	50.90	0.994

SMR Process: Avoidable/unavoidable

Component	Parameter, unit	Design -point	Unavoidable thermodyn. inefficiency	Component	Parameter, unit	Design-point	Unavoidable thermodyn. inefficiency
COMP	η_s (-)	0.85	0.93	REFORM	Mixer	Base case	Isothermal Isobaric
PUMP	η_s (-)	0.85	0.93		\dot{m} (kg/s)	220.3	350
HX-A	ΔT (K)	25	15		T_{41} (°C)	1340	1340
HX-B	ΔT (K)	25	15		T_{31} (°C)	700	800
HX-C	ΔT (K)	25	15		S/M (-)	3.2	3.2
HX-CH4	ΔT (K)	25	15		CH ₄ conversion	0.8323	0.9073
HT-SHIFT	T (°C)	350	300	H2-SEP	H ₂ Separation efficiency (%)	90	99
					\dot{W}_{H_2-SEP} (MW)	4.79	6.00
HX-SHIFT	ΔT (K)	25	15	COMBRET	Air excess (%)	20	5
LT-SHIFT	T (°C)	200	150		T_{41} (°C)	1341	1460
					Heat duty (MW)	12500	0

SMR Process: Endogenous/exogenous

	Parameter Unit	DP	Theoretical conditions	Hybrid conditions		Parameter Unit	DP	Theoretical conditions	Hybrid conditions	
COMP	η_s (-)	0.85	1.0	0.85	REFORM	Mixer	Base case	$T_{31}^T = T_{31}^R$ $T_{23}^T = T_{15}^T$	$T_{31}^T = T_{31}^R$	
PUMP	η_s (-)	0.85	1.0	0.85		\dot{m} (kg/s)	220.3			
HX-A	ΔT (K)	25	-	-		T_{41} (°C)	1340	$T_{41}^T = T_{41}^R$	$T_{41}^T = T_{41}^R$	
HX-B	ΔT (K)	25	$T_{14}^T = T_{31}^R$	$T_{14}^H = T_{15}^H = T_{15}^R$		T_{31} (°C)	700	$T_{42}^T = T_{31}^T$		
HX-C	ΔT (K)	25	$T_{36}^T = T_{42}^T$	$T_{36}^H = T_{36}^R$		S/M (-)	3.2	$\chi_{31}^T = \chi_{31}^R$	$\chi_{31}^H = \chi_{31}^R$	
HX-CH4	(ΔT K)	25	$T_{23}^T = T_{52}^T$	$T_{23}^H = T_{15}^H$		CH ₄ conversion	0.8323	1		
HT-SHIFT	T (°C)	350	$T_{32}^T = T_{32}^R$ $T_{33}^T = T_{33}^R$ $\chi_{33}^T = \chi_{33}^R$	$T_{32}^H = T_{32}^R$ $T_{33}^H = T_{33}^R$ $\chi_{33}^H = \chi_{33}^R$		H2-SEP	H ₂ Sep eff.	90 %	100 %	90 %
HX-SHIFT	ΔT (K)	25	$T_{13}^T = T_{34}^T$	$T_{13}^H = T_{13}^R$		\dot{W}_{H_2-SEP}	(MW)	4.79	$\dot{m}_{52}^T = \chi_{H_2,36}^T \dot{m}_{36}^T$	$\chi_{52}^H = \chi_{52}^R$
LT-SHIFT	T (°C)	200	$T_{34}^T = T_{34}^R$ $T_{35}^T = T_{35}^R$ $\chi_{35}^T = \chi_{35}^R$	$T_{34}^H = T_{34}^R$ $T_{35}^H = T_{35}^R$ $\chi_{35}^H = \chi_{35}^R$		COMBRET	Air excess	20 %	$\frac{\dot{m}_{air}}{\dot{m}_{fuel}} = real$	$\frac{\dot{m}_{air}}{\dot{m}_{fuel}} = real$
	χ (mol %)					T_{41} (°C)	1341			
					Heat duty	12500	(MW)	$\dot{m}_{25}^T = 0$ $\chi_{41}^T = \chi_{41}^R$	$\dot{m}_{25}^T = 0$ $\chi_{41}^H = \chi_{41}^R$	

SMR Process: Splitting the $\dot{E}_{D,k}$

Component	$\dot{E}_{D,k}^{EN} > \dot{E}_{D,k}^{EX}$		$\dot{E}_{D,k}^{UN}$ [MW]	$\dot{E}_{D,k}^{AV}$ [MW]	Splitting $\dot{E}_{D,k}^{real}$ [MW]			
	$\dot{E}_{D,k}^{EN}$ [MW]	$\dot{E}_{D,k}^{EX}$ [MW]			$\dot{E}_{D,k}^{UN}$ [MW]		$\dot{E}_{D,k}^{AV}$ [MW]	
					$\dot{E}_{D,k}^{UN,EN}$	$\dot{E}_{D,k}^{UN,EX}$	$\dot{E}_{D,k}^{AV,EN}$	$\dot{E}_{D,k}^{AV,EX}$
COMBRET	131.76	1.94	99.38	34.32	97.94	1.44	33.82	0.50
H ₂ SEP	–	–	6.68	23.46	–	–	–	–
REFORM	34.66	1.04	31.92	3.78	30.96	0.96	3.70	0.08
HT-SHIFT	0.61	0.11	0.70	0.02	0.59	0.11	0.02	0
HX-SHIFT	7.11	0.21	1.19	6.13	1.01	0.18	6.10	0.03
LT-SHIFT	4.27	-0.54	3.70	0.03	4.23	-0.53	0.04	0.01
HX-A	–	–	1.63	11.11	–	–	–	–
HX-B	17.22	1.28	1.64	16.86	2.45	-0.81	14.77	2.09
HX-C	7.25	2.96	0.35	9.86	0.33	0.02	6.92	2.94
HX-CH ₄	–	–	0.10	0.02	–	–	–	–
COMP	–	–	0.35	0.40	–	–	–	–
PUMP	–	–	0.004	0.006	–	–	–	–

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