GTT-Technologies 12th Annual Workshop

Exergetic efficiency analysis of pyrometallurgical processes

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Outline

Exergetic efficiency analysis

- Definition exergy
- Calculation method

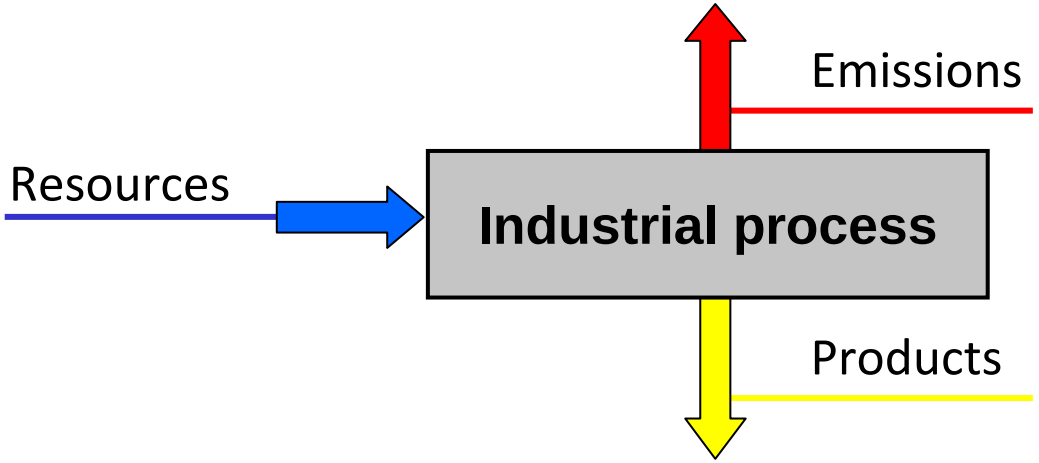
Exergy analysis in pyrometallurgy

- Issues in pyrometallurgical applications
- Practical implementation

Case study: zinc recycling process

- Introduction of the process
- Result of an exergy analysis

Efficiency of industrial processes



Process efficiency = $\frac{\Sigma \text{ products}}{\Sigma \text{ resources}}$

How to quantify the different streams ?

Definition of exergy

The exergy of a stream is the

maximum amount of work

the stream can perform by evolving towards thermodynamic equilibrium with a

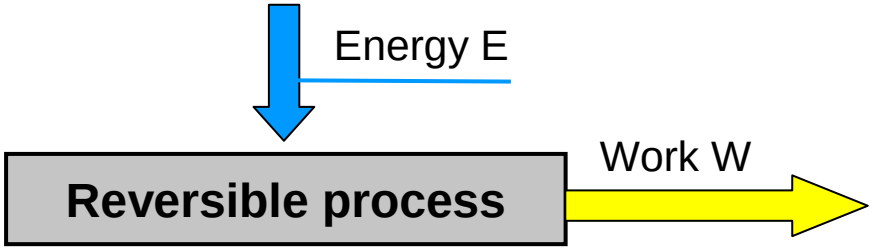
reference environment

through reversible interactions only with this environment

No distinction between mass streams and energy streams

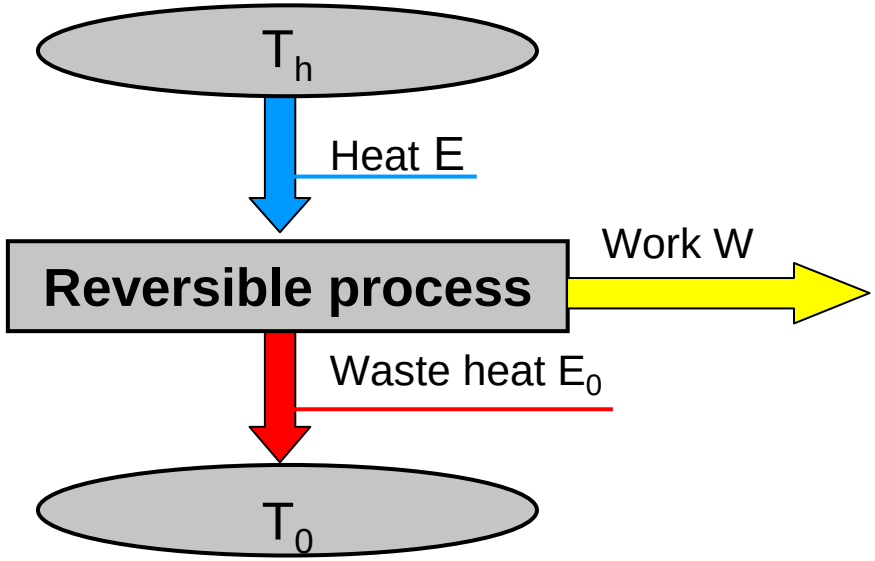
Exergy of energy streams

- Electrical and mechanical energy (E) can be fully transformed into work



$$Exergy\ B = W_{max} = E$$

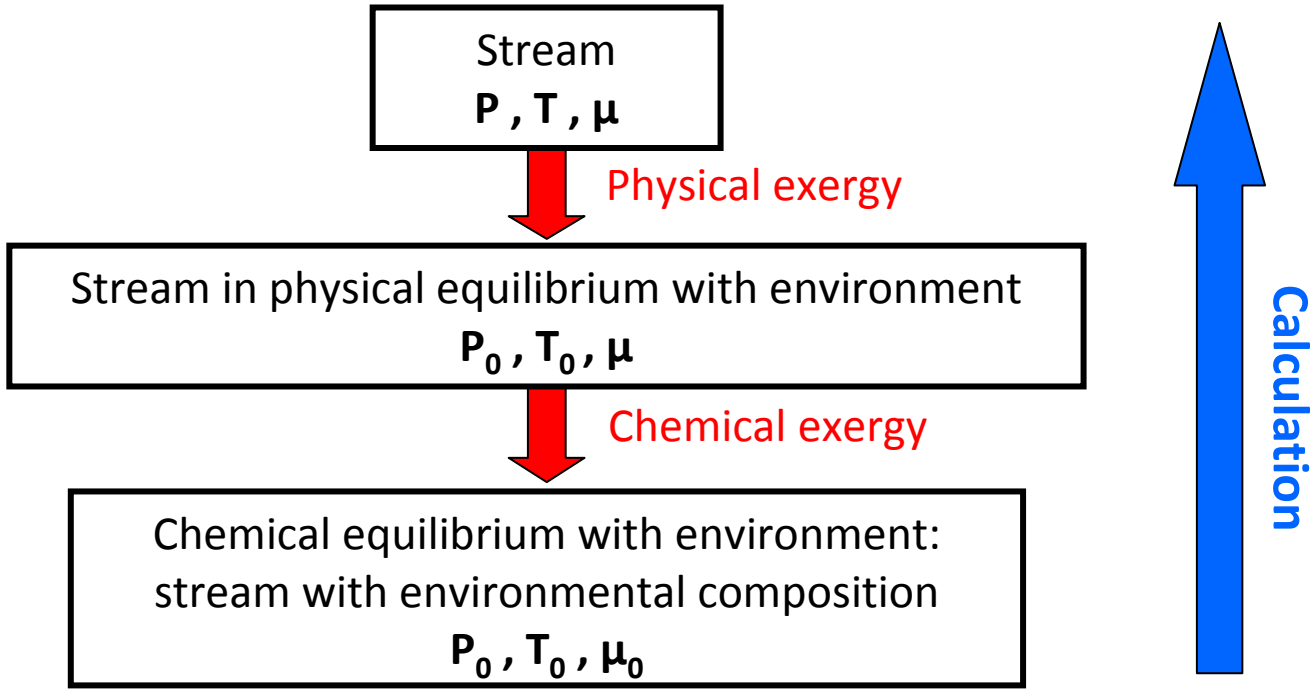
- Thermal energy can only partially transformed into work (Carnot-law)



$$Exergy\ B = W_{max} = E - E_0 = E\left(1 - T_0/T_h\right)$$

Exergy of mass streams

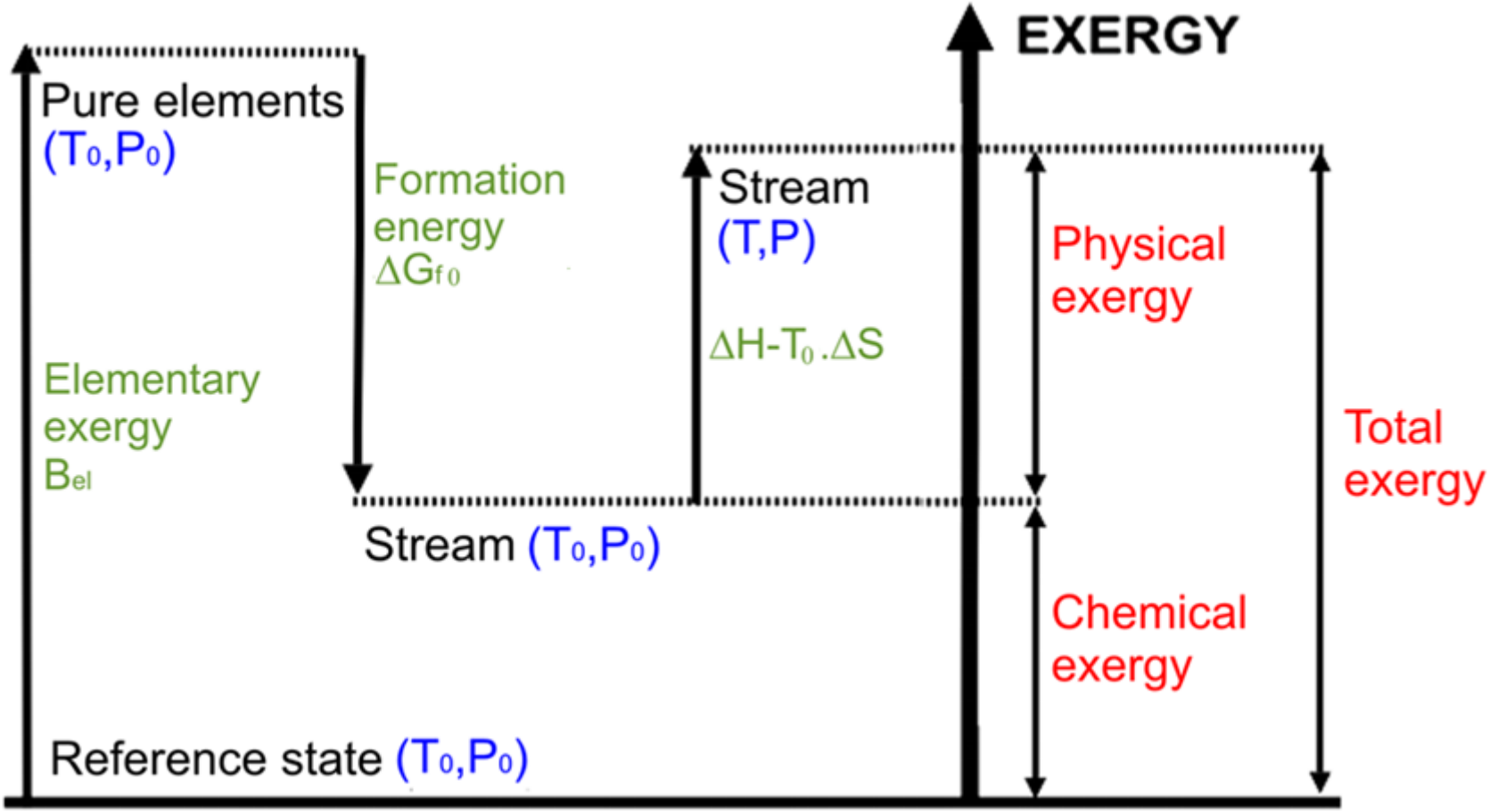
In general: potential to perform work due to inequilibrium with environment (composition, temperature, pressure …)



Standard reference environment (literature)

→ Molar chemical exergy of pure chemical elements B_{el}

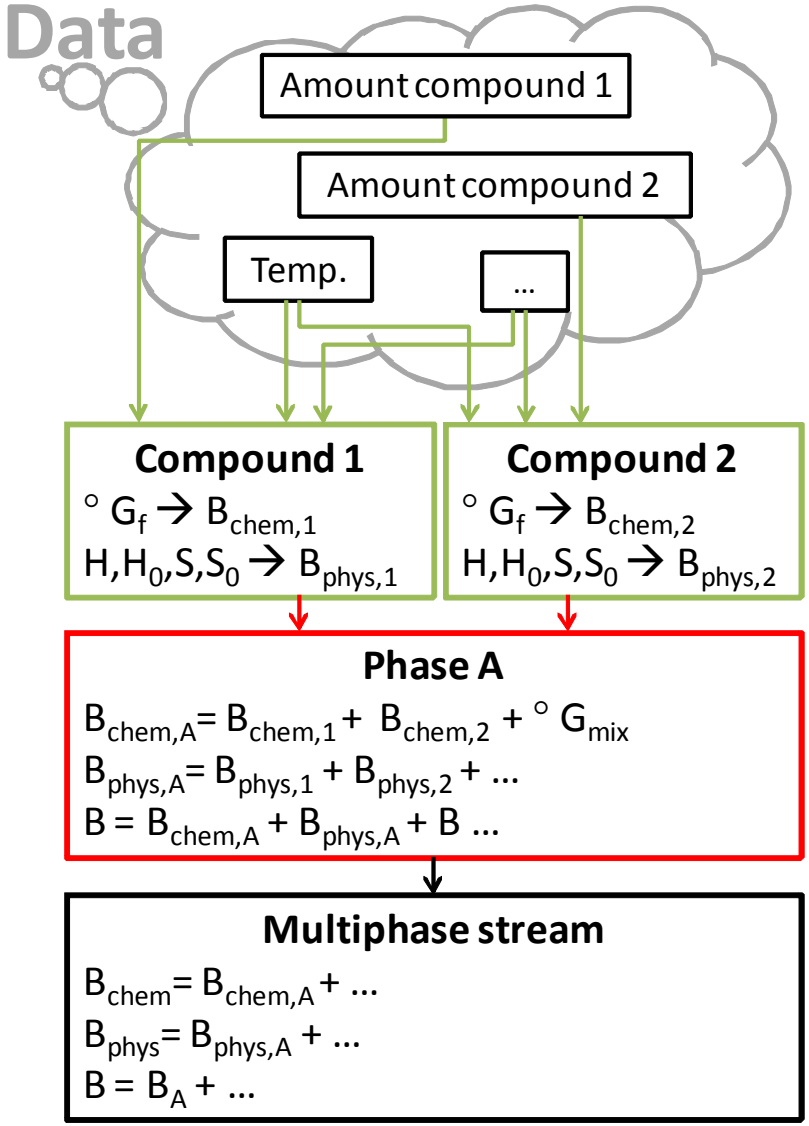
Exergy calculation for single phase stream



Exergy content of multiphase stream = sum of phase exergies

→ effect due to (macroscopic) mixing of phases is often negligible ($=T_0\Delta^{mix}S$)

Typical methodology



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Pyrometallurgical issues

Exergy = generic concept: straightforward implementation for many common simple streams but difficult for streams with complex composition

Issues with high-temperature pyrometallurgical streams:

- Inconsistent descriptions: element- / compound- / phase- / … based
- Non-uniform incorporation of compositional information from different sources

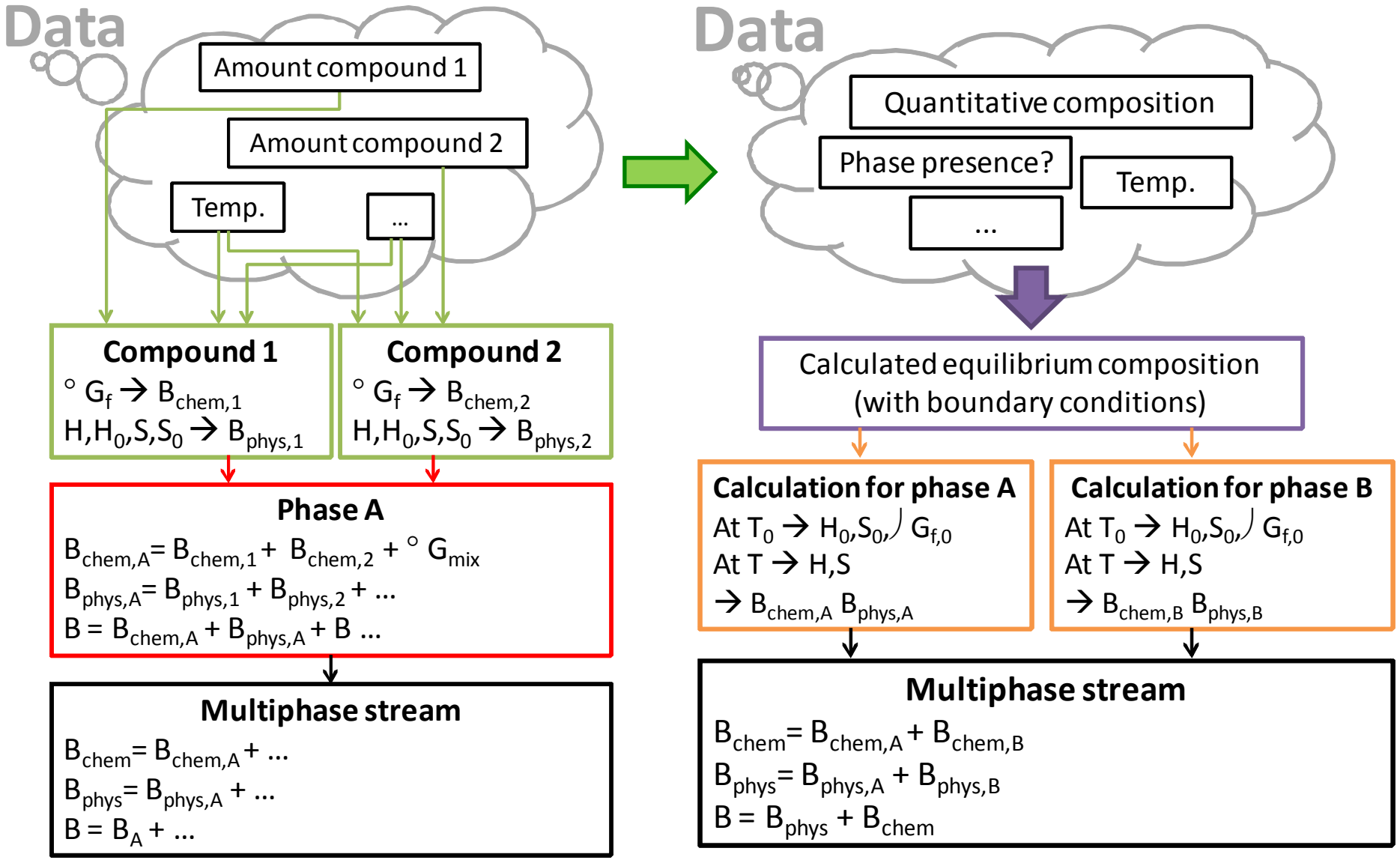
→**Comparison between independent analyses is difficult**

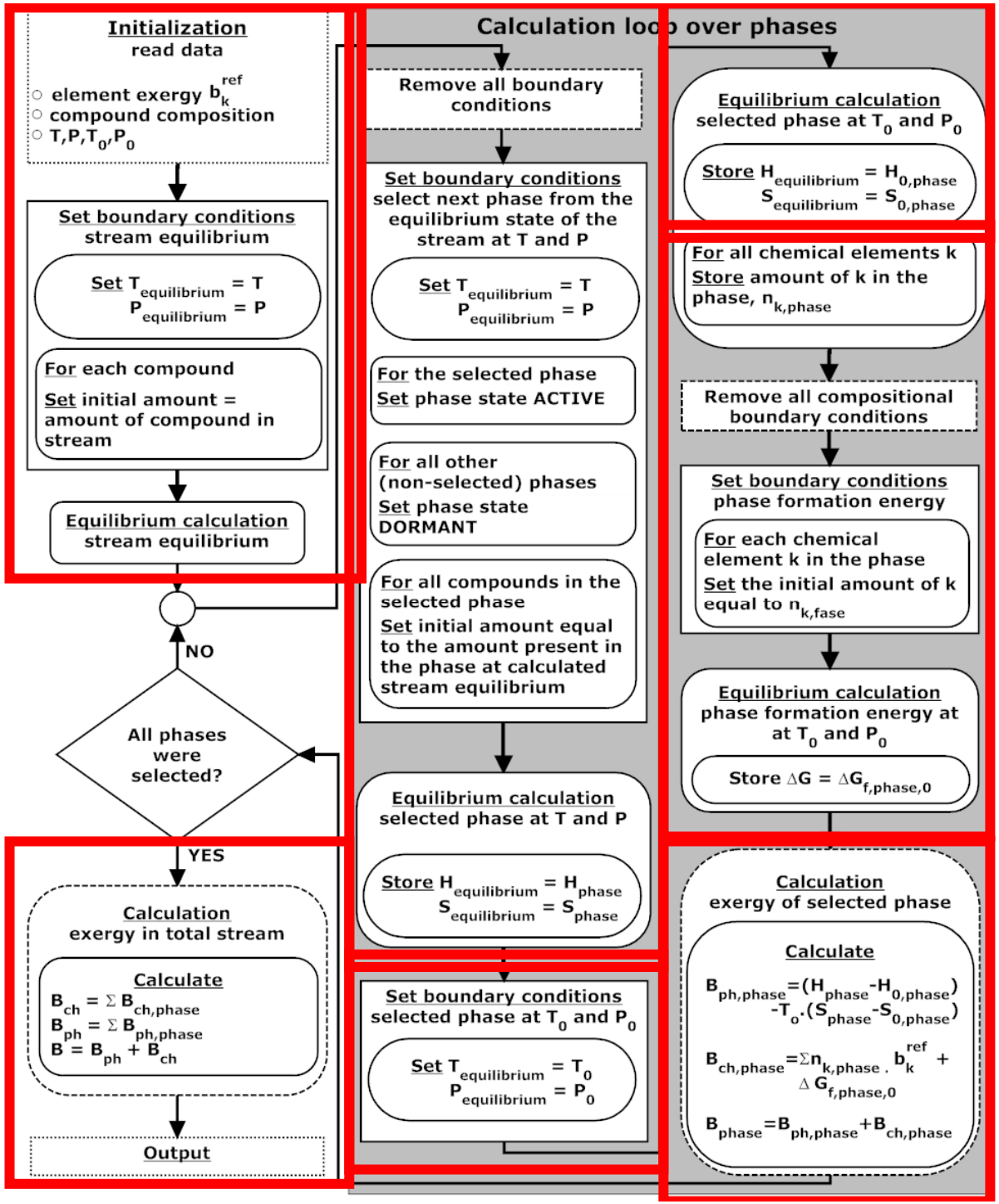
Solution: Use a semi-analytical approach: determine exergy based on a calculated equilibrium composition

- Start from any available composition
- Account for the formation of compounds and (solution) phases
- Use boundary conditions to incorporate quantitative or qualitative knowledge (e.g. measured non-equilibrium phases, measured phase concentrations …)

→**Implemented with ChemApp / FactSage and FACT databases**

Suggested methodology




Initialization
read data
element exergy b_k^{ref}
compound composition
T,P,T_0,P_0
Set boundary conditions
stream equilibrium
Set $T_{equilibrium}$ = T
$P_{equilibrium}$ = P
For each compound
Set initial amount = amount of compound in stream
Equilibrium calculation
stream equilibrium
NO
All phases were selected?
YES
Calculation
exergy in total stream
Calculate
$B_{ch} = \Sigma B_{ch,phase}$
$B_{ph} = \Sigma B_{ph,phase}$
$B = B_{ph} + B_{ch}$
Output
Calculation loop over phases
Remove all boundary conditions
Set boundary conditions
select next phase from the equilibrium state of the stream at T and P
Set $T_{equilibrium}$ = T
$P_{equilibrium}$ = P
For the selected phase
Set phase state ACTIVE
For all other (non-selected) phases
Set phase state DORMANT
For all compounds in the selected phase
Set initial amount equal to the amount present in the phase at calculated stream equilibrium
Equilibrium calculation
selected phase at T and P
Store $H_{equilibrium} = H_{phase}$
$S_{equilibrium} = S_{phase}$
Set boundary conditions
selected phase at T_0 and P_0
Set $T_{equilibrium} = T_0$
$P_{equilibrium} = P_0$
Equilibrium calculation
selected phase at T_0 and P_0
Store $H_{equilibrium} = H_{0,phase}$
$S_{equilibrium} = S_{0,phase}$
For all chemical elements k
Store amount of k in the phase, $n_{k,phase}$
Remove all compositional boundary conditions
Set boundary conditions
phase formation energy
For each chemical element k in the phase
Set the initial amount of k equal to $n_{k,fase}$
Equilibrium calculation
phase formation energy at at T_0 and P_0
Store $\Delta G = \Delta G_{f,phase,0}$
Calculation
exergy of selected phase
Calculate
$B_{ph,phase} = (H_{phase} - H_{0,phase}) - T_o.(S_{phase} - S_{0,phase})$
$B_{ch,phase} = \Sigma n_{k,phase} . b_k^{ref} + \Delta G_{f,phase,0}$
$B_{phase} = B_{ph,phase} + B_{ch,phase}$

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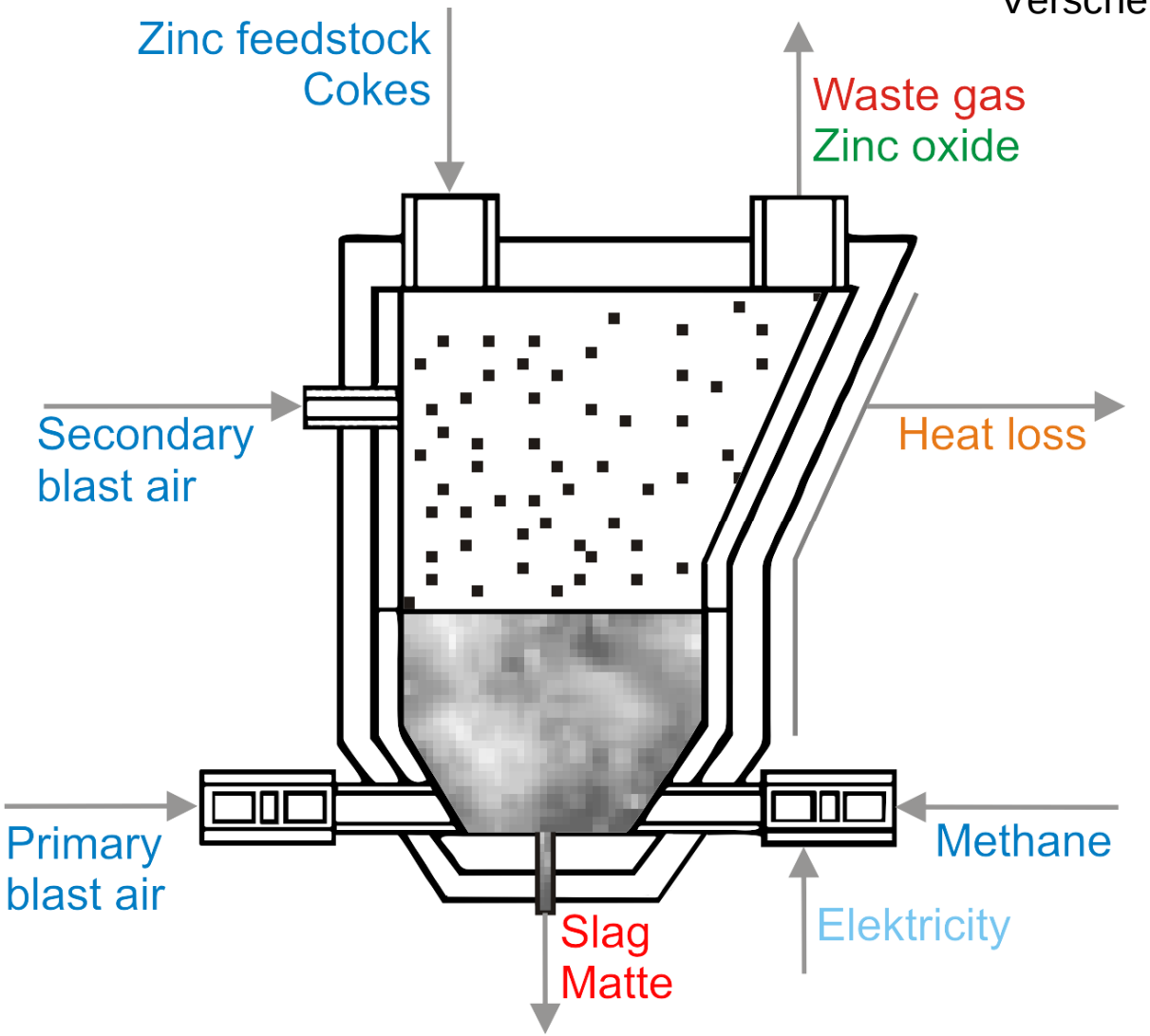
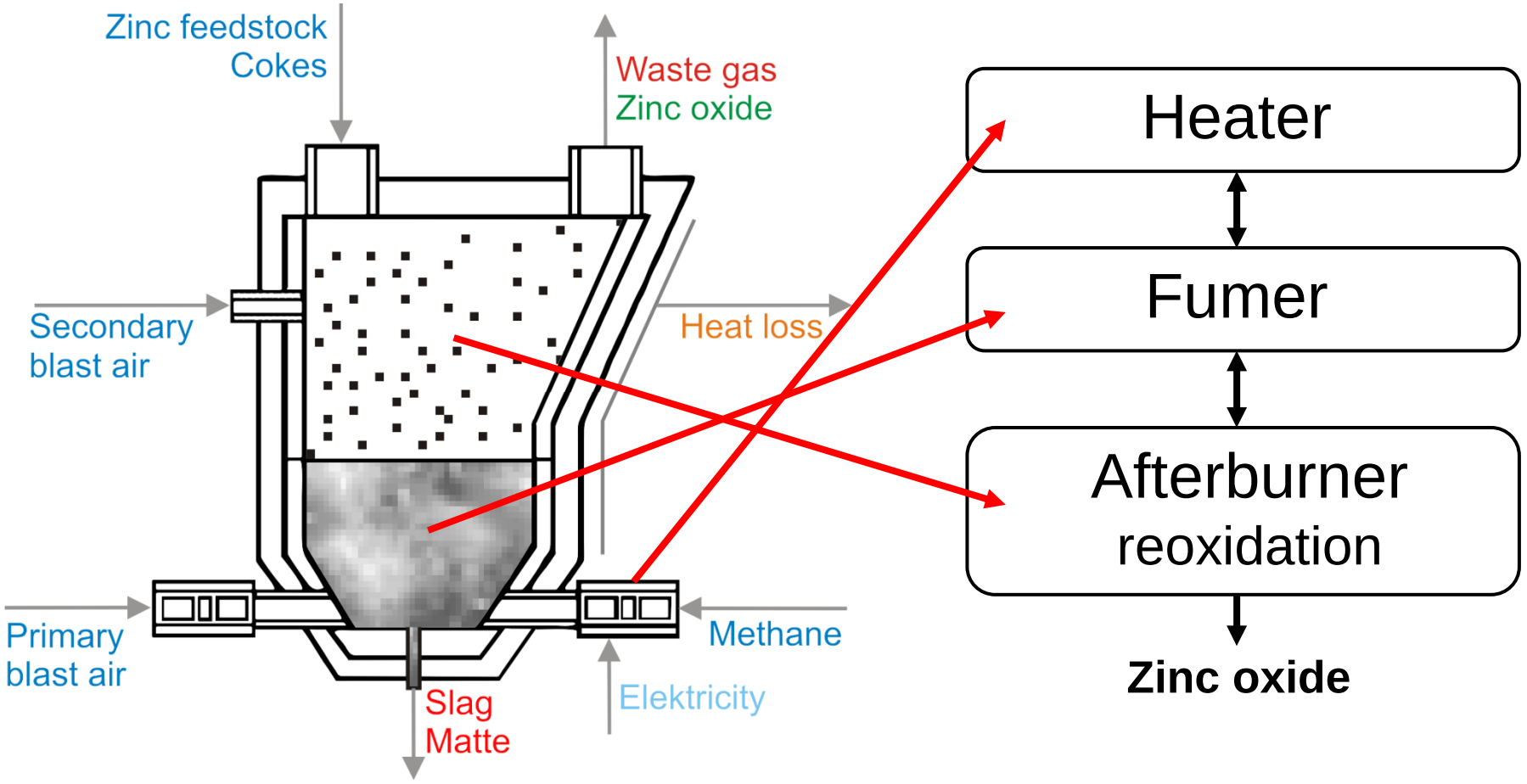
Zinc recycling process

Verscheure et al. (2007)

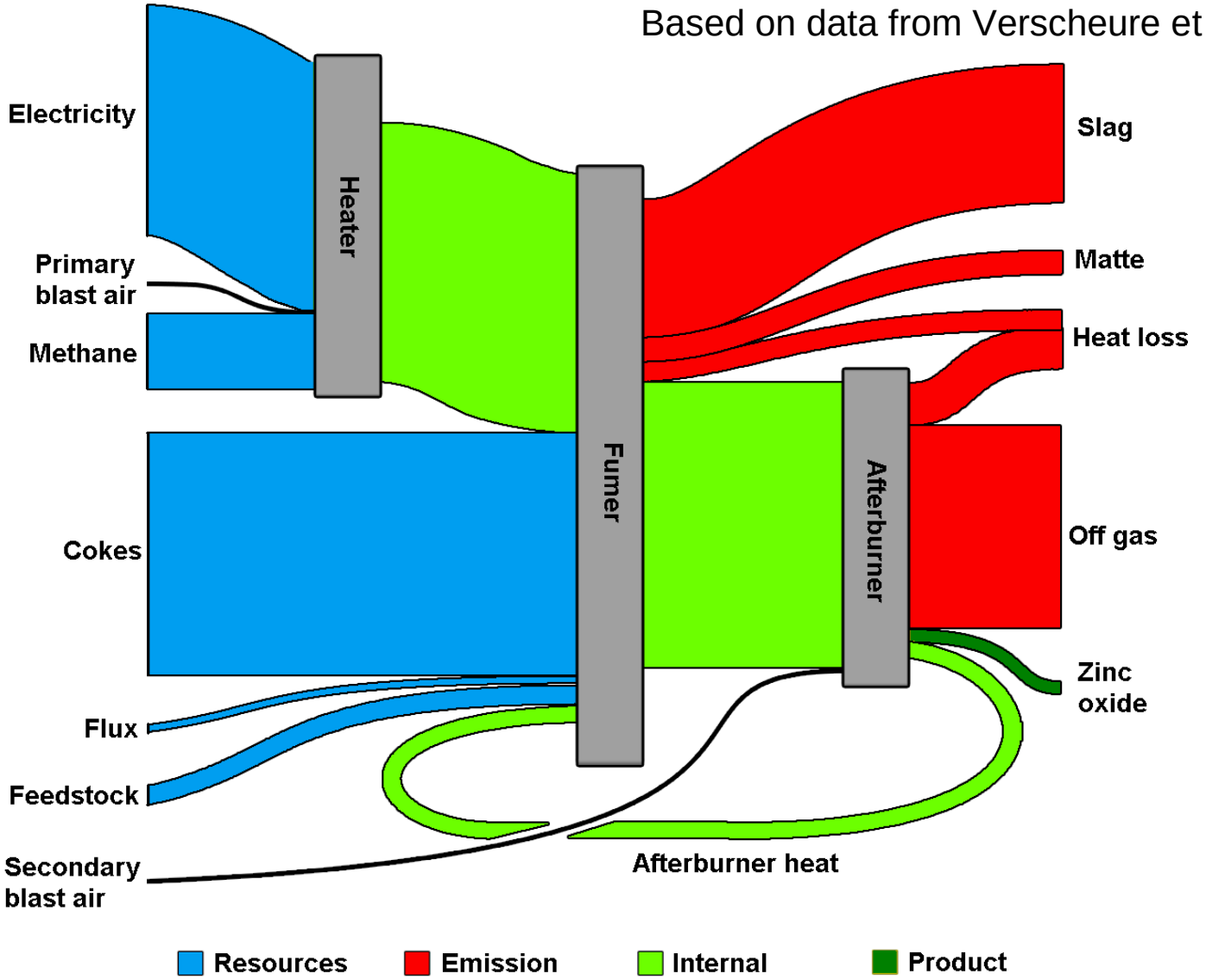


Zinc recycling process - model



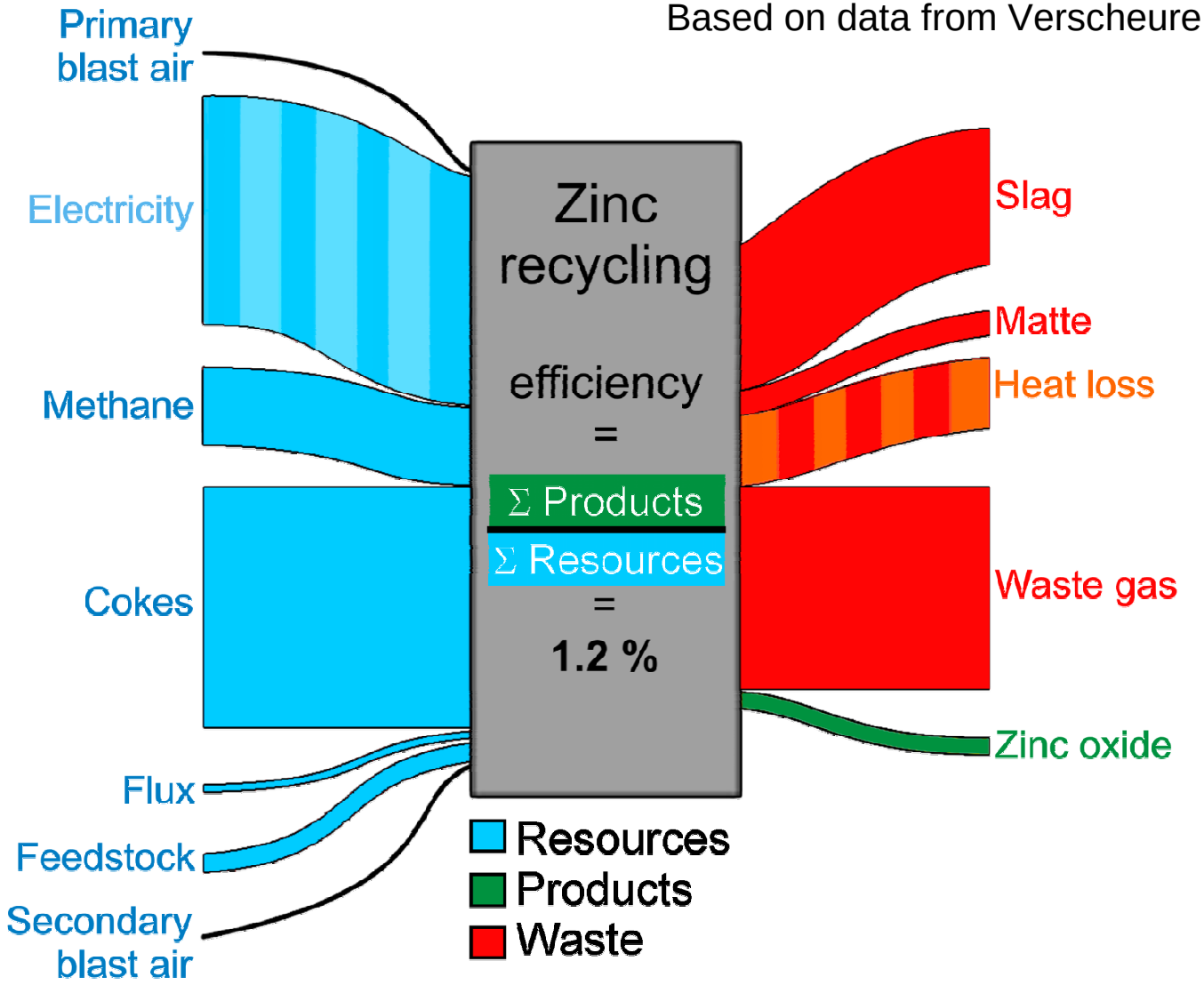
Zinc recycling process - model

Based on data from Verscheure et al. (2007)



Exergy analysis – base case

Based on data from Verscheure et al. (2007)



Conclusions

- Exergy analysis allows an unambiguous assessment of the efficiency of a process
- Translating the theoretic concept into a widely applicable and practical methodology is not straightforward
- A methodology for exergy calculations on complex pyrometallurgical process streams is suggested and implemented using FactSage/ChemApp
- A case-study on zinc recycling proces shows briefly the potential of exergetic efficiency analysis

Thanks for your attention

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