



Second Generation MethylMethAcrylate

Concepts of process design

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MMAtwo
workshop

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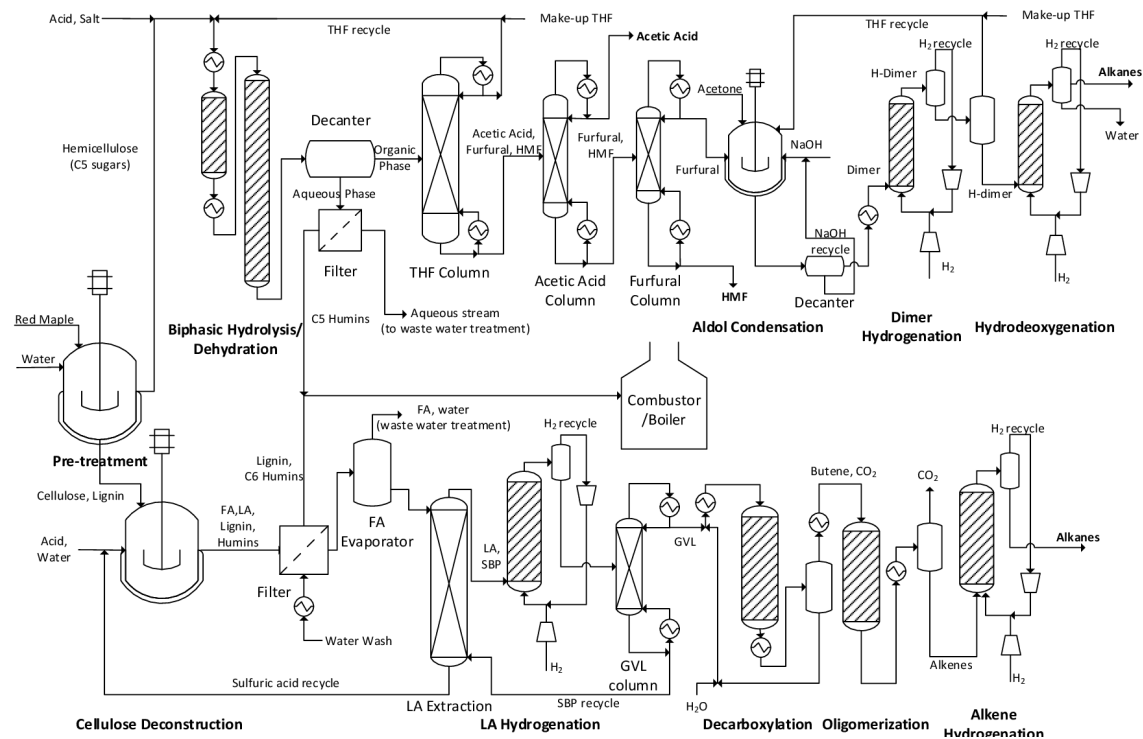
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Process design



- Can the process be further improved?

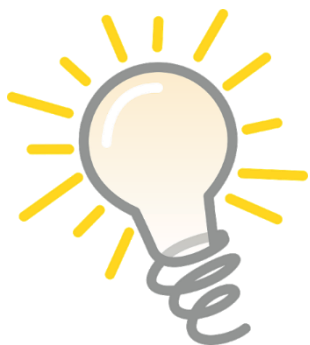


from J. Q. Bond et al., *Energy Environ. Sci.*, 2014, 7, 1500



Typical process development approach

- Core technology first, design process around it in the final stage
- COSTS & energy optimization to be done as final touch
- Idea → Laboratory → Pilot Scale → Mass scale





Typical process development approach

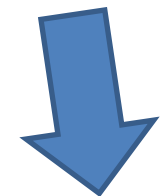
- Am I actually improving anything with my process?
- Am I on the right track towards “best” process?
(many solutions may be possible)
- What’s the practical value of the innovation?



Process X



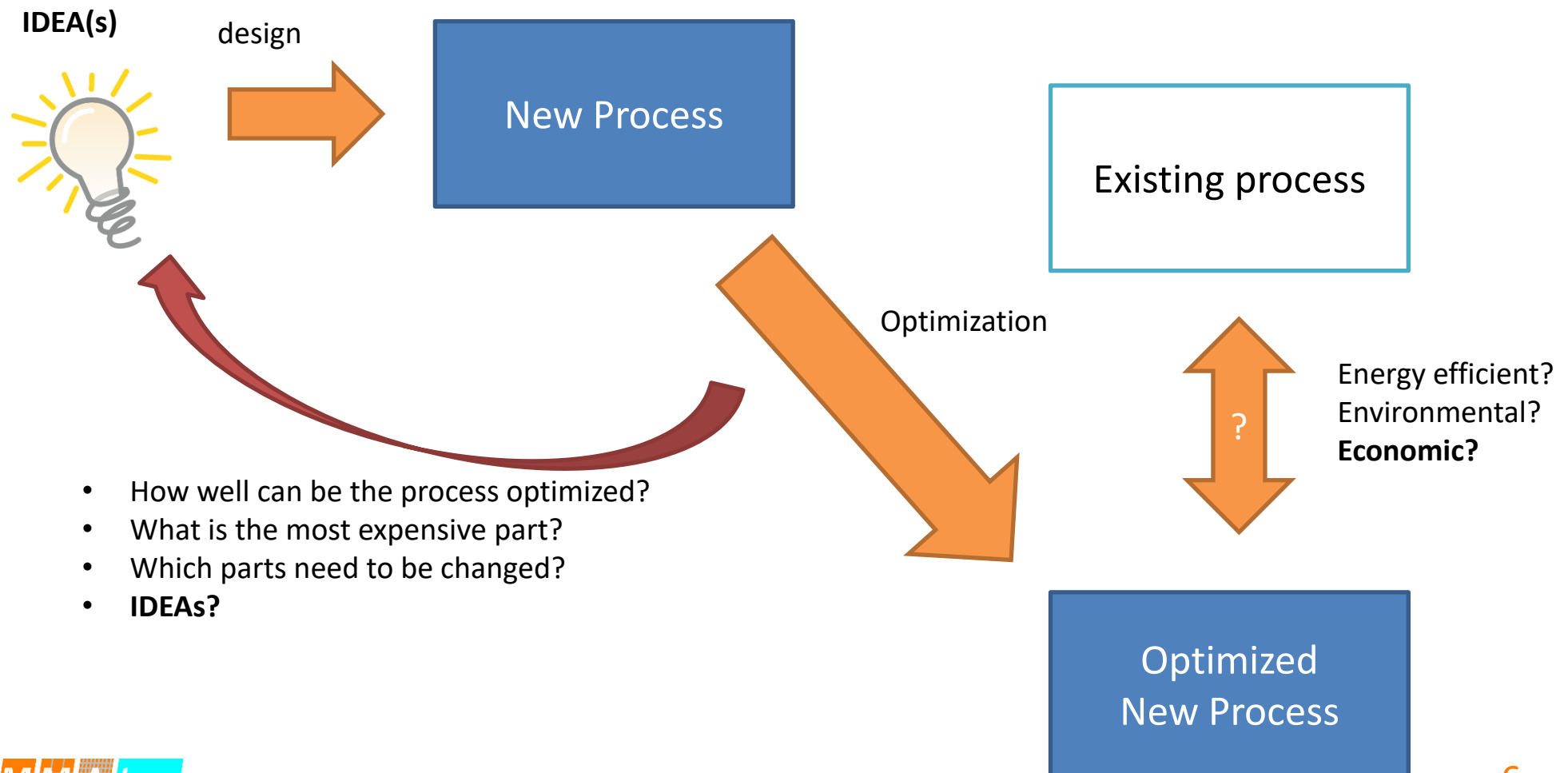
Process Y



Process Z



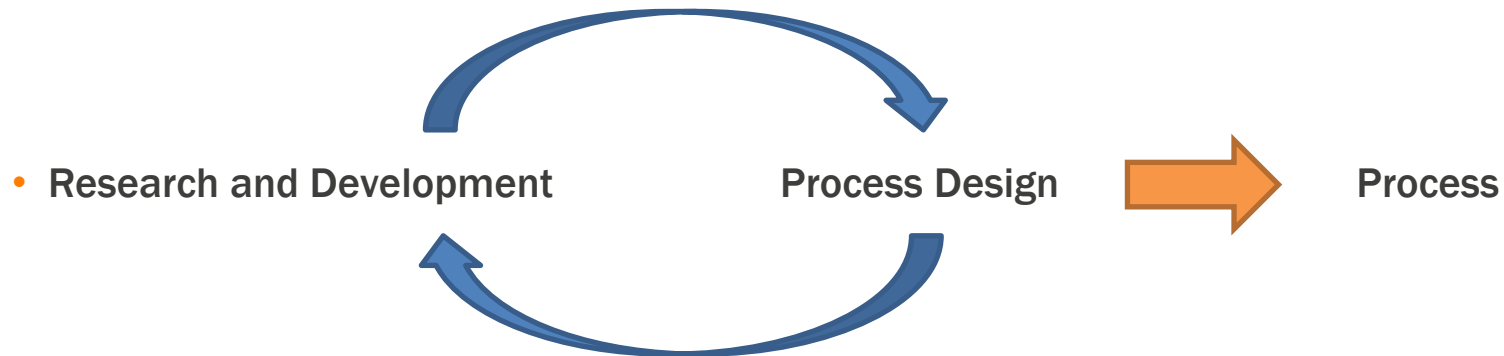
Modified process development approach





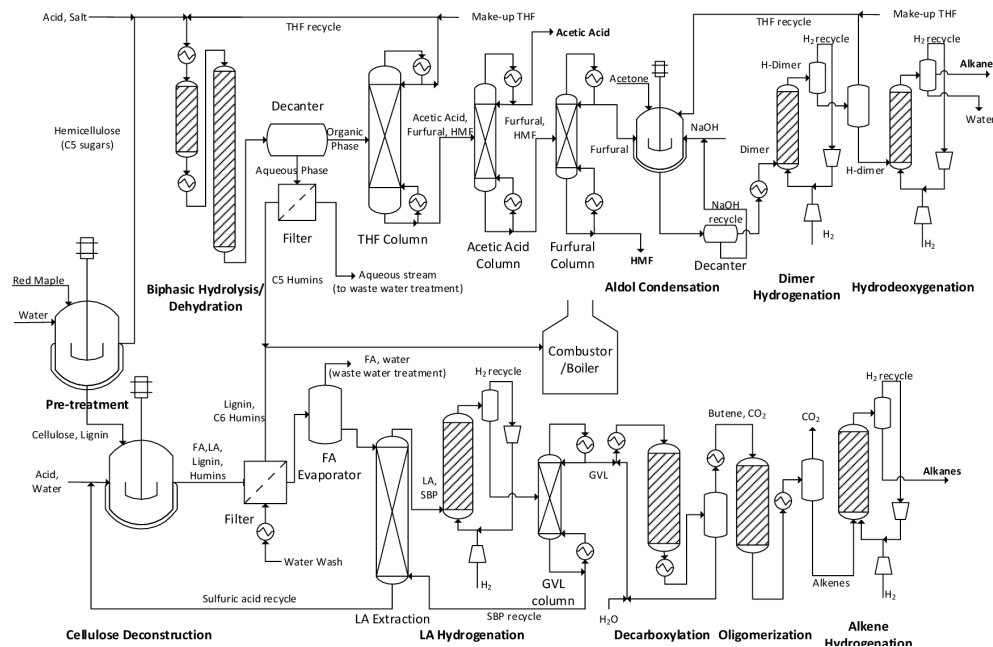
Modified process development approach

- Successful process design is an iterative process:



- Cooperation of scientists and process engineers is essential

Concepts of process design



**Material processing efficiency
(products vs. by-products, raw
material loss)**

Energy consumption

Environment

Equipment costs

Economy



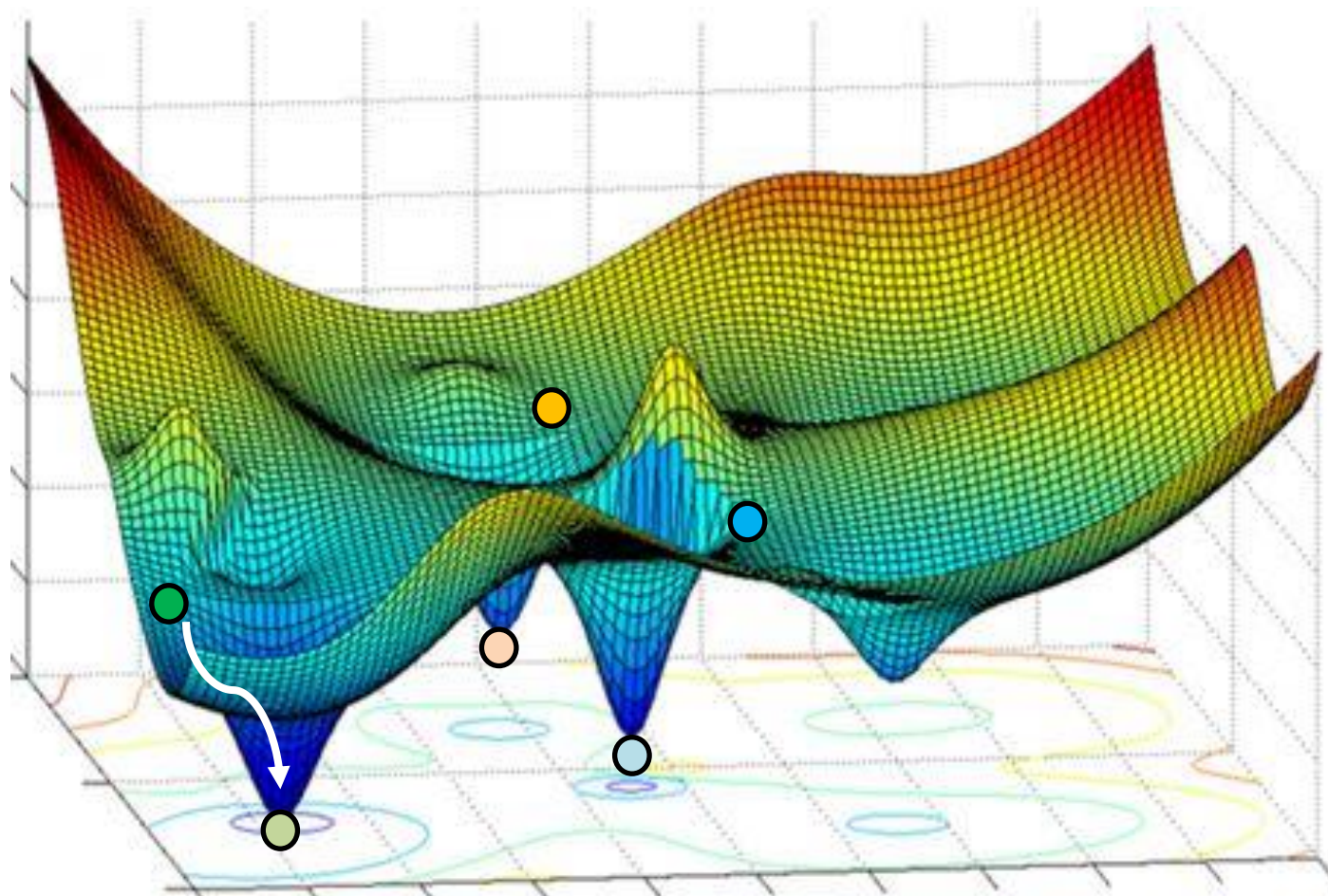
Concepts of process design

- Can we say if there's any room for reasonable improvement for the existing process? **YES**
- **Concept of perfect process exists we can measure how far our process is in terms of energy & material processing efficiency**
- Can we say which parts are crucial to be improved during optimization? **Likely YES**
- **Imperfection of the process is sum of imperfections of its parts**
- Can we say what other process choice is to do the trick? **ultimately NO**
- **Example:** What is the best process to separate methyl-methacrylate and ethyl-acrylate?
  - distillation expert: choose distillation!
  - crystallization expert: choose crystallization!
  - extraction expert: chose extraction!
- But structured process design approaches exist nevertheless



Process design as loss function minimization

- Process idea to optimized design



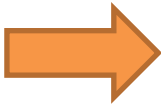
- Distillation
- Crystallization
- Extraction



Perfect process?



Process energy

- Electric energy (power by shaft-work): **20 EUR/MWh**
- Heat: **6 EUR/MWh of natural gas**
- Thermodynamics:  **work is more precious than heat**

Heat has certain “quality” to it



1200 °C

price of fuel



30 °C

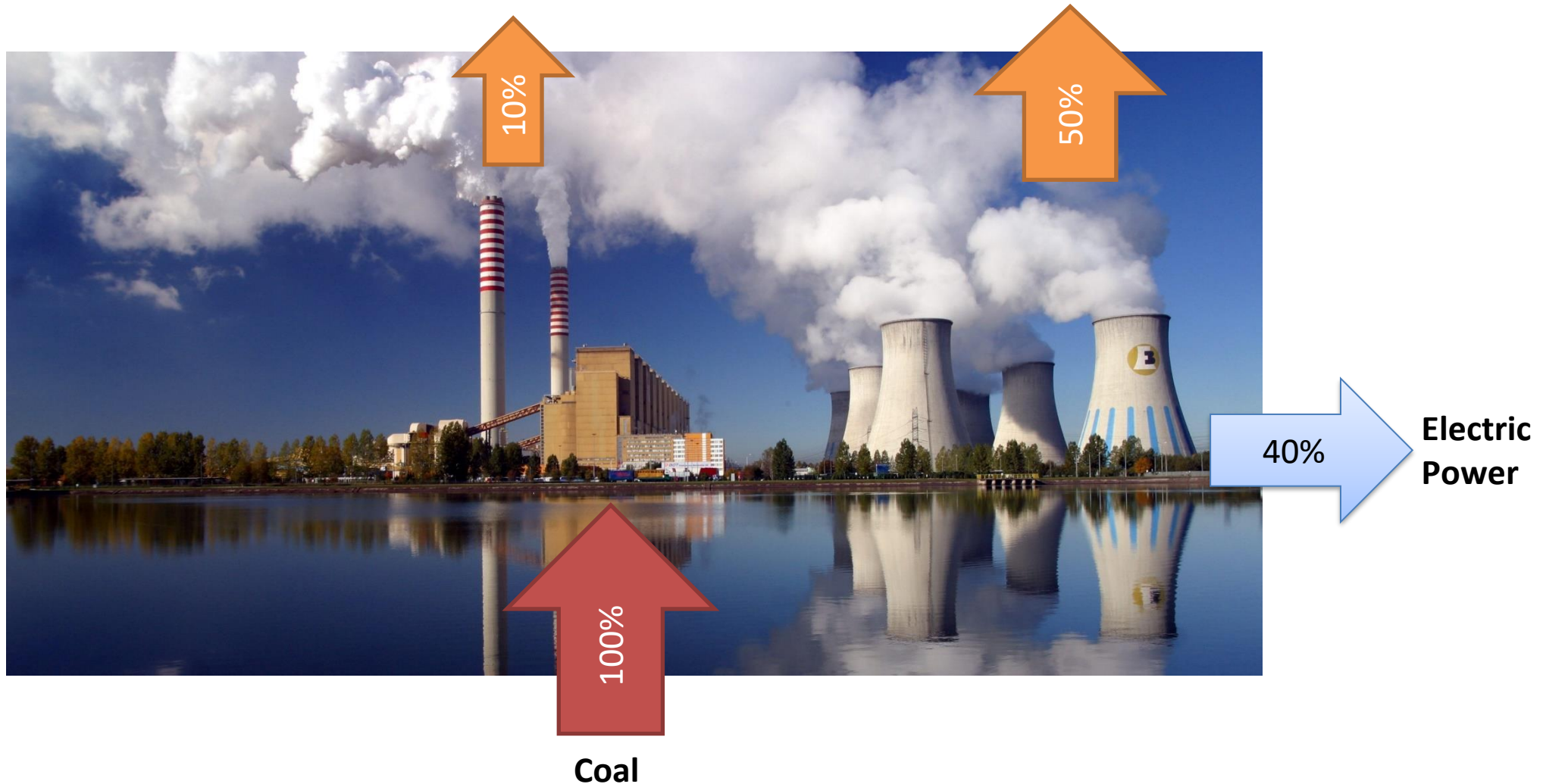
Price = 0 EUR (useless, even some added costs)



Heat to Power

Flue gas (150°C)

Cooling water evaporate (30°C)

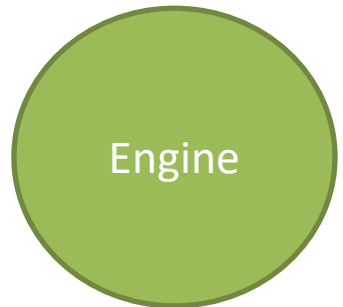




Perfect vs. real engine

Flame (1200°C)

Steam (350°C)



Electric Power



Cooling water (25°C)

PERFECT ENGINE

$$W_{max} = Q \left(1 - \frac{T_{COLD}}{T_{HOT}} \right)$$

$$\Delta S = 0$$

$$\left(1 - \frac{T_{COLD}}{T_{HOT}} \right)$$

Heat “quality”

REAL ENGINE

$$\Delta S = S_{IRR}$$

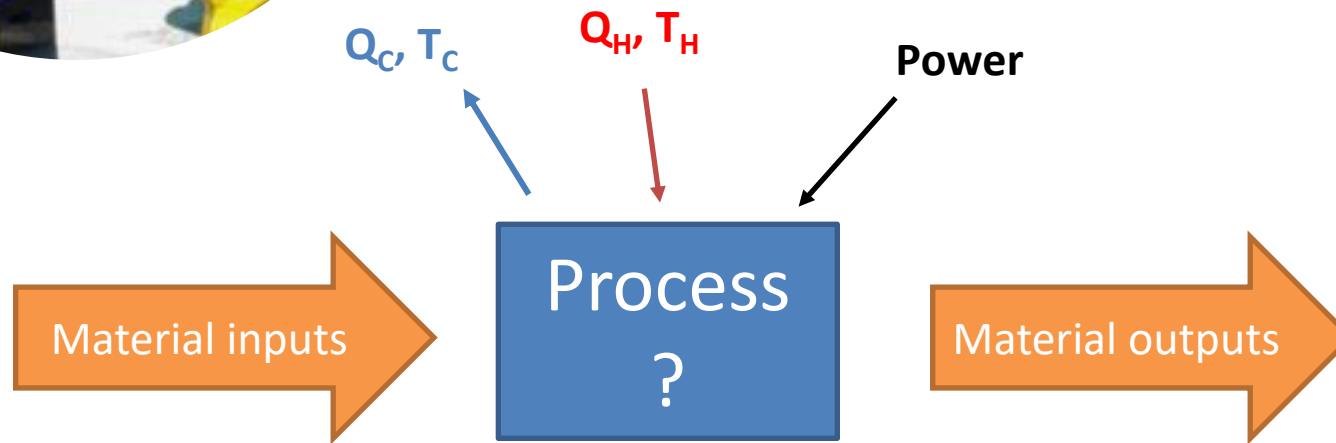
$$W_{real} = W_{max} - W_{lost}$$

$$W_{lost} = S_{IRR} \cdot T_{COLD}$$

Entropy is bad



Perfect vs. real process



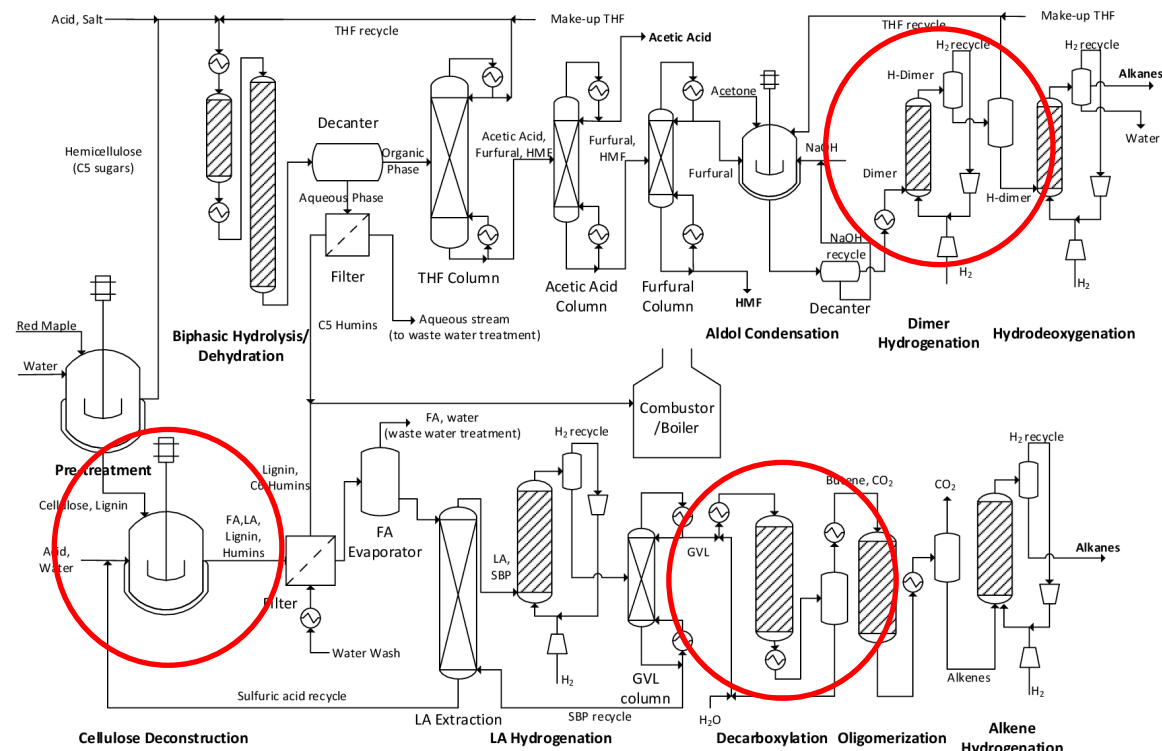
$$\sum_{\text{in the system}} \left[Si + \frac{\dot{Q}_i}{T_i} \right] + S_{IRR} = \sum_{\text{out of the system}} \left[Sj + \frac{\dot{Q}_j}{T_j} \right]$$

$$\sum_{\text{in the system}} \left[Gi + \dot{Q}_i \left(1 - \frac{T_0}{T_i} \right) + \dot{W}_k \right] = \sum_{\text{out of the system}} \left[Gj + \dot{Q}_m \left(1 - \frac{T_0}{T_m} \right) + \dot{W}_n \right] + W_{lost}$$



Guided process improvement

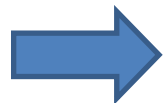
- Can be done for whole process or any of its part (it's just balances)
- Simply, minimize generation of entropy (minimize work loss / minimize exergy loss)
- Re-think operations that have large exergy loss (large entropy generation)



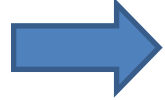


How to reduce entropy

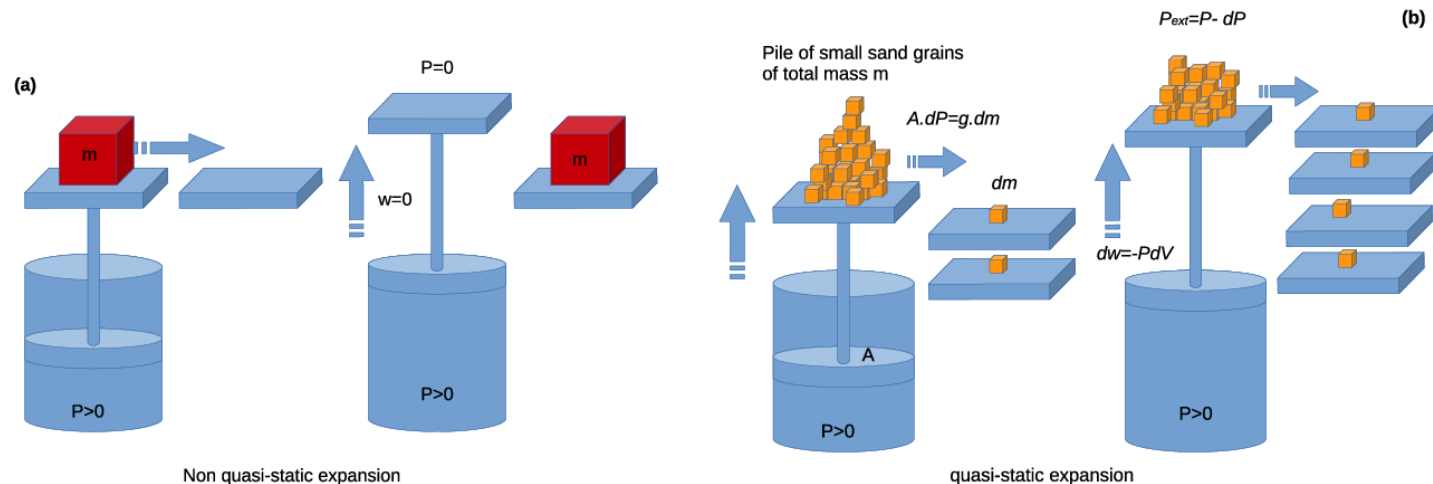
- reduce entropy = closer to "equilibrium like" = reduce driving forces
- Apply only slightly more driving force than minimum
- Reuse forces generated in the process



Staging (think of distillation column, ... or any separation column)



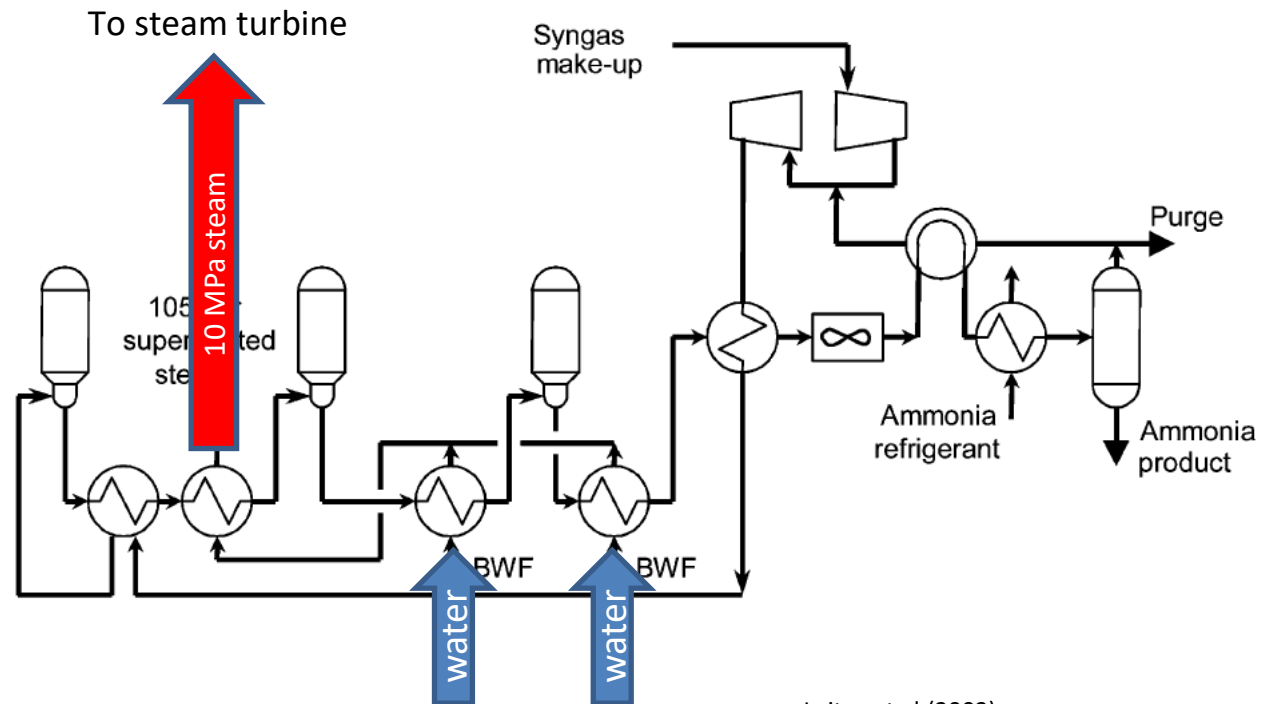
Counter-current operations (think about heat exchangers)





Example: ammonia production

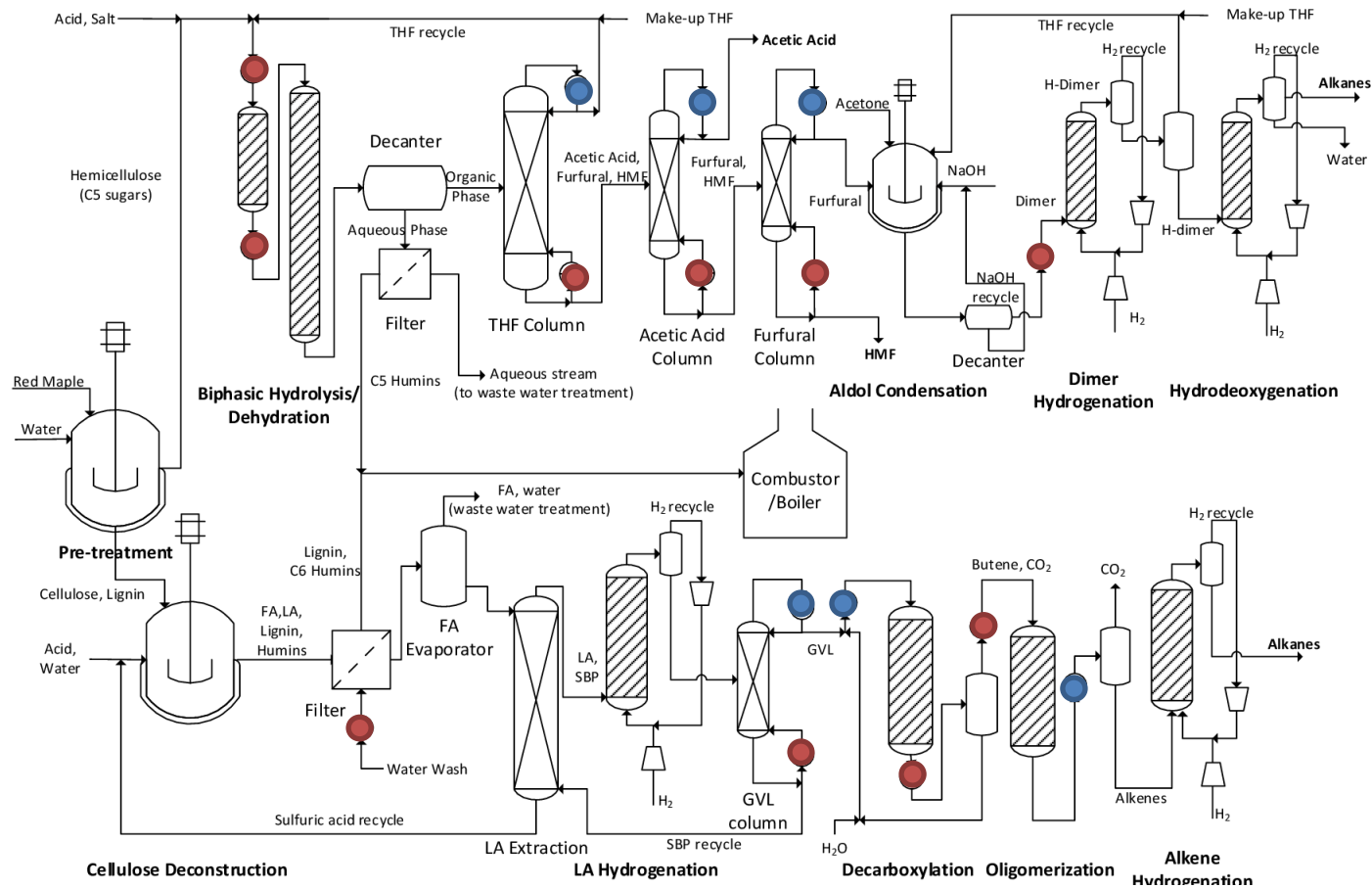
- $3\text{H}_2 + \text{N}_2 = 2\text{NH}_3$
- Very exothermic reaction
- Le Chatelier's principle:
cool down as much as possible!
- Energy efficiency:
not so fast!
- Reactor in 3 stages
 $T_1 > T_2 > T_3$
- Cuntercurrently **water** to **steam**
- **Steam** to turbine (to recover work)



Leites et al.(2003)



Example: heat integration

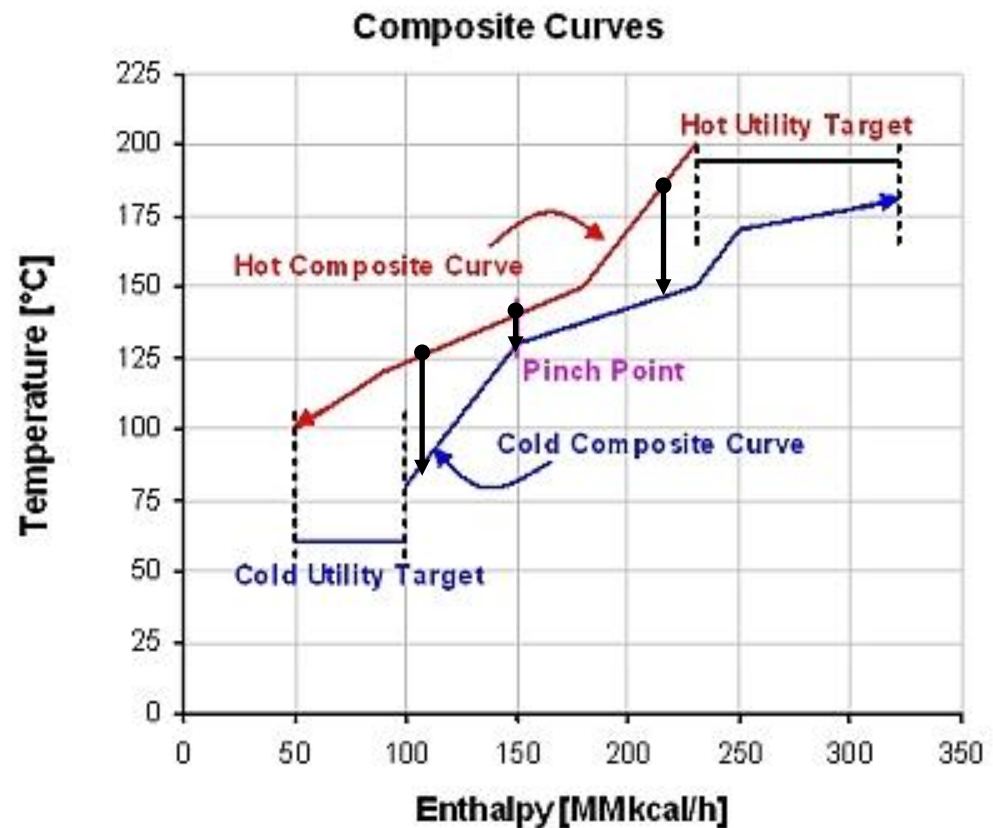




Example: heat integration

Again:

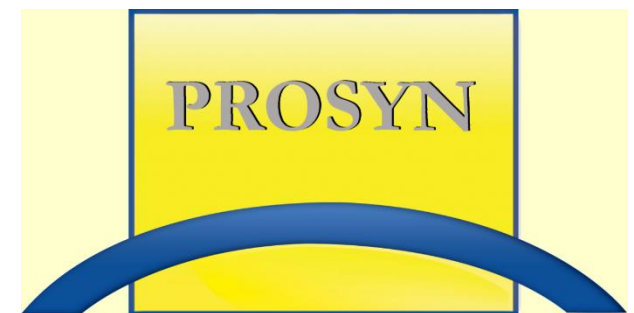
- Apply only slightly more driving force than minimum
- Reuse as much force generated in the process as possible
- Counter-current operations
- Savings on **hot utility** ("HEAT") and **cold utility** consumption





Real process improvement

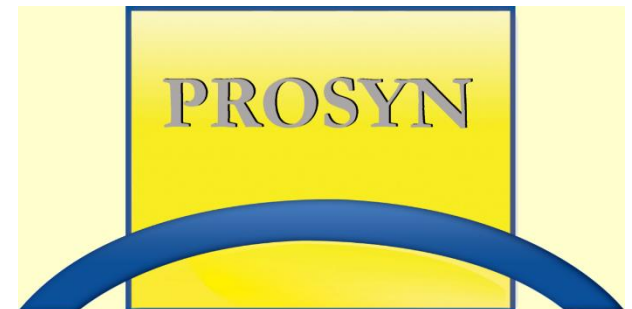
- Any efficiency improvement reflects the entropy minimization.... one way or another
- Incremental process optimization can get you only that far... (till some local minimum)
- Sometimes new technology needs to be chosen for some part of the process or the process as whole
- New starting point for the optimization
- Designer ingenuity
- **Heuristic approach for automatic process synthesis: PROSYN (PDC)**





Key - takeaways

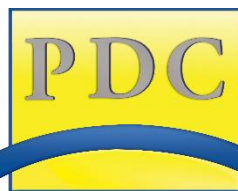
- Successful process design is an iteration between designers and R&D
- We can objectively say how “bad” a process is to see if we can improve something
- Thermodynamics can be useful for systematic guided process improvement
- **Entropy is bad**
- Process technology choice is ultimately on the designer view of the problem, but helping-out tools for starter exists





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