Karim Ben Hicham
Christian Kuckelkorn
Christopher Kypke
Niklas Nickel
Elvis Sim

AixSTRAWdinary
Driving the chemistry of tomorrow

Aachener Verfahrenstechnik

RWTH AACHEN UNIVERSITY

AixSTRAWdinary – Chemocatalytic Production of Butadiene from Lignocellulosic Biomass

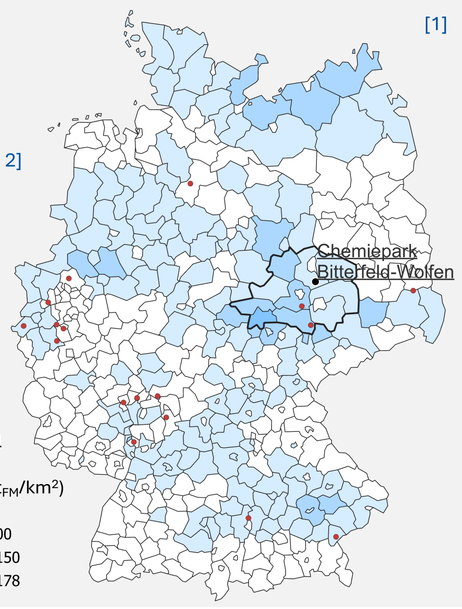
Concept: As traditional butadiene production emits significant CO_2, we developed a sustainable, two-step, cereal-straw-based, chemocatalytic process rigorously modelled in Aspen Plus.

Feedstock Selection

1. Cereal Straw

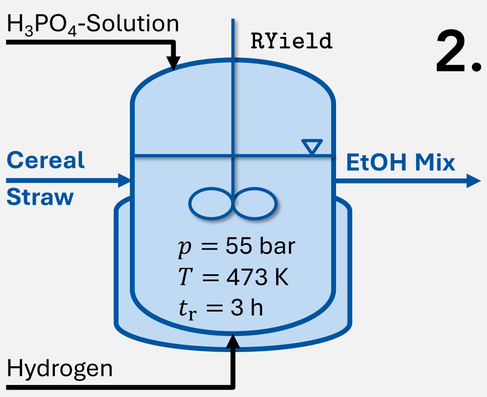
- Most underutilized biomass in Germany [1, 2]
- vs. other 1st & 2nd generation biomasses:
  + No land-use change [3]
  + No competition with food industry
- Centralized plant (**Bitterfeld-Wolfen**)
  ⟹ Only 60 km mean transport distance

Mobilizable biomass potential
~6.5 Mt_{DM}/a [1, 2]



Reaction 1: Chemocatalytic Hydrogenolysis

2. Ethanol Production



One-pot, selective hydrogenolysis of pretreated cellulose to ethanol [4]

vs. Fermentation
+ Fewer CO_2 emissions [5]

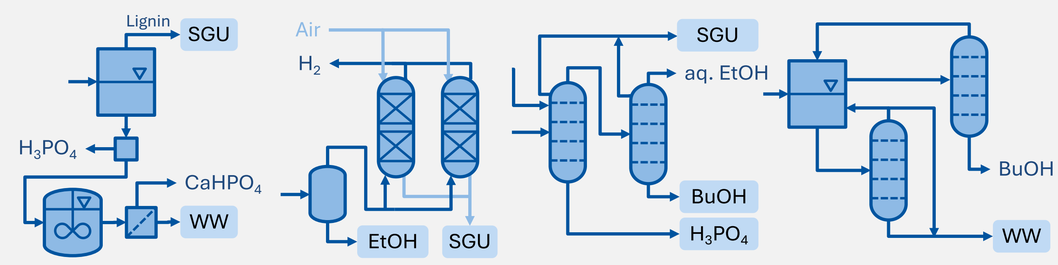
vs. Gasification
+ Lower CAPEX and OPEX [5]

Catalyst: Nickel on Carbon (Ni@C) with H_3PO_4 [6]

Separation / Purification System

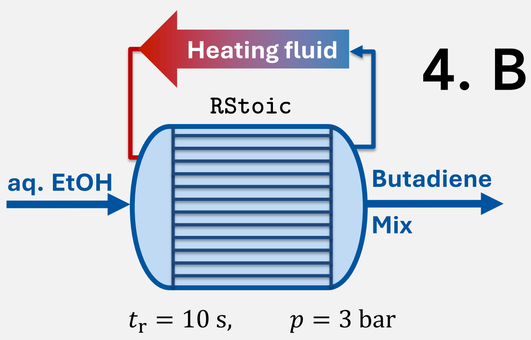
3. Ethanol-Mixture Separation

H_3PO_4 Recovery | H_2 Recovery | EtOH Separation | BuOH Purification



Reaction 2: LEBEDEV Process

4. Butadiene Synthesis



Single-step, gas-phase reaction
Kinetic model implemented [7]

ζ_{EtOH} = 99.8% σ_{BD} = 84.1% [9]

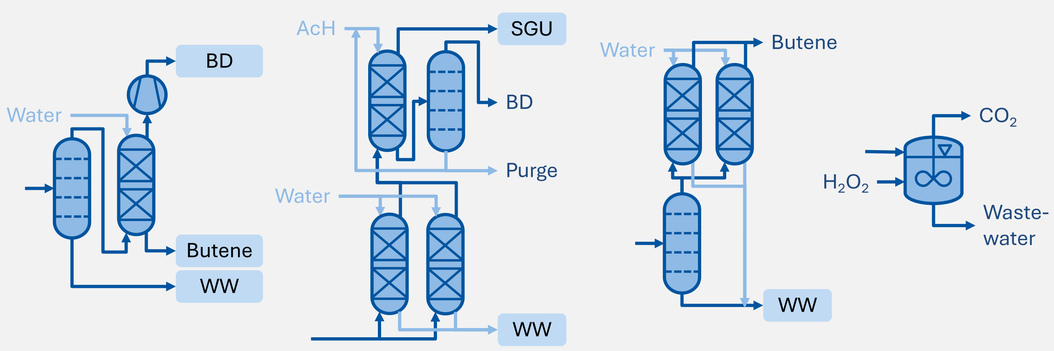
vs. OSTROMISLENSKY process
+ Lower CAPEX [7]
+ Improved Sustainability [7]

Catalyst: K_2O:ZrO_2:ZnO/MgO-SiO_2 [8]

Separation / Purification System

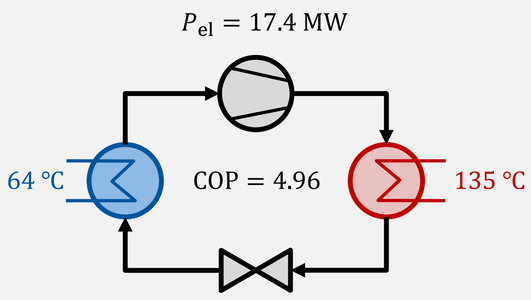
5. Butadiene-Mixture Separation

Butadiene Separation | Butadiene Purification | Butene Purification | Wastewater Treatment



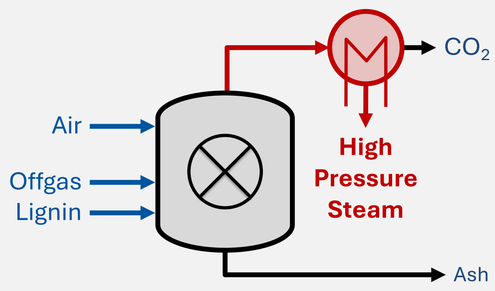
Process Integration

6. Energy Recovery



Industrial Heat pump

→ **16.7 MW** district heating
→ Achieves **~95%** heat integration

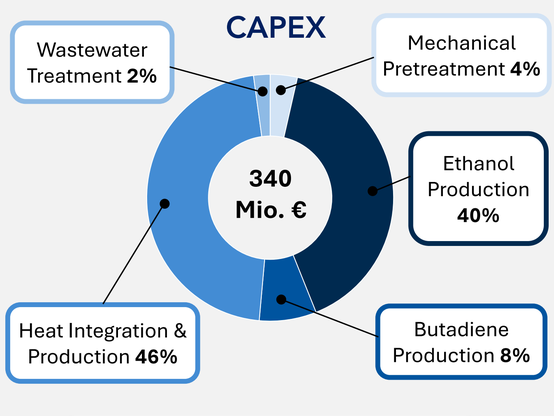


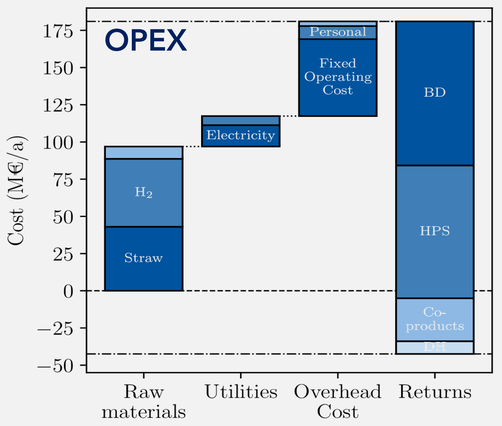
Steam Generation Unit

→ Generates **all hot utilities**
→ **215 t/h** excess HPS

Process Analysis

7. Economic Analysis





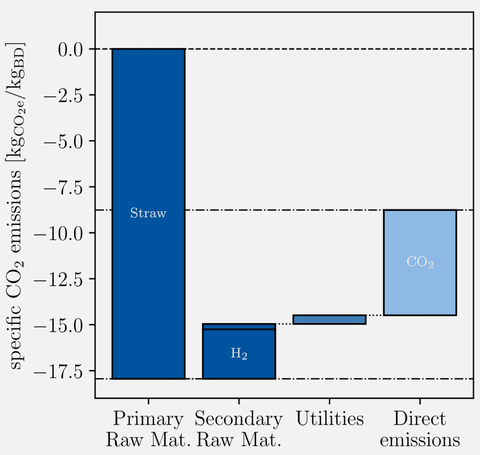
Minimum Selling Price
1.56 €/kg_{BD}
Bio-Processes: 1.4 – 2.6 €/kg_{BD} [10, 11]

Payback Time
10 years @ i = 5% p.a.

Selling Price
1.90 €/kg_{BD}

Process Analysis

8. Sustainability Assessment



- Scope 3 upstream (cradle-to-gate) carbon footprint analysis
- Social benefits: supports local stakeholders through utilization of excess straw

CO_2 Footprint
–8.8 t_{CO_2}/t_{BD}
Conventional: 1.7 t_{CO_2}/t_{BD} [12]

References

1. Ressourcen Datenbank, *Deutsches Biomasseforschungszentrum gGmbH* (2023)
2. A. Brosowski et int. D. Thrän, *Energy, Sustainability and Society* (2020)
3. C. Weiser et int. D. Thrän, *Applied energy* (2014)
4. Z. Gong et int. L. Shuai, *Catalysts* (2022)
5. A. Devi et int. S. Upadhyayula, *Bioprocess and Biosystems Engineering* (2021)
6. Q. Liu et int. L. Ma, *ChemSusChem* (2019)
7. K. Wang et int. N. Tsubaki, *Fuel* (2024)
8. S. Da Ros et int. J. C. Pinto, *Applied Catalysis* (2017)
9. A. Brosteanu et int. I. Banu, *UPB Scientific Bulletin* (2022)
10. S. Rodgers et int. J. McKechnie, *Journal of Cleaner Production* (2022)
11. S. Farzad et int. J. Görgens, *Bioresource technology* (2017)
12. ChemPLANT Task Description, *Verein Deutscher Ingenieure e.V.* (2024)

Acknowledgements

kjVI www.kjVI.de
chemPLANT

Imprint

RWTH Aachen University
Aachener Verfahrenstechnik (AVT)

Chair for Fluid- and Process Systems Engineering
Forckenbeckstraße 51
52074 Aachen

You want the full aixperience?
Visit us on: **aixstrawdinary.de**
Or scan the code: