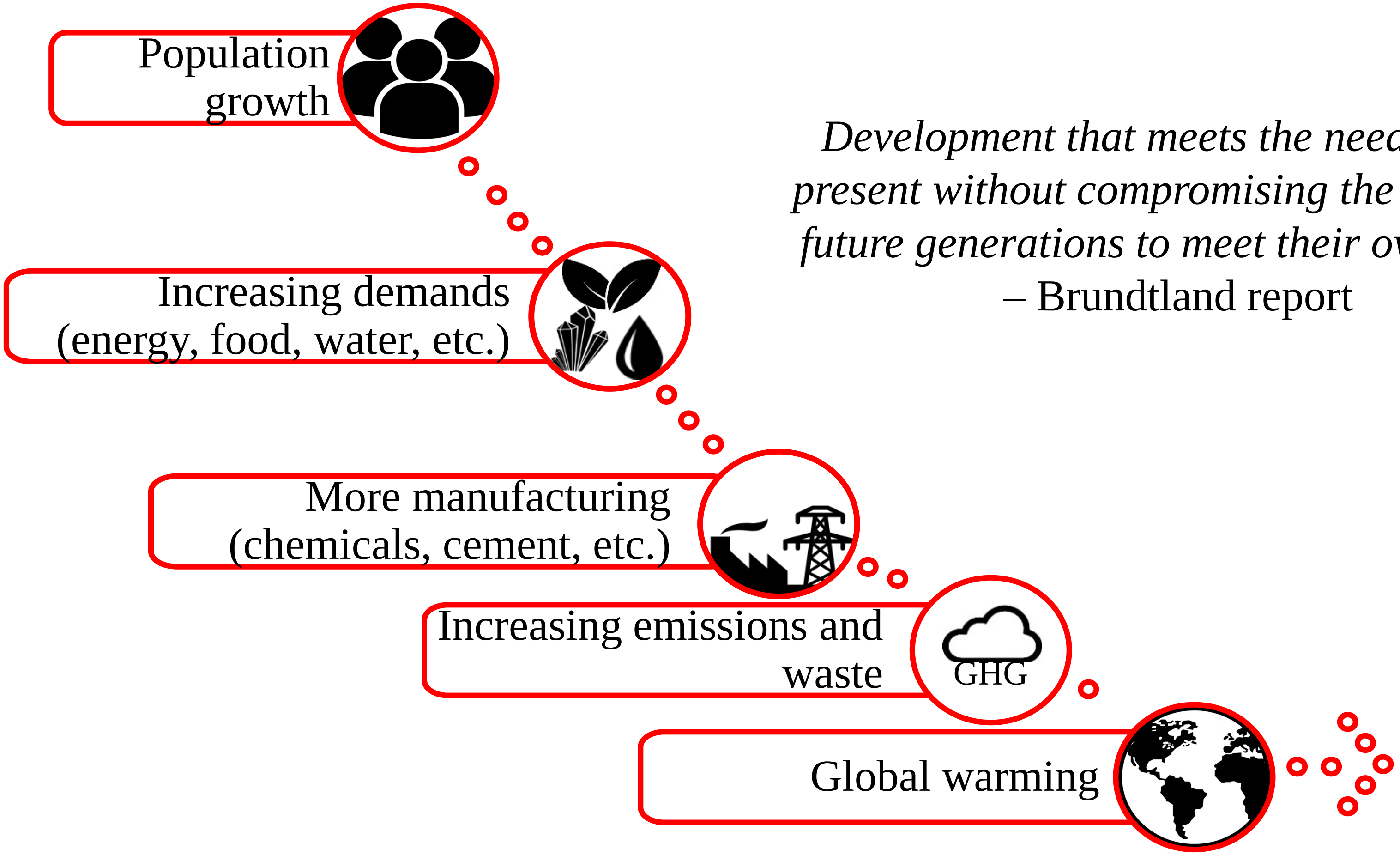
Sustainable CO_2 Capture & Conversion Technologies

Rebecca Frauzem
Supervisors: Rafiqul Gani and John M. Woodley

Overview

- Introduction
- 3-stage approach
- Framework
- Application
- Conclusions
- Outlook

Global scenario



Population growth

Increasing demands (energy, food, water, etc.)

More manufacturing (chemicals, cement, etc.)

Increasing emissions and waste

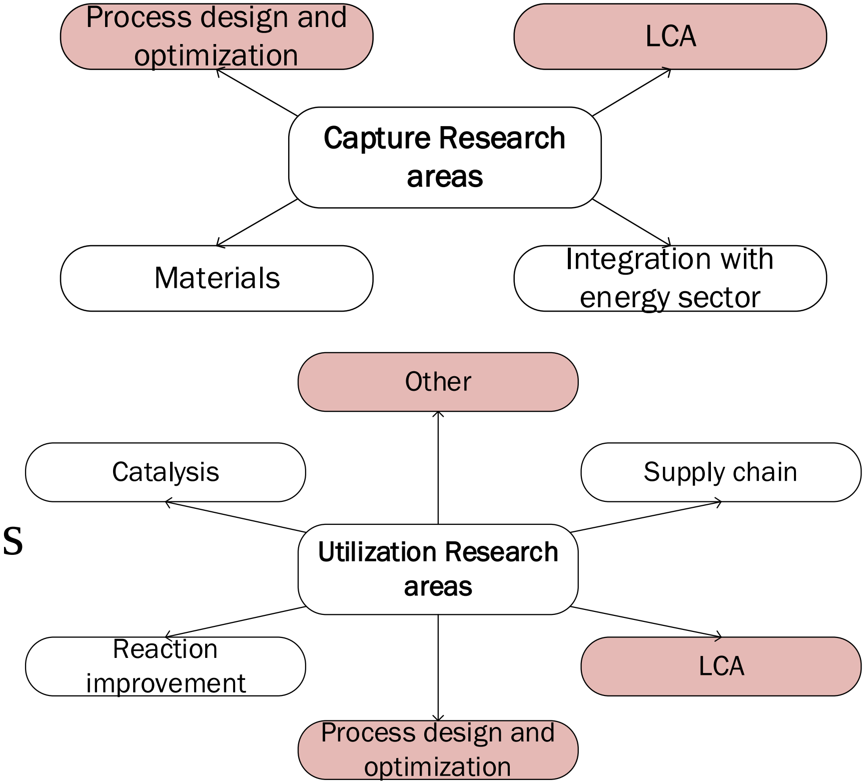
Global warming

Development that meets the needs of the present without compromising the ability of future generations to meet their own needs
– Brundtland report

United Nations Population Fund, 2015 & 2016.

CO_2 reduction strategies & CCU

- Carbon capture and storage (CCS)
  - +Long-term storage
  - –Offers no economic incentive
- Carbon capture and utilization (CCU)
  - +Value-added products
  - –Mostly immature processes
- Improved energy efficiency
  - +Truly emission reducing
  - –Lack of technology



Capture Research areas

Process design and optimization

LCA

Materials

Integration with energy sector

Utilization Research areas

Other

Catalysis

Supply chain

Reaction improvement

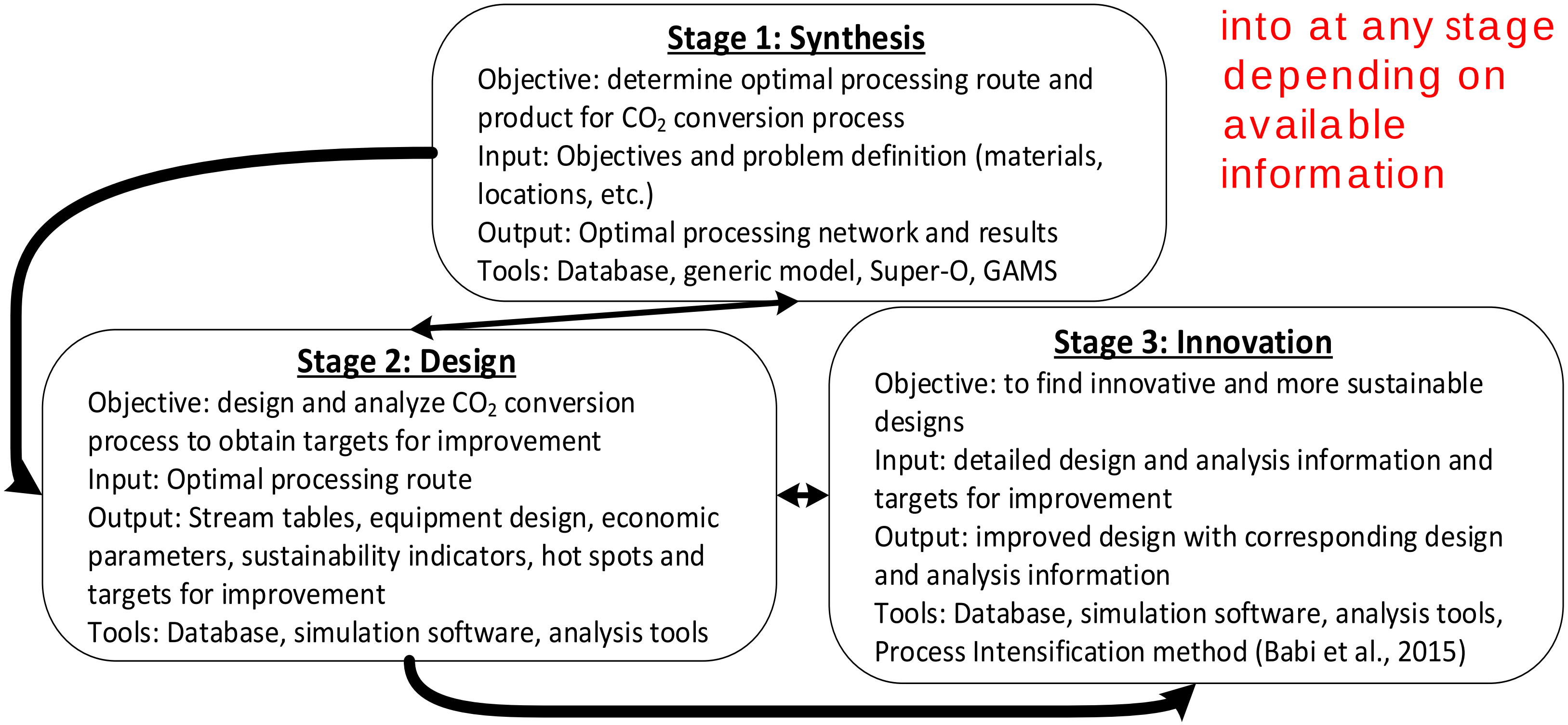
LCA

Process design and optimization

Motivation & objectives

- Need sustainable capture and utilization processes
- Constrained by:
  - Early stage technology → limited information
  - Limited reaction and catalyst information
- Method used here:
  - 3-stage framework to decompose problem
  - Assisted by computer-aided methods and tools
  - Sustainability analysis

3-stage approach



Stage 1: Synthesis

Objective: determine optimal processing route and product for CO_2 conversion process

Input: Objectives and problem definition (materials, locations, etc.)

Output: Optimal processing network and results

Tools: Database, generic model, Super-O, GAMS

Stage 2: Design

Objective: design and analyze CO_2 conversion process to obtain targets for improvement

Input: Optimal processing route

Output: Stream tables, equipment design, economic parameters, sustainability indicators, hot spots and targets for improvement

Tools: Database, simulation software, analysis tools

Stage 3: Innovation

Objective: to find innovative and more sustainable designs

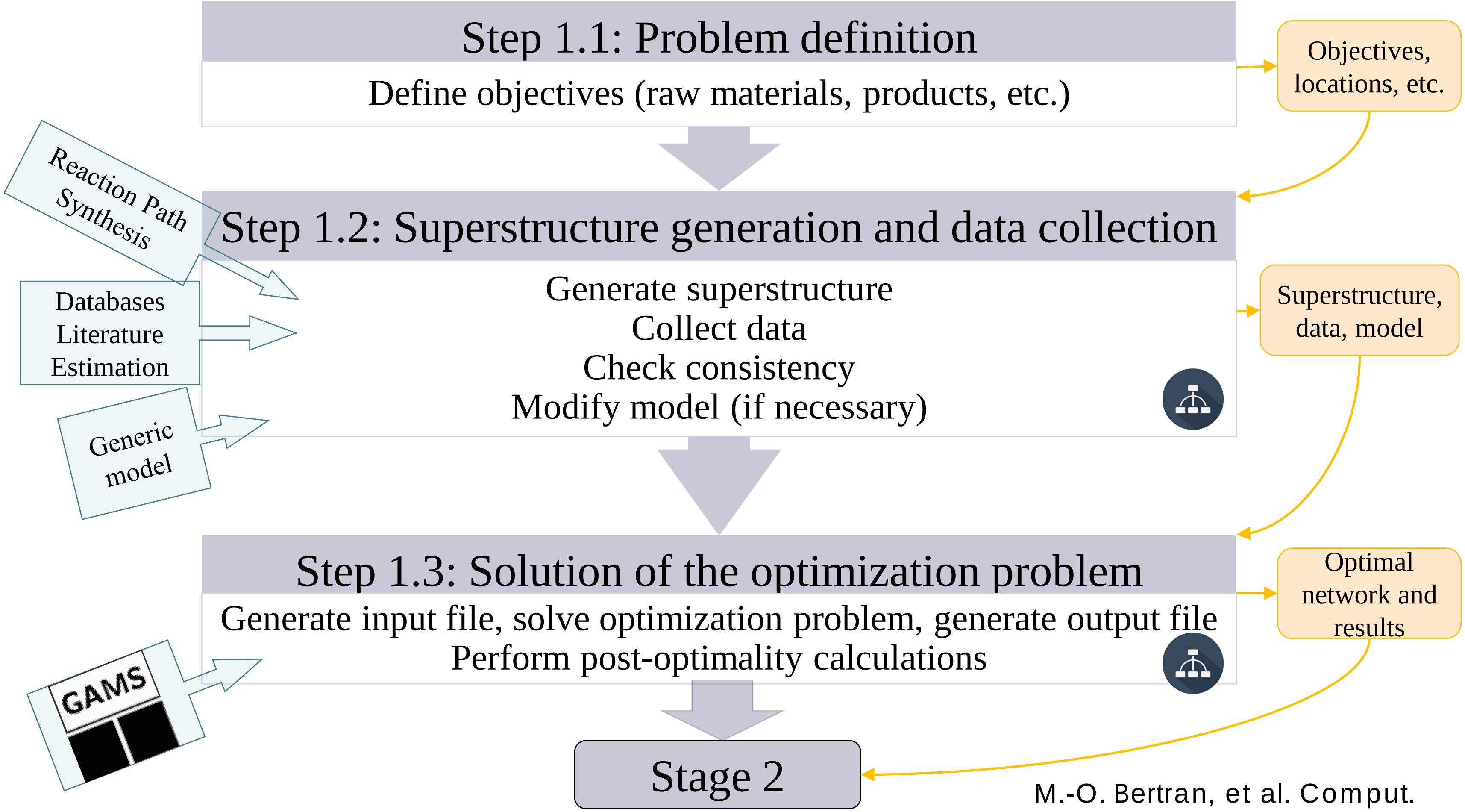
Input: detailed design and analysis information and targets for improvement

Output: improved design with corresponding design and analysis information

Tools: Database, simulation software, analysis tools, Process Intensification method (Babi et al., 2015)

Can be stepped into at any stage depending on available information

Framework – Stage 1



Step 1.1: Problem definition

Define objectives (raw materials, products, etc.)

Objectives, locations, etc.

Step 1.2: Superstructure generation and data collection

Reaction Path Synthesis

Databases
Literature
Estimation

Generic model

Generate superstructure
Collect data
Check consistency
Modify model (if necessary)

Superstructure, data, model

Step 1.3: Solution of the optimization problem

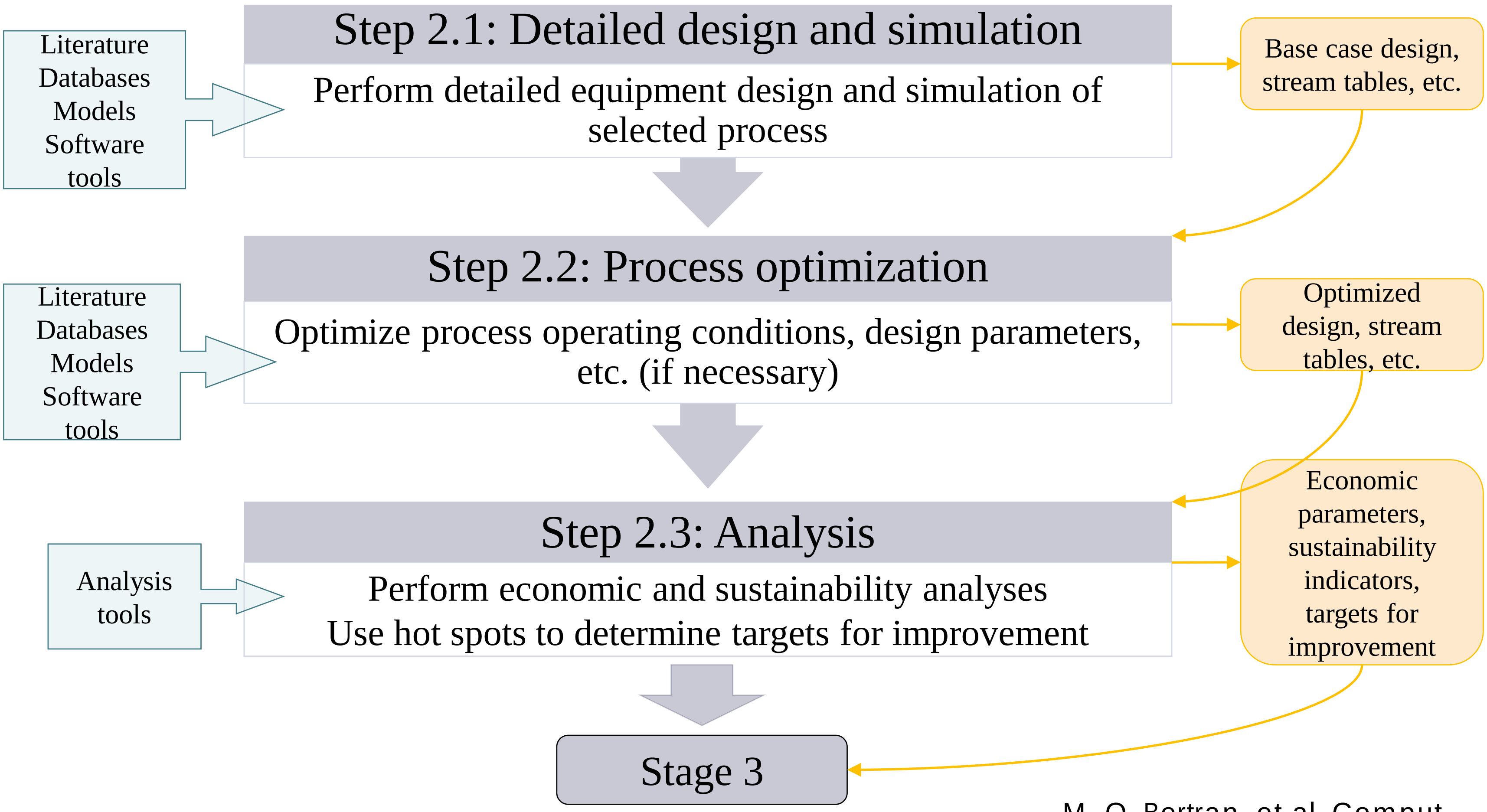
Generate input file, solve optimization problem, generate output file
Perform post-optimality calculations

Optimal network and results

Stage 2

M.-O. Bertran, et al. Comput. Chem. Eng., 2017.

Framework – Stage 2



Literature
Databases
Models
Software
tools

Step 2.1: Detailed design and simulation

Perform detailed equipment design and simulation of selected process

Base case design, stream tables, etc.

Literature
Databases
Models
Software
tools

Step 2.2: Process optimization

Optimize process operating conditions, design parameters, etc. (if necessary)

Optimized design, stream tables, etc.

Analysis tools

Step 2.3: Analysis

Perform economic and sustainability analyses
Use hot spots to determine targets for improvement

Economic parameters, sustainability indicators, targets for improvement

Stage 3

M.-O. Bertran, et al. Comput. Chem. Eng., 2017.

Framework – Stage 3

- Use the targets from Stage 2 analysis
- Use of Process Intensification (PI) and unique process integration
  - Innovative designs
  - Improved sustainability
- PI involves phenomena-based method developed by Babi et al. (2015) *Computers and Chemical Engineering*

Important methods and tools

- Reaction Path Synthesis (RPS) → determine all feasible reactions from CO_2 to desired products
- Database → facilitate the storage and retrieval of data
- Generic model → allow solution of a variety of problems
- Simulation library → enable easy reuse of simulations

Tools

Reaction Path Synthesis

Step	Criteria	Result
1	C, H, O compounds, max chain length 7, max 2 functional groups	> 100 products
2	All chemically feasible reactions CO2 to the target products	> 1000 reactions
3	Only thermodynamically feasible reactions	> 150 reactions
6	Kinetic information available in literature	> 20 reactions

Database

Number of feedstocks	4
Number of products	13
Number of steps	25
Number of intervals	91
Number of components	36
Number of utilities	3
Number of reactions	37

Simulation Library

Number of Simulations	>60
Products produced	11
CO_2 feedstocks considered	4

Application

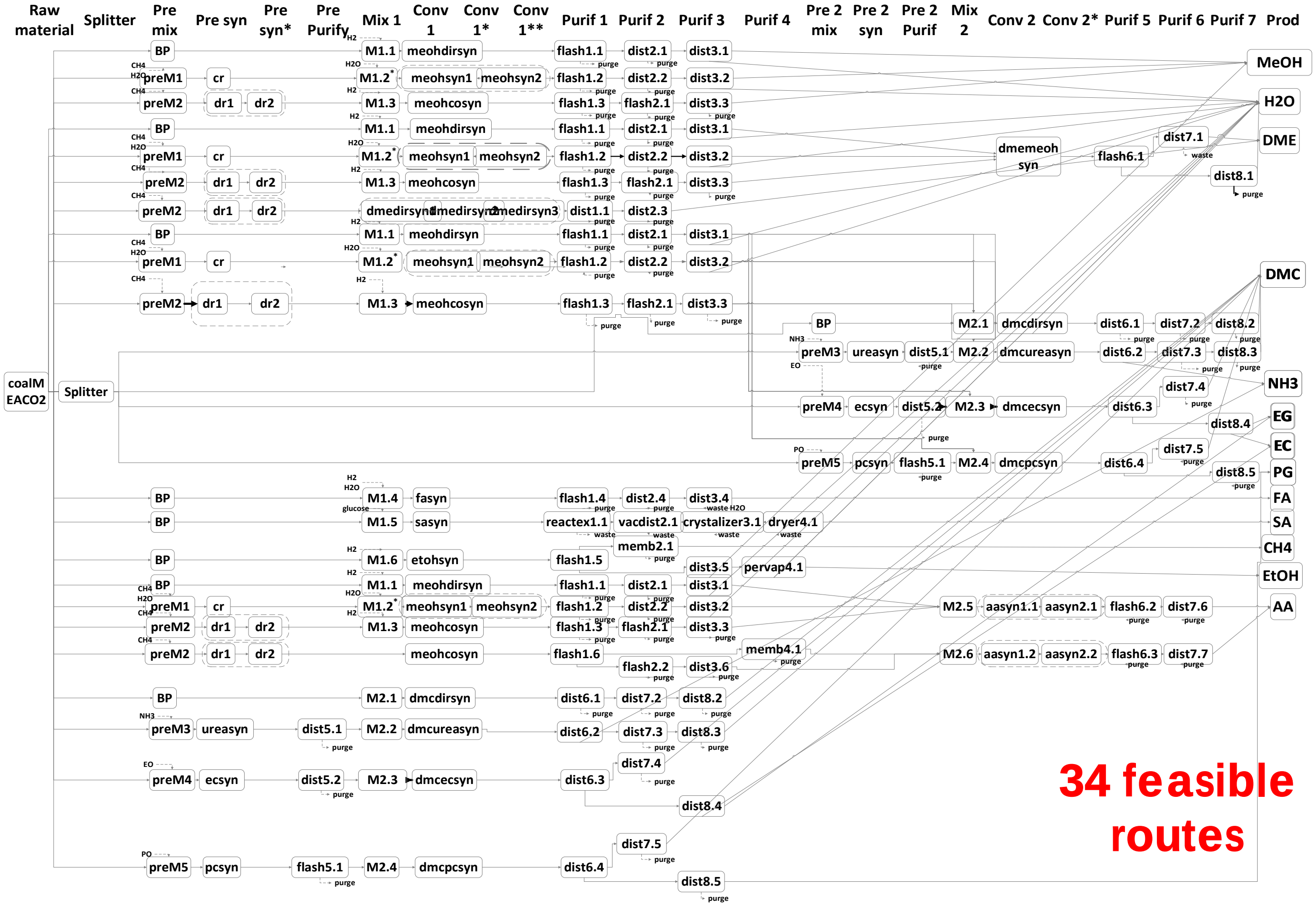
- Goal: sustainable CO_2 conversion processes
- Raw material: captured CO_2 (Fjellerup MSc Thesis, 2015)
- Reactions & products: determined via Reaction Path Synthesis (RPS)

Superstructure

115 Intervals

23 Steps (w/ RM & Prod)

13 Products



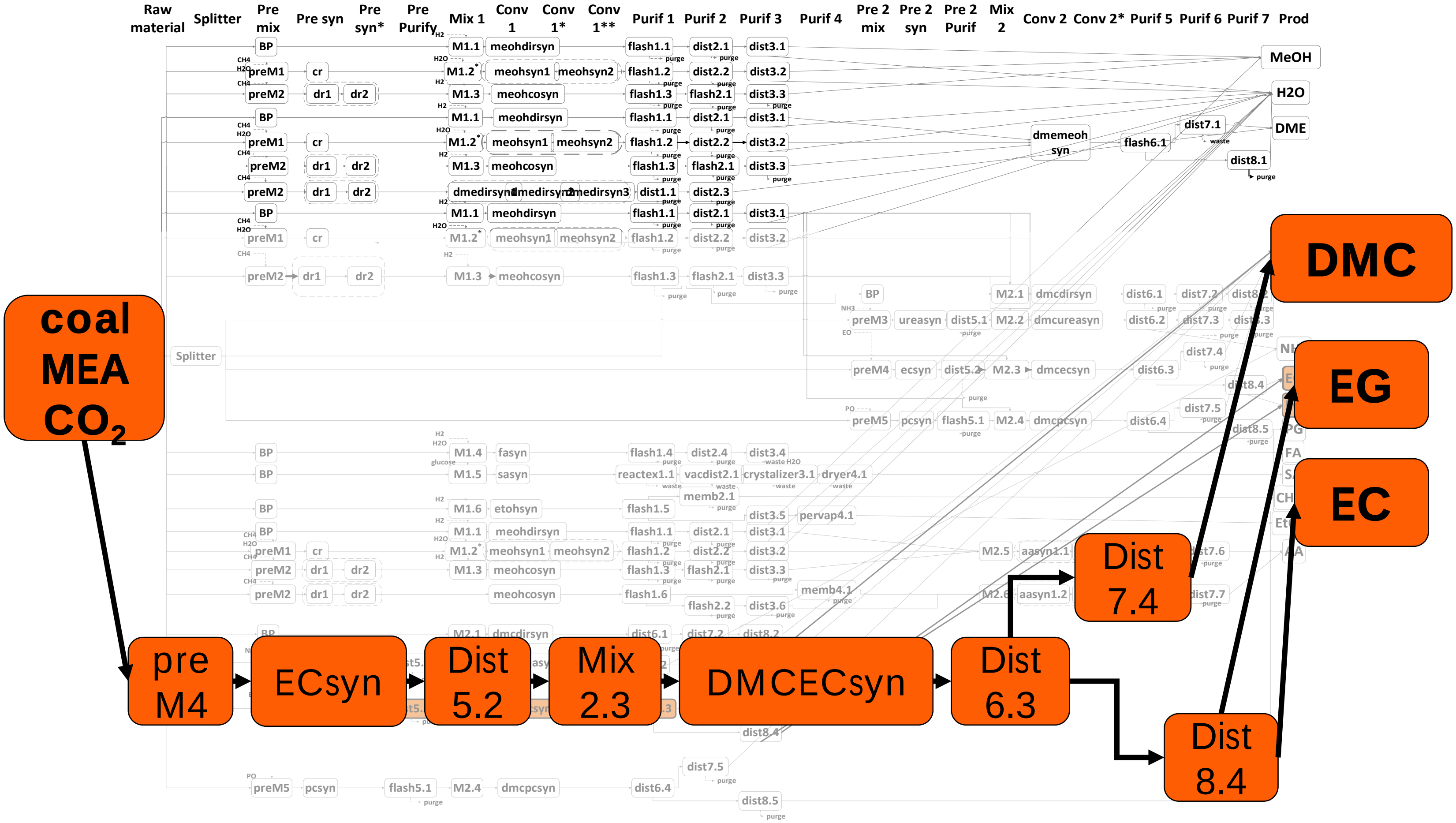
1 Feed

34 feasible routes

Rebecca Frauzem, PhD – Sustainable CO_2 Capture & Conversion Technologies

KT Consortium Annual Meeting, 2017

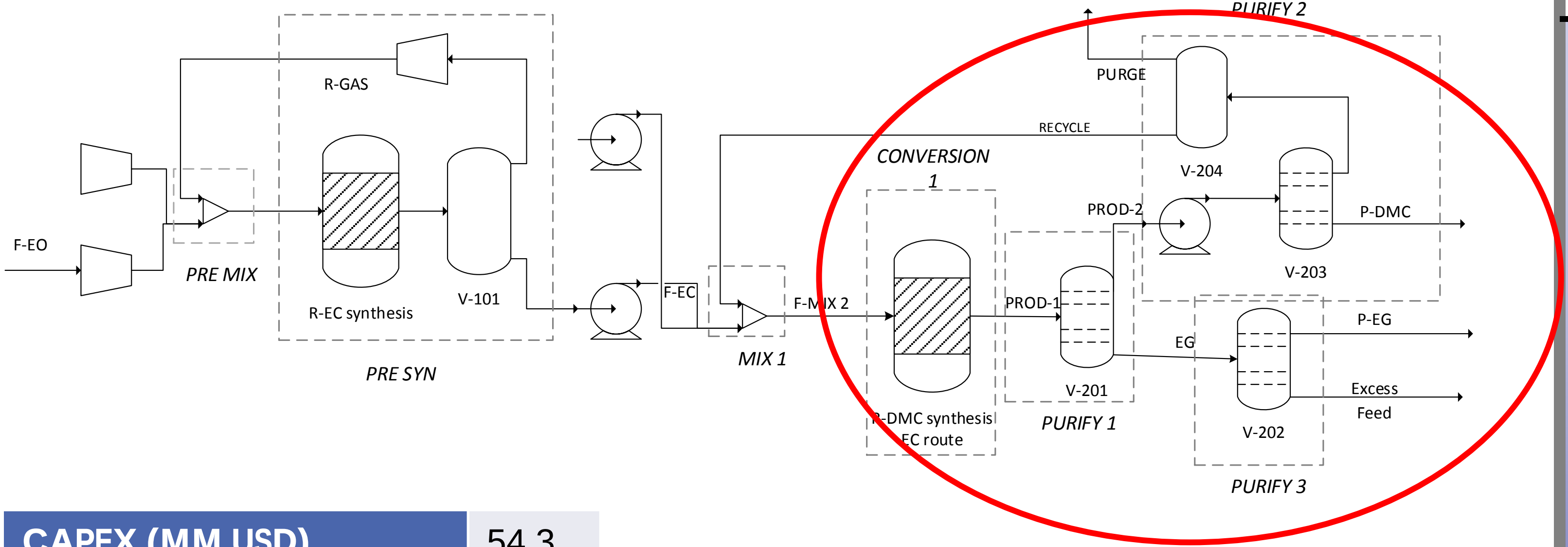
Stage 1 results



Stage 1 results

	Scenario 3
Objective function (OF)	Sales – OPEX – CAPEX
Number of equations (NEQ)	4,255,204
Number of variables (NV)	4,229,505
Number of discrete variables (NDV)	426
Problem type	MIP
Solver	CPLEX
Execution time (seconds)	10.499
Sales (MM USD/y)	100.4
OPEX (MM USD/y)	65.8
CAPEX (MM USD)	20.5
Profit (MM USD/y)	32.55

Stage 2



CAPEX (MM USD)	54.3
OPEX (MM USD/y)	57.8
NetCO$_2$ (kgCO$_2$/kgDMC)	-0.36
Yield	1.7

Bottleneck: energy intensive separation

→ Target for improvement

P. Kongpanna, et al. Comput. Chem. Eng., 2016.

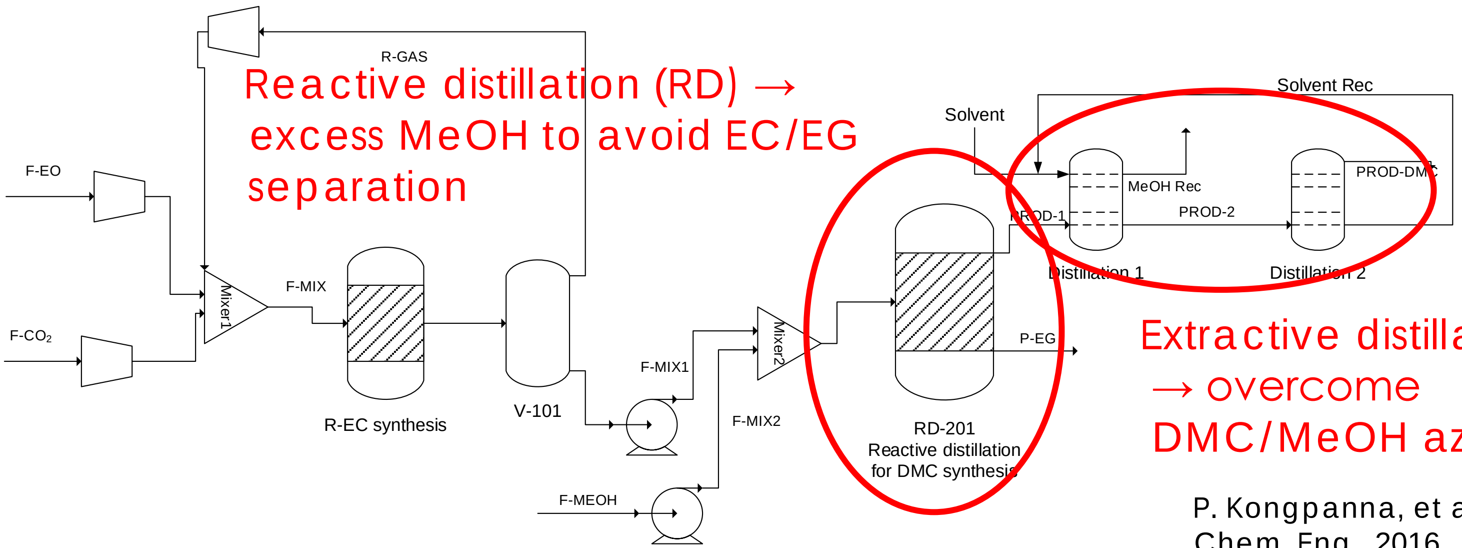
Stage 3

Address target for improvement → Process intensification (Babi et al, 2015)

Material costs dominate

Less equipment

	Intensified	Base case
CAPEX (MM USD)	39.6	54.3
OPEX (MM USD/y)	57.7	57.8
NetCO$_2$ (kgCO$_2$/kgDMC)	-0.38	-0.36
Yield	1.7	1.7

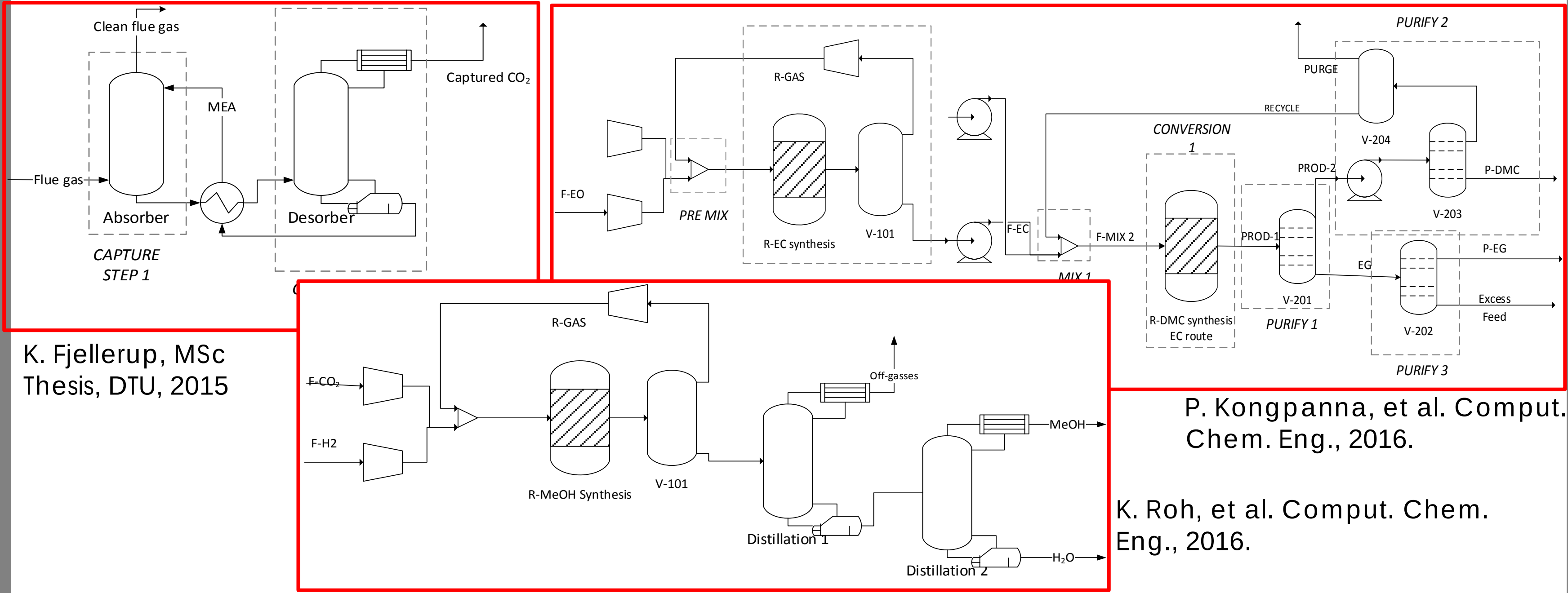


Reactive distillation (RD) → excess MeOH to avoid EC/EG separation

Extractive distillation (ED) → overcome DMC/MeOH azeotrope

P. Kongpanna, et al. Comput. Chem. Eng., 2016.

Integrated capture and conversion



K. Fjellerup, MSc Thesis, DTU, 2015

P. Kongpanna, et al. Comput. Chem. Eng., 2016.

K. Roh, et al. Comput. Chem. Eng., 2016.

	Capture	Methanol	DMC	Combined
CAPEX (MM USD)	0.1	19.4	54.3	73.8
OPEX (MM USD/y)	0.9	2.1	57.8	60.8
NetCO_2	0.13 $kg_{CO2}/kg_{captured}$	-0.7 kg_{CO2}/kg_{MeOH}	-0.36 kg_{CO2}/kg_{DMC}	-0.7 kg_{CO2}/kg_{DMC}

Conclusion

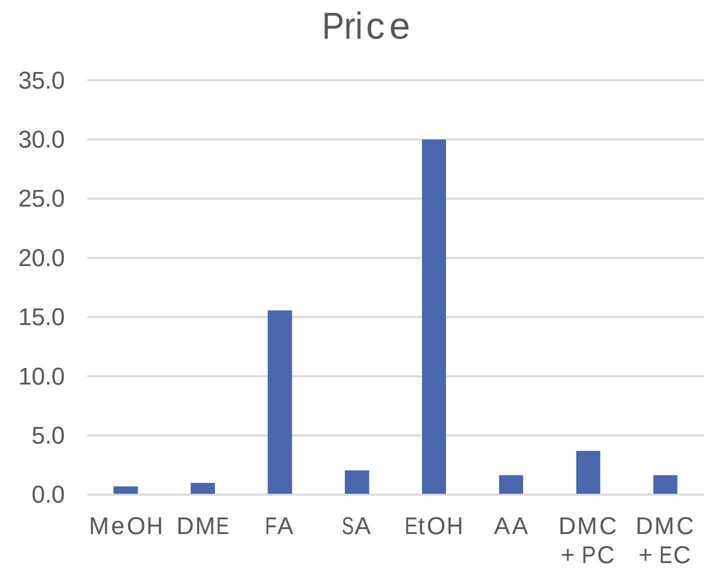
- 3-stage framework for the sustainable design of CO_2 capture and utilization processes
- Incorporates various computer-aided methods and tools
- Database and simulation library to facilitate storage and retrieval

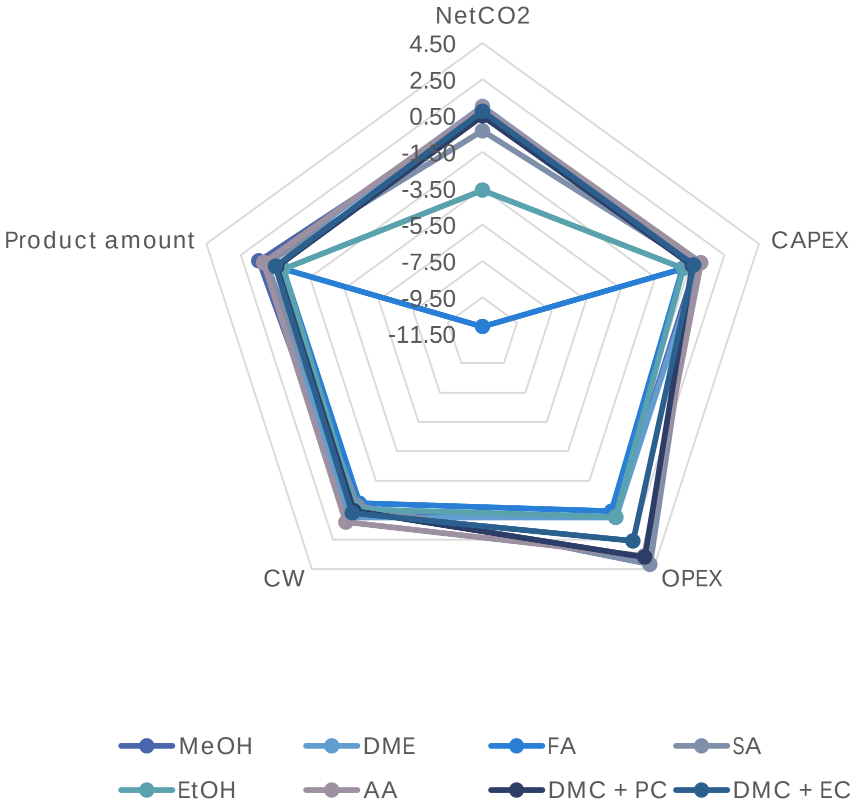
Future work

- Consider various scenarios to understand influence of price, demand, etc.

1. Operating cost – utility cost
2. Operating cost
3. Capital cost + operating cost
4. **Product price**
5. Demand
6. Location
7. Price sensitivity

Future work – Scenario 4

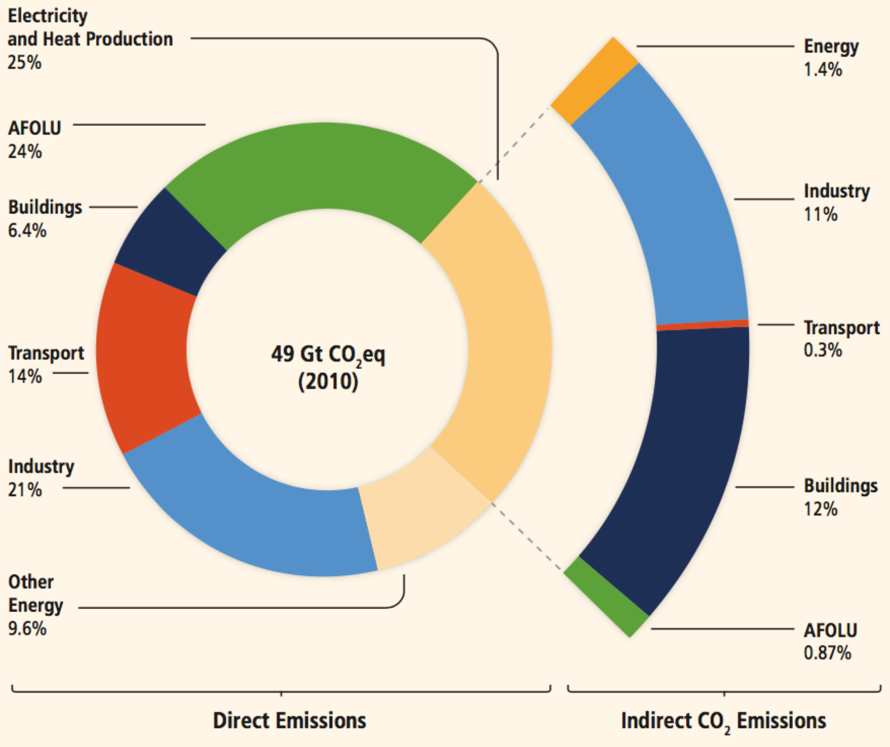




Outlook

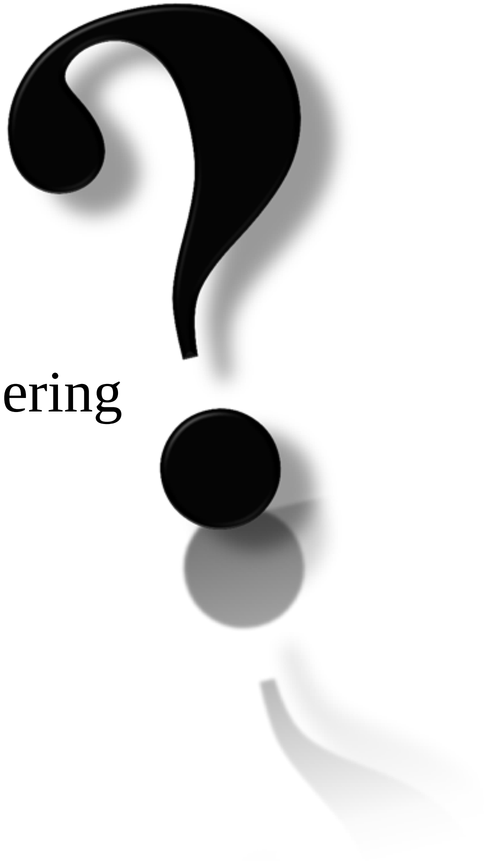
- Current reduction potential of conversion technology < 10%

⇒ A combined approach to tackling CO_2 emissions is necessary



IPCC, 2014. *Climate Change 2014: Mitigation of Climate Change*

Thanks for listening!



Rebecca Frauzem

Department of Chemical and Biochemical Engineering

Technical University of Denmark

2800 Kgs. Lyngby

Denmark

* rebfra@kt.dtu.dk

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