AVEVAWORLD

PARIS

Covestro's path towards sustainable polymer materials production

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Digital Process Technology & Knowledge Management

Modeling & Conceptual Design (DPK-M&D)

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• B.Sc./M.Sc. Mechanical Engineering & Business Administration	**2010 – 2016** RWTH Aachen University	**2011 – 2017** RWTH Aachen University	• B.Sc. Mechanical Engineering • M.Sc. Chemical Engineering
• Project Management for Logistics and Digitalization Projects	**2016 – 2017** Air Liquide Project Management	**2017 – 2022** Aachener Verfahrenstechnik – Process Systems Eng.	• Ph.D. Process Systems Engineering • Optimization-based process development
• Process Lead Engineer for Project Engineering of isocyanate plants	**2017 – 2024** Covestro Deutschland AG Project Engineering	**2022** Cambridge CARES	• Research visit • Bayesian optimization for process development
• Process development for circular economy processes • Bringing models and data into production	**2024 – now** Covestro Deutschland AG Modelling & Conceptual Design	**2022 – now** Covestro Deutschland AG Modelling & Conceptual Design	• Process development for circular economy processes • Bringing models and data into production

These changes shape the needs from entire industries and value chains

Lightweight & corrosion protection in transportation

Eco-Efficient production processes

Energy efficiency in construction

Enabling materials in electronics

Cost effectiveness in renewable energies

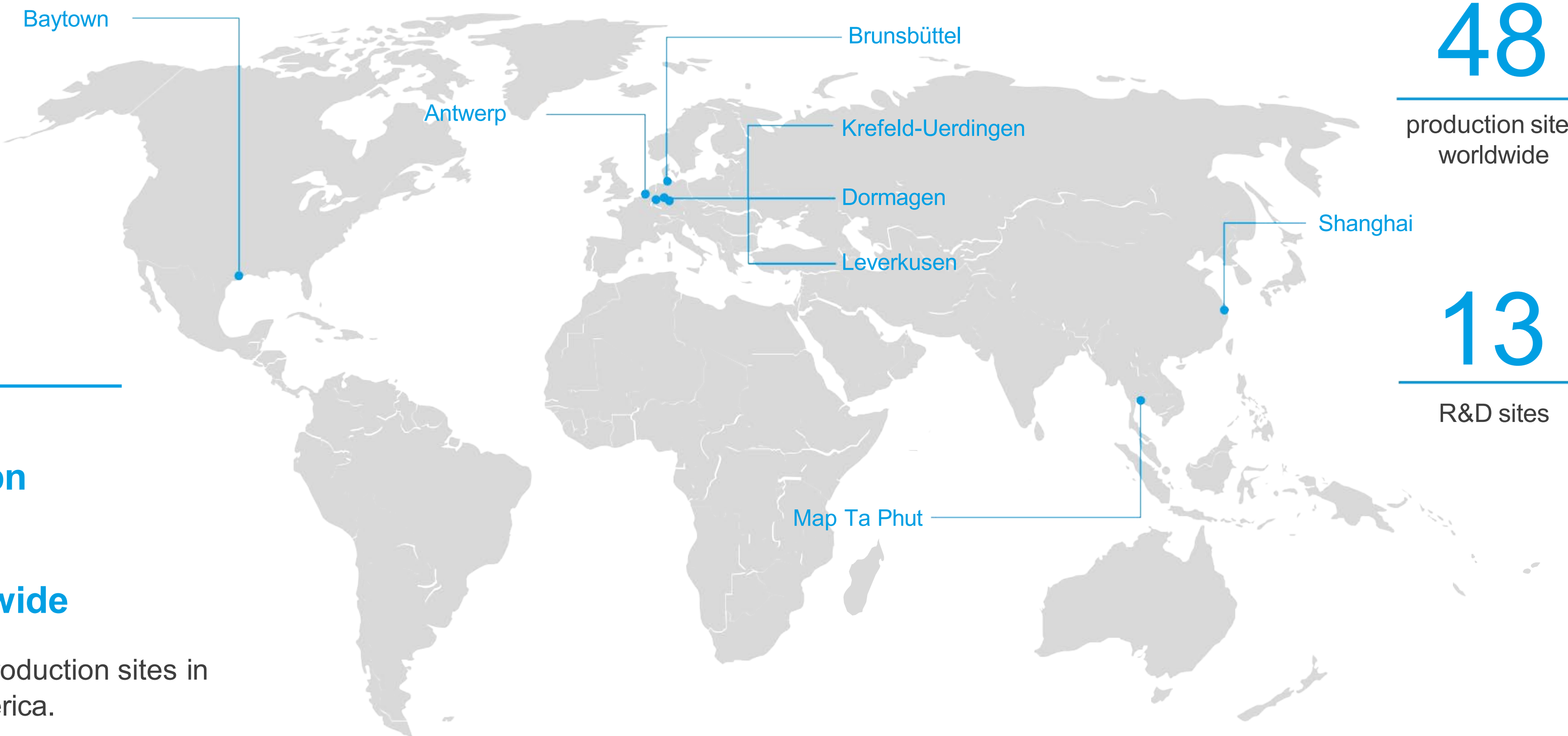
High performing materials for convenience & health

Covestro is a world leading polymer material producer

4.9 m t
Greenhouse gas emissions
(CO_2 equivalents)

Sales (2023)

€14.4 bn



48
production sites worldwide

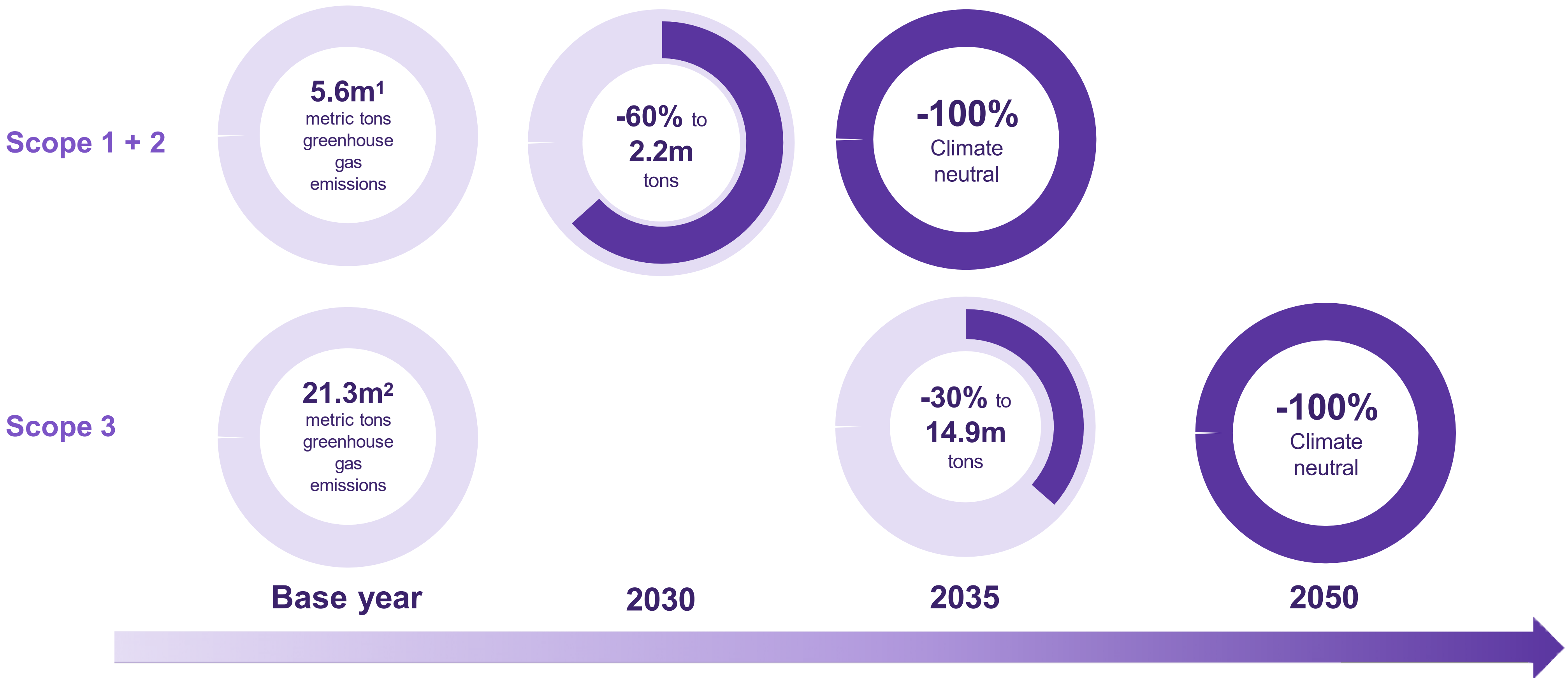
13
R&D sites

Covestro worldwide

Covestro counts 48 production sites in Europe, Asia and America.

Covestro sets itself ambitious climate goals

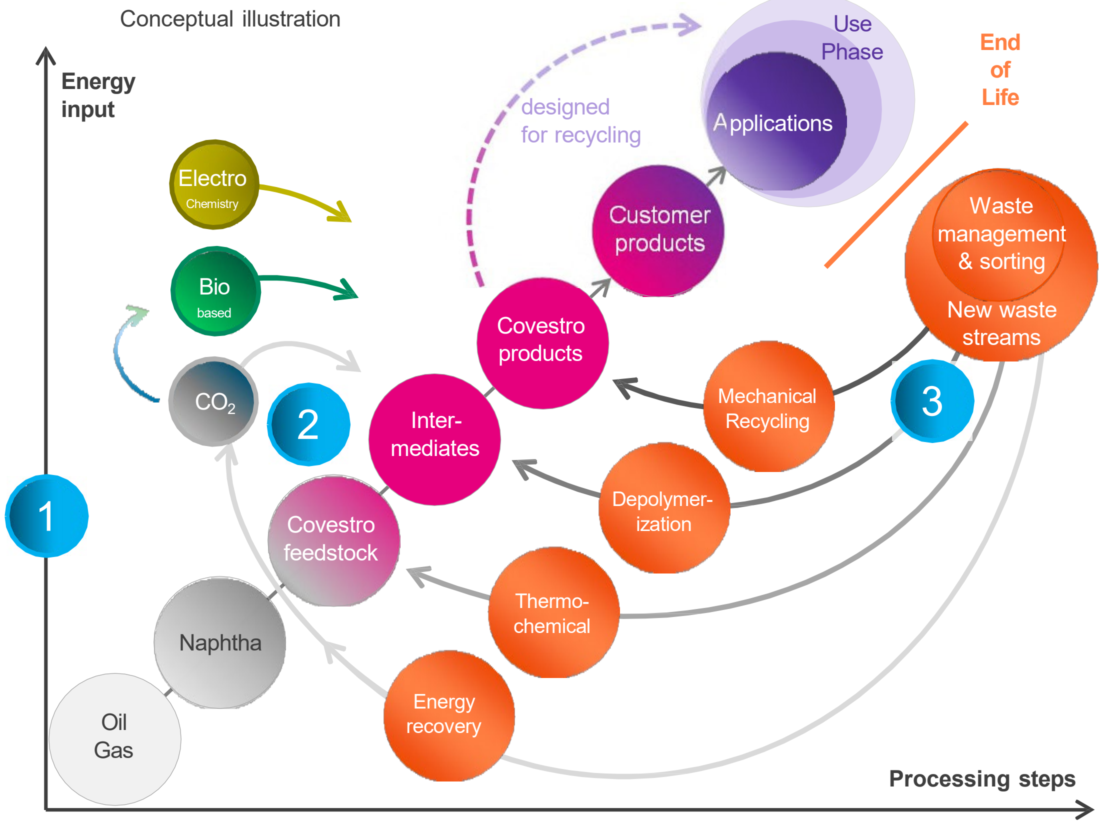
Climate neutrality targets for GHG emissions



1) Reference year 2020
2) Reference year 2021

Closing material and carbon loops for a circular economy

Circular and climate neutral economy



Covestro approach to circularity

1 Renewable energy & efficiency

2 Alternative raw materials

NEnzy

Bio4PURdemo

…& many more!

3 Recycling for end-of-life solutions

PUReSmart

Polycarbonates Recycling

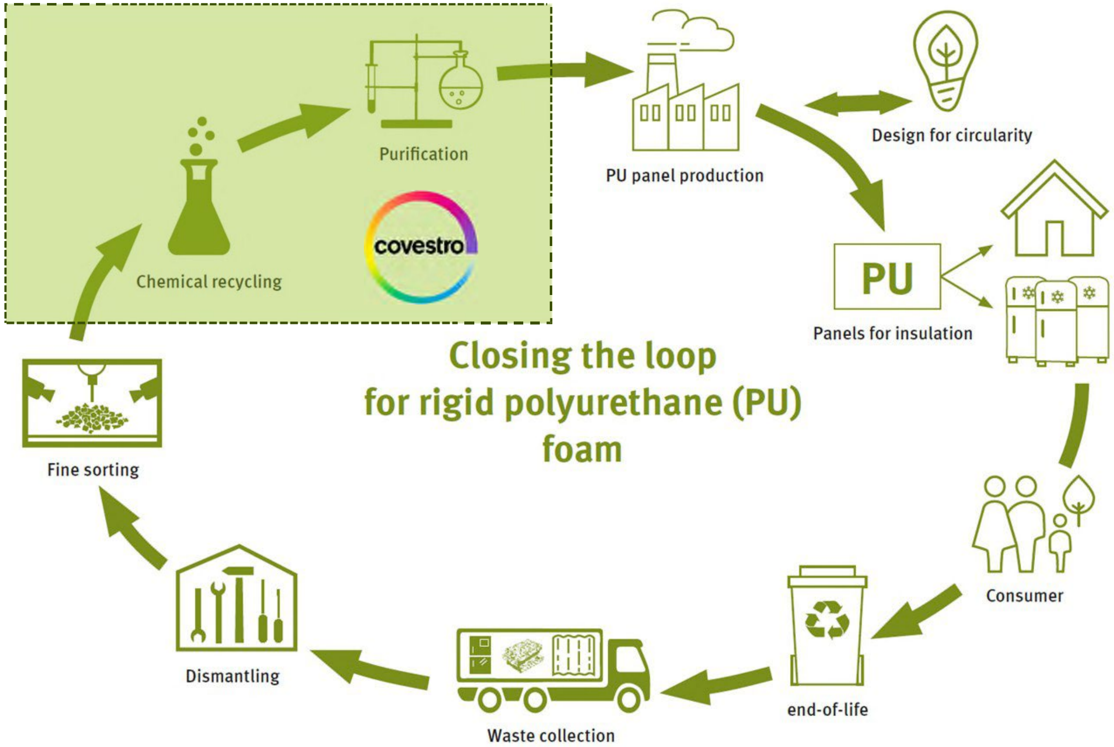
CIRCULAR FOAM

…& many more!

Notes: Shown recycling technologies and energy recovery are illustrative examples only

Recycling of rigid polyurethane (PU)

Dedicated circular value chain



Roll-out in the EU could bring by 2040:

- 1 mt per year less waste
- 2.9 mt per year less CO_2 emissions
- 150 m€ less cost for incineration

Innovation Action

Coordinated by covestro

24 partners from 9 countries

48 months: 10.2021-09.2025

The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101036854

Two chemical recycling technologies in focus:

Chemolysis and catalytic pyrolysis followed by downstream purification

Step 1: **Polymer cleavage**

Chemolysis

Breaking polymeric materials down into individual components (monomers or other intermediates) via **chemical reactions**.

Using solvents, catalysts, heat at **moderate temperatures** and sometimes pressure.

OR

Catalytic pyrolysis

Thermal degradation of polymeric materials into individual components (monomers or other intermediates) at high temperatures.

Step 2: **Downstream processing** (purification of components in depolymerisation mixture)

Good results in both steps are paramount:

- depolymerisation should lead to high yields of targeted molecules with few (or no) side-products
- efficient separation in the downstream step is required to obtain materials of high purity.

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Covestro and AVEVA strive for a long-term partnership

Covestro…

requires process simulation tools ready for the **digital** transformation.

What we need …

- Advanced numerics
- Easy integration of plant data (OSI PI)
- Custom modeling (special know-how)
- Steady-State
- Dynamics for further studies beneficial
- Smooth migration, no work disruption

Cooperation Covestro / AVEVA
Started in 2017

Goals

(1) Early evaluation of software
(2) Configuration of tool to our requirements

Methods

(1) Regular monthly meetings with experts from AVEVA & Covestro
(2) Fast troubleshooting together with AVEVA experts and customer support

AVEVA…

develops next-generation simulation tool AVEVA Process Simulation designed from the ground up to be ready for digitalization.

AVEVA requires …

- Customer feedback in the chemicals sector to further develop the software

New processes feature new modeling challenges

Fossil-based

- Large simulations with many recycle streams
- Mostly non-polar raw materials diluted in organic solvents
- Rigorous heat exchanger modeling
- Modeling of high-temperature thermal separations (e.g. distillation)
- Online Models

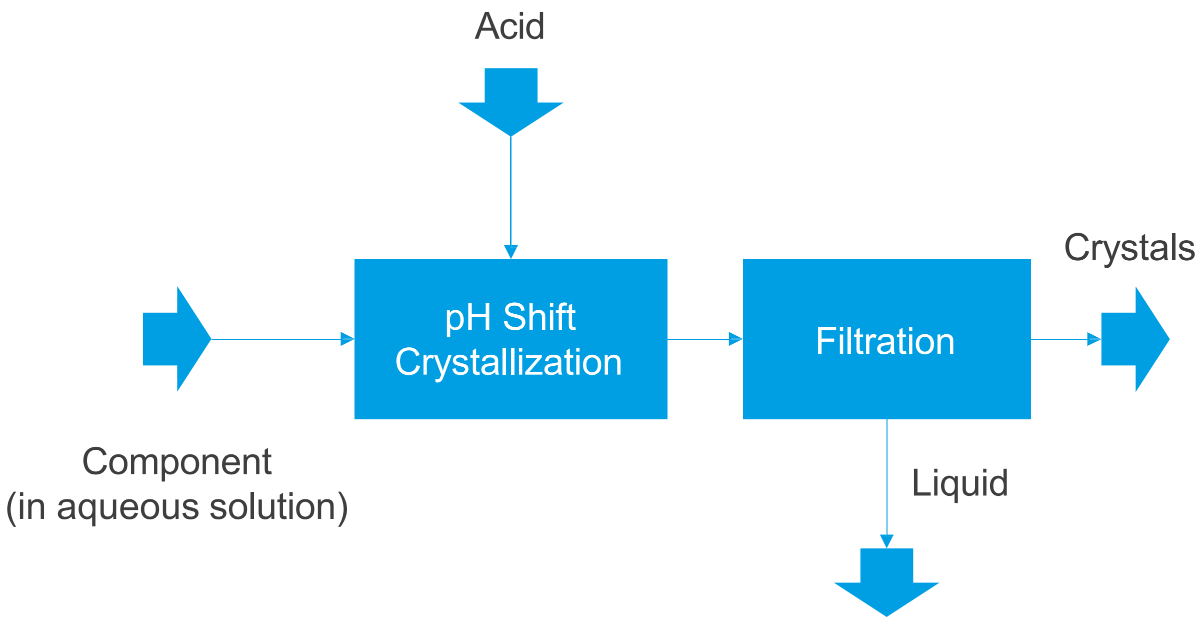
Circular Economy

- Easy description of less-known components
- Modeling of aqueous electrolyte mixtures
- Solids modeling
- Modeling of low-temperature thermal separations (e.g. crystallization, extraction)
- Custom modeling

Crystallization and filtration are unit operations commonly used

Example

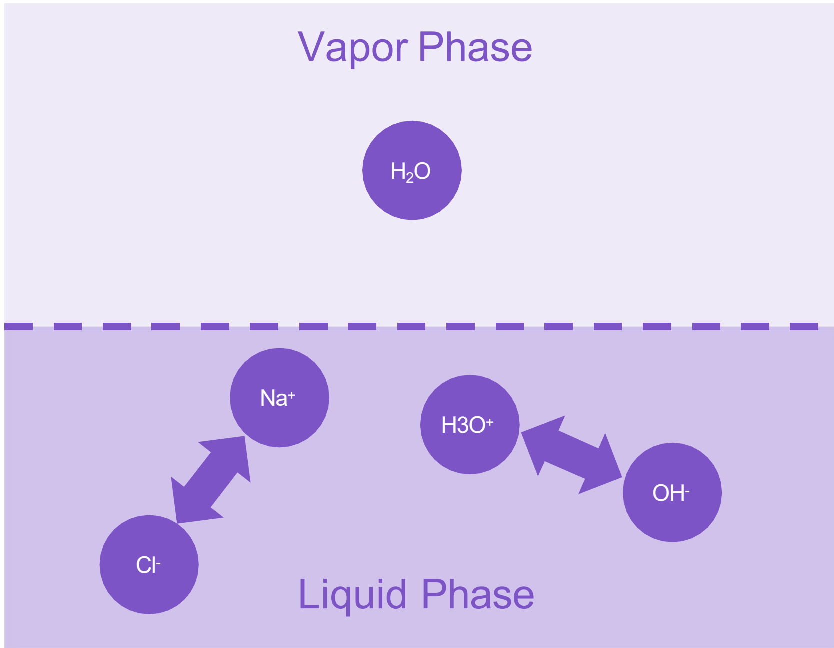
- Components are dissociated in aqueous solutions which are modelled as electrolytes
- To separate these components it requires pH shift towards lower pH values by adding an acid this lowers the solubility of the component in the aqueous phase
- The crystals are afterwards filtered by mechanical filters



Our models underly certain assumptions

- The model uses electrolyte non-random two-liquid (eNRTL) method (when no electrolytic ions are present in the fluid, the eNRTL method reduces to the NRTL method)
- Dissociation and crystallization is modelled as temperature-dependend equilbrium reaction
- The filter is a custom-modelled unit operation
- pH value is specified and the amount of acid is calculated based on the pH value. The amount acid specifies the concentration of H_3O^+ ions

$$\mathrm{pH} \approx -\log_{10}\left(c(H_3O^+)\right)\left[\frac{mol}{L}\right]$$

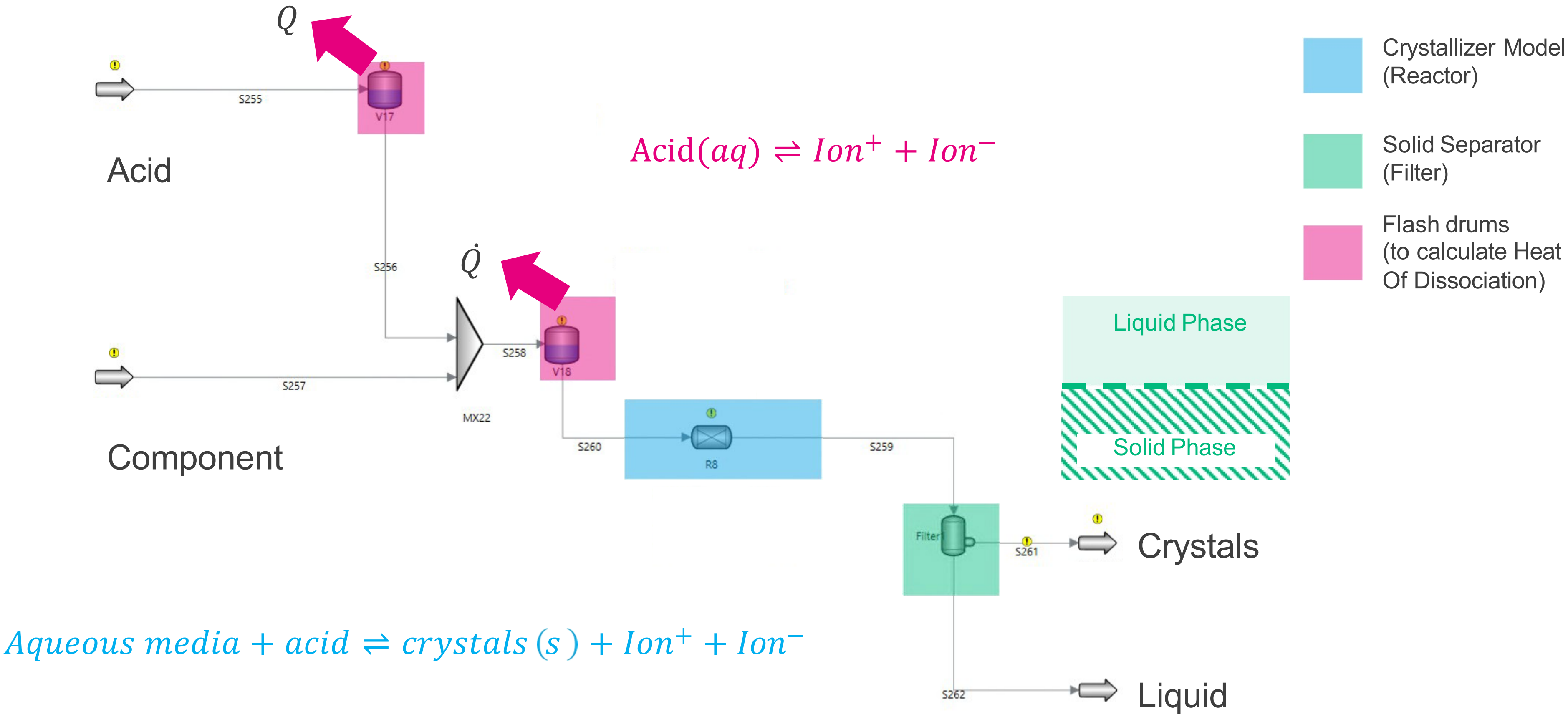


Dissociation in liquid phase:
(Example)

$$2\mathrm{H_2O} \rightleftharpoons H_3O^+ + OH^-$$

$$\mathrm{NaCl} \rightleftharpoons Na^+ + Cl^-$$

Example of APS Flowsheet

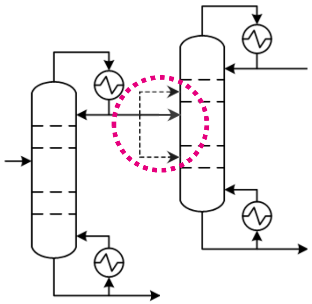


Optimization of distillation column sequences

… under uncertainties

Motivation

Waste with varying composition …



… requires robust process design

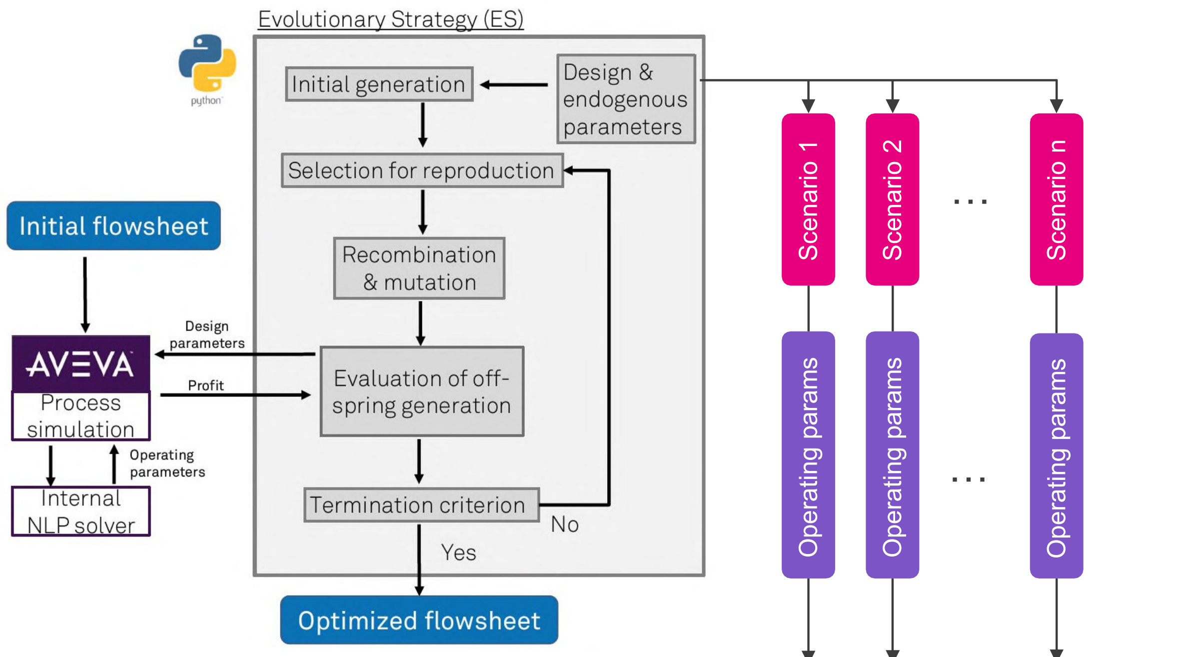
Composite end-of-life (EoL) material from **varying sources**

Uncertainty in composition of EoL material

Cost-optimal column sequence dependent on EoL material

Stochastic optimization for handling of uncertainties

Approach



Optimization of profit: $\max \left[\frac{1}{n}\sum_{i=1}^{n} Profit\ scenario_i\right]$

$Profit\ scenario_i =$ *Sales – Utility costs – Disposal costs − Depreciation*

Lotz, Patrick, et al. "Design of chemical recycling processes for PUR foam under uncertainty." *Computer Aided Chemical Engineering*. Vol. 53. Elsevier, 2024. 1471-1476.

Optimization of distillation column sequences

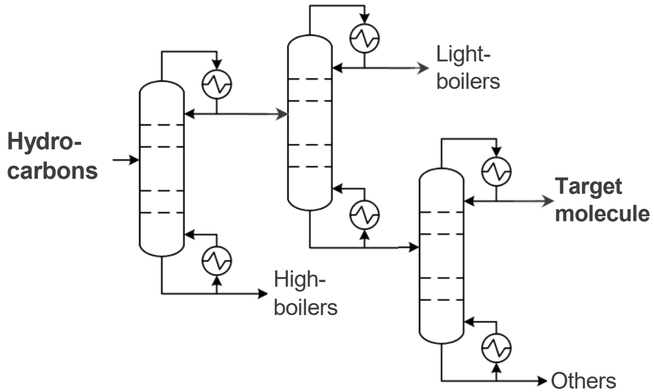
… under uncertainties

Case study

Description of case study

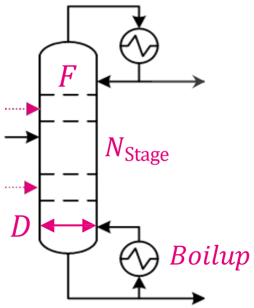
- Thermal separation of **10 hydrocarbons**
- High recovery at **purity of 99.5%** of target molecule
- Scenarios: Uncertainty of **+/- 10%** in feed
  - ➢ Amount of target molecule
  - ➢ Amount of low-boilers
  - ➢ Amount of high-boilers

  } 8 different scenarios

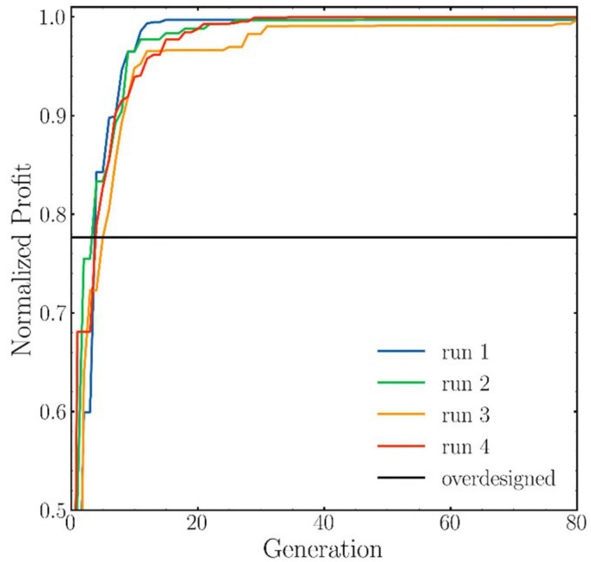


Optimization parameters

- Design parameters (same for all scenarios)
  1. **Number of stages**
  2. Position of **feed stage**
  3. Column **diameter**
- Operating parameters (adapted to scenario)
  1. **Boil-up** / **reflux** ratios
  2. **F-factors**



Results



- **Interfaces via Python or Real-time System** connect APS to 3rd party solver
- Stochastic optimization enables **efficient handling of uncertainties**
- **Robust approach / simulation** required for robust optimization
- Handling of **high number of optimization variables** possible

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Chemical Industry | GERMANY

AVEVA Process Simulation enables us to develop highly customized process models and with that supports design and operation decisions to make circularity become true.

Challenge

- pH-Shift crystallization process with temperature changes in a medium with complicated thermodynamics
- High variation in raw material composition making a robust process design challenging

Solution

- Highly customizable process model to consider most important phenomena
- Flexible interface between APS and 3rd party software to enable robust optimization

Results

- **Customized process model including a complicated thermodynamic model, which enables a reliable design of the plant**
- **Cost-optimal design of a distillation sequence that can cope with an uncertain feed composition**