

The Path of AVEVA Process Simulation @Covestro

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Covestro – a leading supplier of premium polymers



Efficient insulation material



Comfortable foams



Light weight and durable parts



Polycarbonates for lifesaving medical devices



Specialties for durable Photovoltaics



Polyurethane resins for rotor blades

...

Circular economy as guiding principle



Circularity as key

Circular economy is the key to protect **climate and environment** as well as to preserve **limited resources**.

We drive circularity with a **strategic program** and anchor it in the whole organization.

By switching to green electricity and alternative raw materials we want to achieve a fossil-free production.

With innovative technologies we aim to **improve recycling processes**.

*Alternative raw materials:
make use of biomass, CO₂
and end-of-life products*



*Innovative recycling:
develop new technologies*

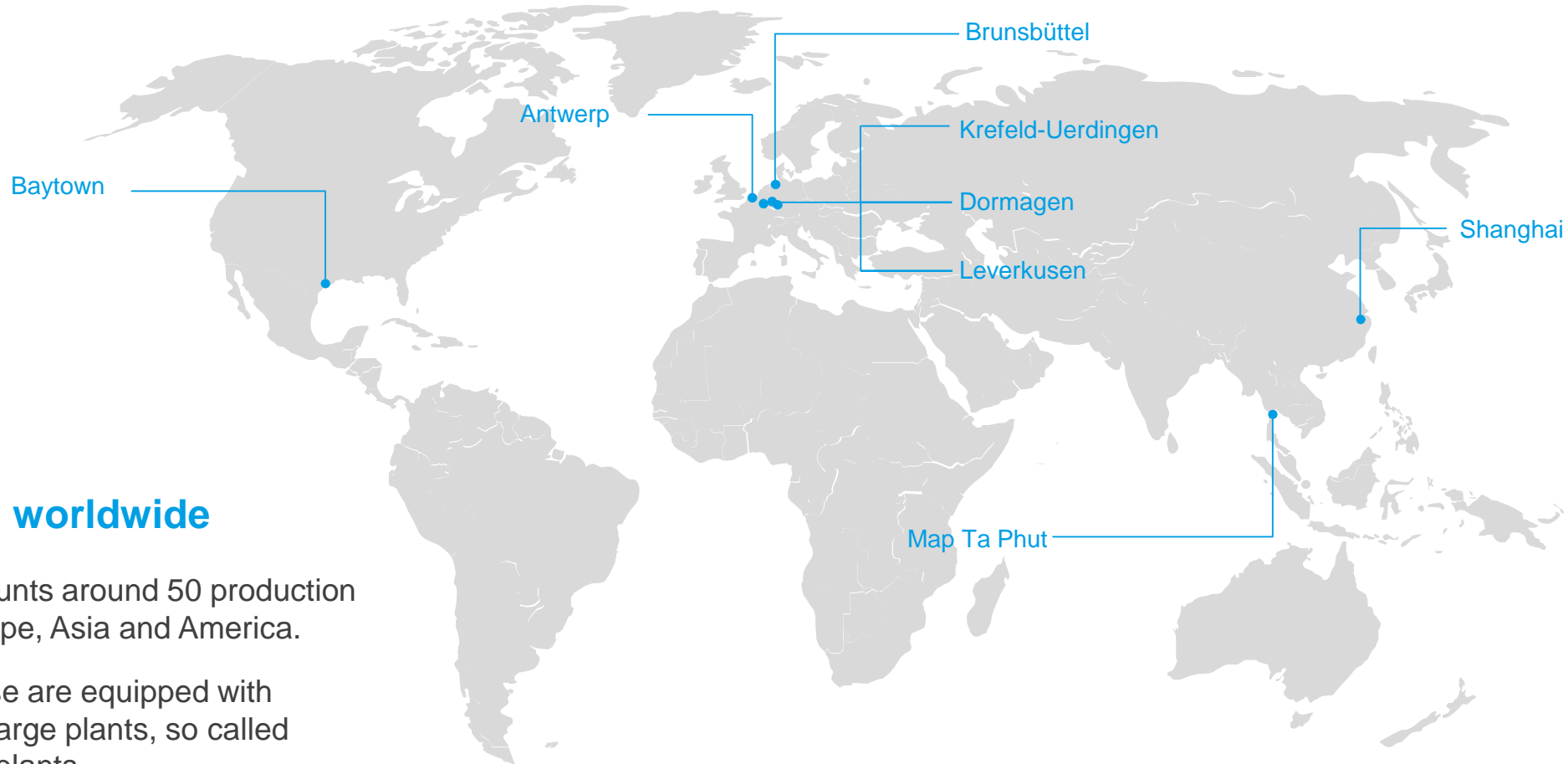


*Renewable energies:
convert sites to green
electricity*



*Joint solutions:
find new ways to
create value*

Our presence



50

production sites worldwide

8

sites with world-scale production plants

13

R&D sites

Covestro worldwide

Covestro counts around 50 production sites in Europe, Asia and America.

Eight of these are equipped with particularly large plants, so called world-scale plants.

Agenda



Hand-in-Hand: Cooperation for 7 years



Selected Examples



Covestro's view on APS

Modelling challenges in our two worlds



Large Scale Production

- Large simulations
- High level of detail
- Rigorous heat exchanger modeling
- Online Models
- VLLE modeling
- Electrolytes Modeling
- Steady-state and dynamic case studies
- Custom modeling



Circular Economy

- Large simulations
- Easy description of less-known components
- Solids modeling
- Modeling of unconventional unit operations
- VLLE modeling
- Custom modeling



Partnership for Next-Generation Process Simulation



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 in one tool
- Smooth migration, no work disruption



Cooperation SimCentral / AVEVA

Started in 2017

Goals

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



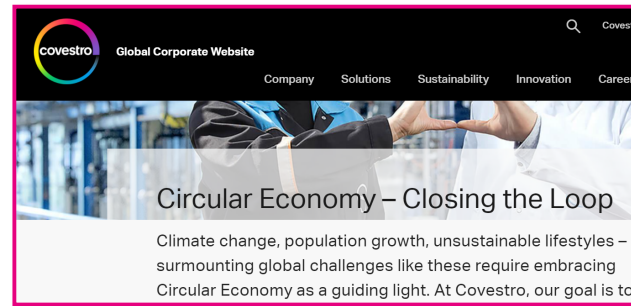
AVEVA...

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

AVEVA vision

- Find reference customers in the chemicals sector to test and promote the software
- Find partners to develop the new software

The Path of AVEVA Process Simulation @Covestro



Circular Economy

- Design of new processes
- Complex & unconventional thermodynamics
- Shift to bioprocesses, solids processes, hybrid processes
- Need for custom modeling

Model migration project:

- ~20 important models in commercial simulator
- ~100 active users
- Switch from sequential-modular to equation-oriented design

- Electrolytes**
- Small dynamic simulations**
- Online models**
- Rig. heat exchanger**
- Case study tool**



2018

2019

2020

2021

2022

2023

2024

Rigorous Heat Exchanger Modeling

Showcase: Falling Film Evaporator (FFE)

- Design and Rating of FFE based on apparatus' geometry

Challenge:

- Complex model
- Two inhomogeneous phases
- Custom correlations for heat transfer coefficients and pressure drops

AVEVA developed Heat Transfer library with first prototype of a heat transfer cell

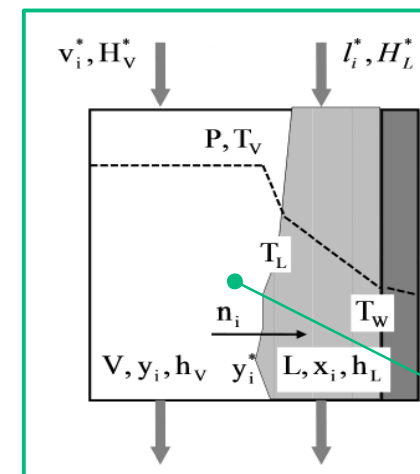
Open feature requests:

- Modeling of inhomogeneous two phases
- Container models for common configurations



Detailed modeling with HXCells

Custom correlations



Inhomogeneous two phases (not yet available)

Simulation of failure scenarios

Showcase: Pressure safety valve (PSV)

- Detailed PSV model for safety investigations
- Objectives:
 - Does the PSV have the correct dimensions?
 - How does popping influence downstream units?

Challenge:

- Specifications are often highly individual
- Numerically demanding (1 Phase ↔ 2 Phases)

AVEVA ...

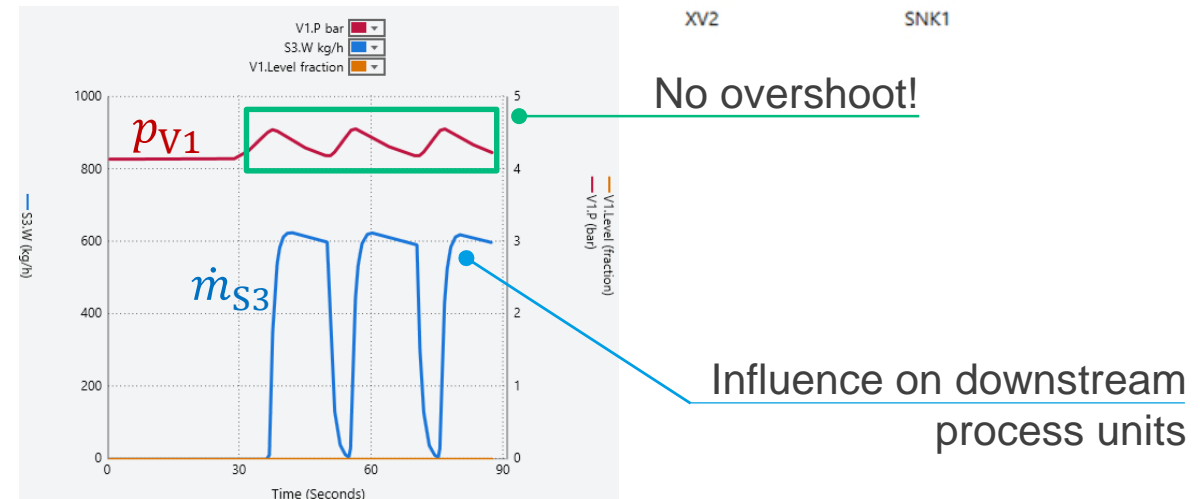
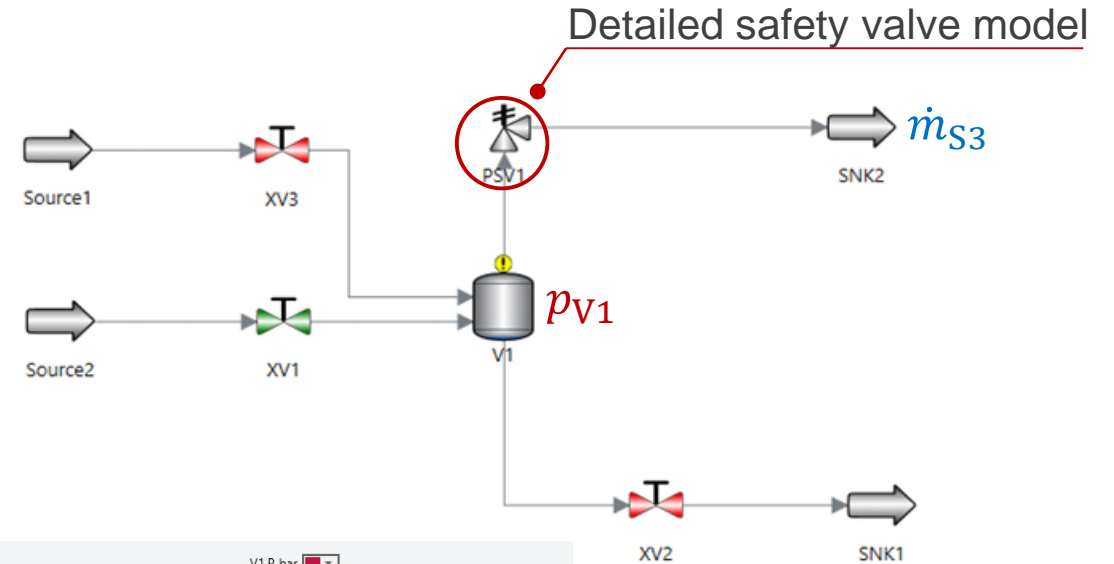
- modified and extended model equations
- Supported modelling to improve robustness

Solution:

- Customized PSV model

Open request:

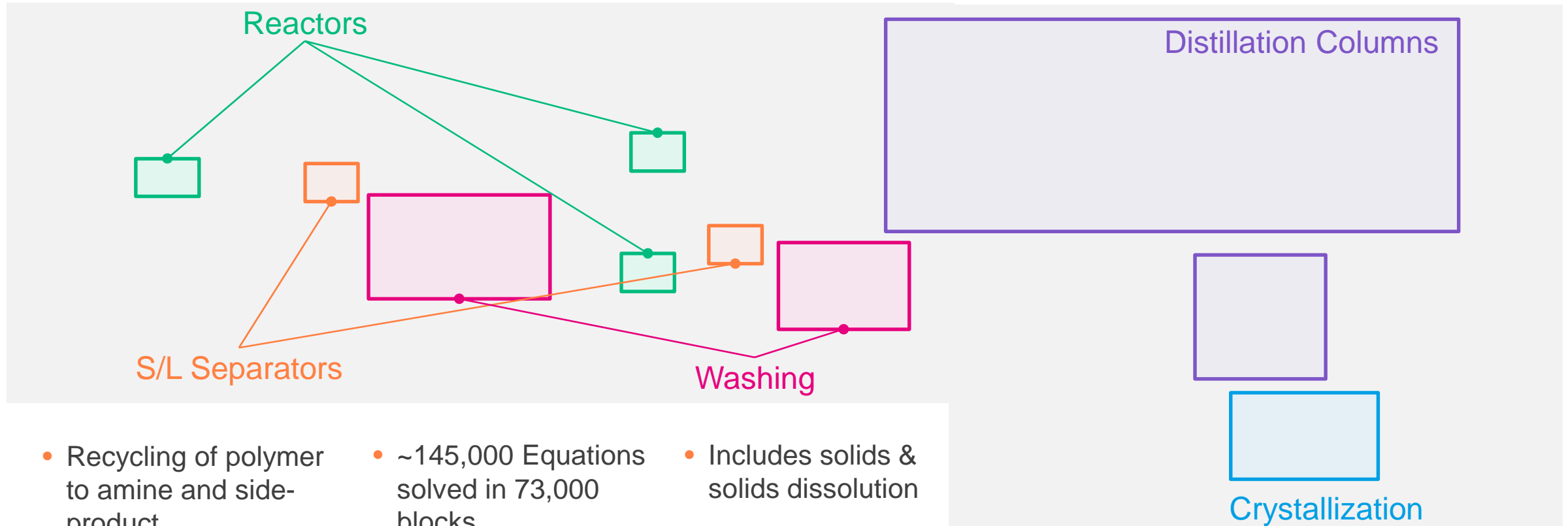
- Improved robustness for more complicated scenarios



Process Development with AVEVA towards Circular Economy



Showcase: Polymer Recycling



- Recycling of polymer to amine and side-product
- ~145,000 Equations solved in 73,000 blocks
- Includes solids & solids dissolution

- Connection to Excel for mass balance & cost estimation reports works well

What we particularly like about APS



OSIsoftPI-integration

- Direct integration with plant data
- Using process data to reconcile model is easy

Python Interface

- Completely flexible interaction with simulation possible
- Automation promises huge productivity gains

Exchangeable Fluids

- Exchange of fluid simple and robust
- Enables scalability of standard process models

Detherm / DPP

- Open interfaces allow integration of best-in-class tools
- Common thermodynamic backbone based on Detherm / DPP

Collaboration with AVEVA

- **Quick support available (usually < 1 business day)**
- **Regular exchange with developers**

Customizable Flowsheet

- Drag important variables / specs to canvas
- Simple and transparent use of flowsheet equations

What we wish for the future



Reduced hardware requirements for large simulations

(min. 32 GB RAM)

Continued quick and effective support

More powerful heat transfer library

(inhomogeneous two phases)

Larger unit operation library for solids processing

(e.g., filtration, washing, drying)

Improved handling of electrolyte systems

(switch true/app. components)



7 years of intensive experience with APS

- Rolling out software that is in development has huge potential, but there can be unforeseeable delays
- Migrating models is labor intensive, but beneficial for Know-How transfer
- Being able to view all model equations is a clear benefit
- Not all of our process simulation needs are (yet) fulfilled

Outlook

- Looking forward to February 2025 version (Performance improvements, Falling Film Evaporator)
- Close collaboration was and still is essential
- Continued quick and effective support

Covestro...

requires process simulation tools ready for the digital transformation.



AVEVA...

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

With AVEVA Process Simulation as next-generation simulation tool we are well equipped for our digital transformation



**THANK YOU FOR YOUR
ATTENTION**