


# Experience on Aveva Process Simulation by Covestro

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# Covestro – leading in the world of plastics

## Strong

- €10.7 bn in sales
- 16,500 employees[1]




## Useful

- Plastics, pre-products and solutions
- For many industries



## Global

- 33 production sites globally
- Close to customers and partners



## Innovative

- 1,200+ employees in research and development
- 80 years of ideas and inventions





Financial year 2020
[1]calculated as full-time equivalent (FTE)

# Key industries in focus

## Automotive and transportation



19%

## Construction



16%

## Wood and furniture



17%

## Electrics and electronics



13%

## Chemicals



7%

## Sports/leisure, cosmetics, health and others

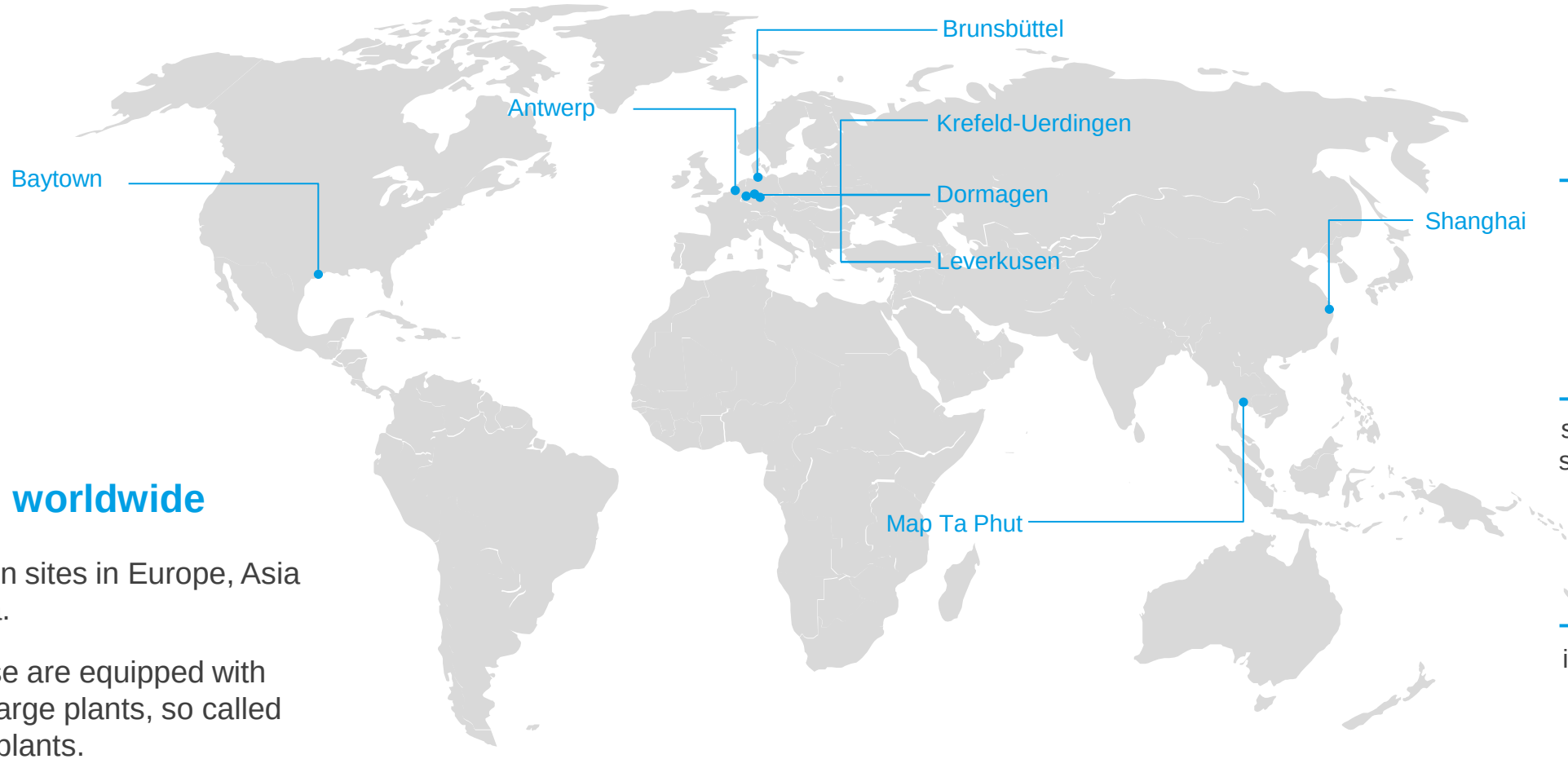


28%



Percentages: Share of total sales in financial year 2020

# Our presence




## Covestro worldwide

33 production sites in Europe, Asia and America.

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

**33**
production sites worldwide

**8**
sites with world-scale production plants

**4**
innovation hubs

# Why is CAPE[1] Simulation so important for Covestro?

[1] CAPE = Computer Aided Process Engineering

## Highly complex world-scale chemical processes

Large number of process units (reactors, columns, pumps, compressors)

Complex thermodynamics (non-ideal VLE & VLLE, many components)

Many recycle streams (trace components are highly relevant)

Tight heat integration (complex interaction of utilities & process)



Our three key points for digitalization in process simulation:

1. **Use** and importance of Process Simulation will **increase in the future**
2. **Quality of simulator** and **ease of use** is key driver for digitalization
3. **Complete Lifecycle** of a plant must be supported by simulation software

# Covestro/AVEVA
# Partnership for Next-Generation Process Simulation

## Covestro…

is looking to make process simulation discipline ready for the digital transformation.

### Our vision

- Simulate the entire process lifecycle
- Process Design
- Equipment Design
- Advanced Process Control
- Plant Support & Debottlenecking

### What we need

- Advanced numerics
- Access to plant data (OSI PI)
- Custom modeling (special know-how)
- Steady-State & Dynamics in one tool
- Smooth migration, no work disruption

**Cooperation SimCentral**
Started in 2017

**Goals**
Early evaluation of software
Configuration of tool to our requirements



## AVEVA…

is providing solutions for 1D, 2D, 3D engineering and simulation.

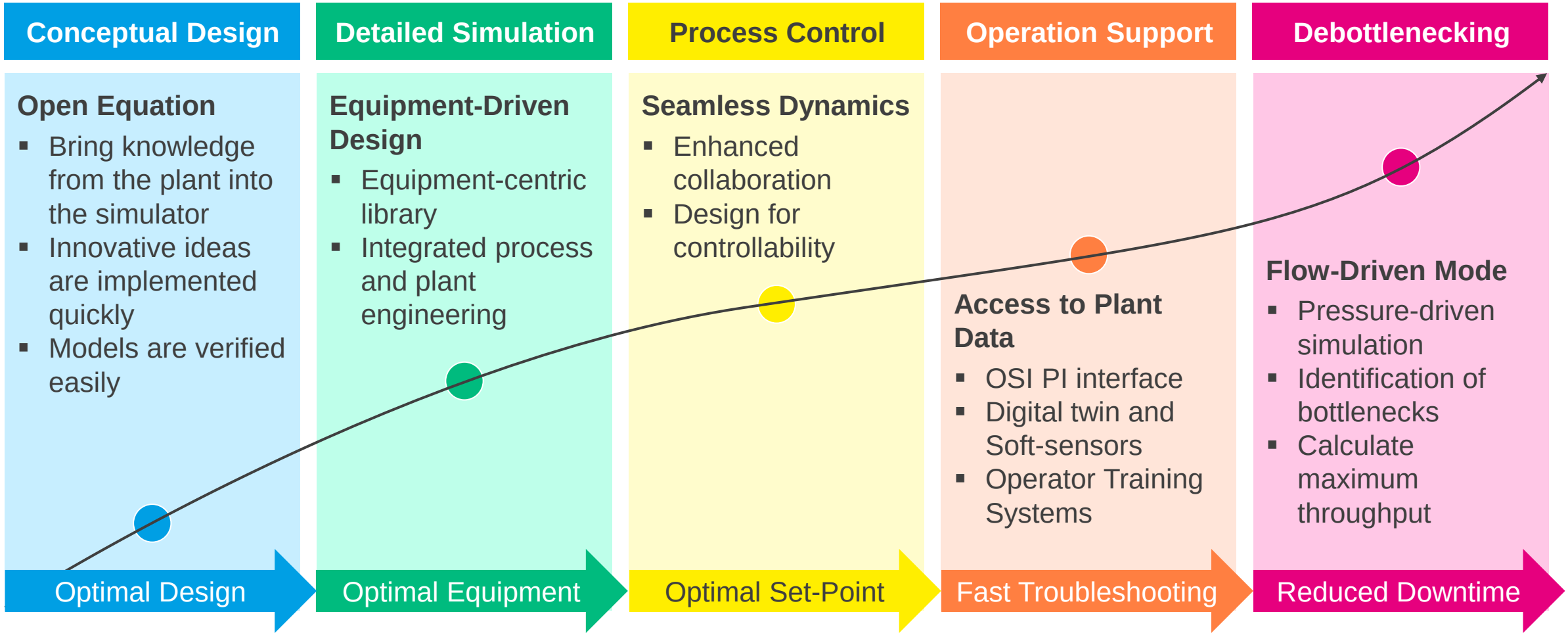
### AVEVA vision

- Develop the next-generation Simulation tool **APS** (**SimCentral**). Designed from the ground up to be **ready for digitalization**.
- Find reference customers in the chemicals sector to promote the new software.

### What AVEVA offers

- Technical excellence
- Close support & training
- Regular progress meetings

# Supporting the Process Model Lifecycle



# Key Features of SimCentral and their relevance for Covestro

### Flexible Thermodynamics

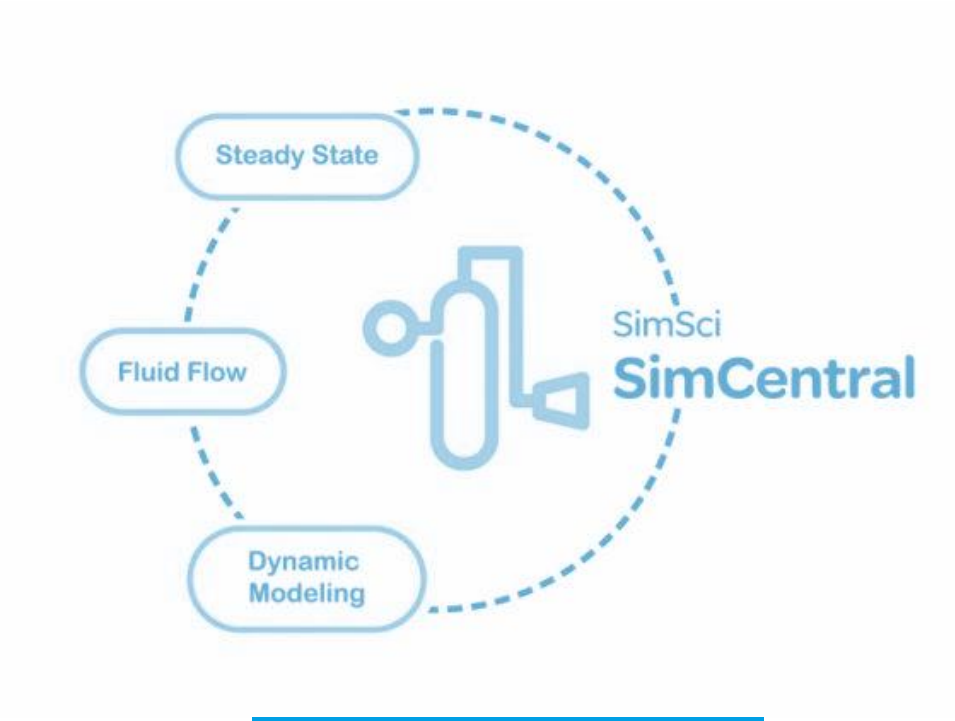
The implementation of the open **IK-CAPE thermodynamics** provide a frame of reference which simplifies migration from legacy simulators.

### Equation-Oriented Solver

The robust **equation-oriented solver** using state-of-the-art numerics allows for efficient calculation of our flowsheet models.

### Steady-State & Dynamics

**Seamless switching** between stationary and dynamic modes increases use across engineering domains and will drive innovation.




### Ease of Use

The **highly interactive** simulator enables rapid exploration of the problem without drowning the user with too much details (user roles)

### Open Modeling

Being able to see and modify the **underlying mathematical equations** enables the process engineer to include advanced customization

### Library Approach

Being able to share and document user-defined models very easily **increases re-use**, reliability and quality of custom solutions.

### Scalable Architecture

The **open platform** architecture of SimCentral allows for expansion into other fields of process simulation

# Examples

1. **Large models**
2. **Challenging thermodynamics**
3. **Custom modelling**





# Large-Scale Flowsheet Simulation

Showcase: MDI Process Simulation

**MDI model:**

>60 components

~50 unit operations

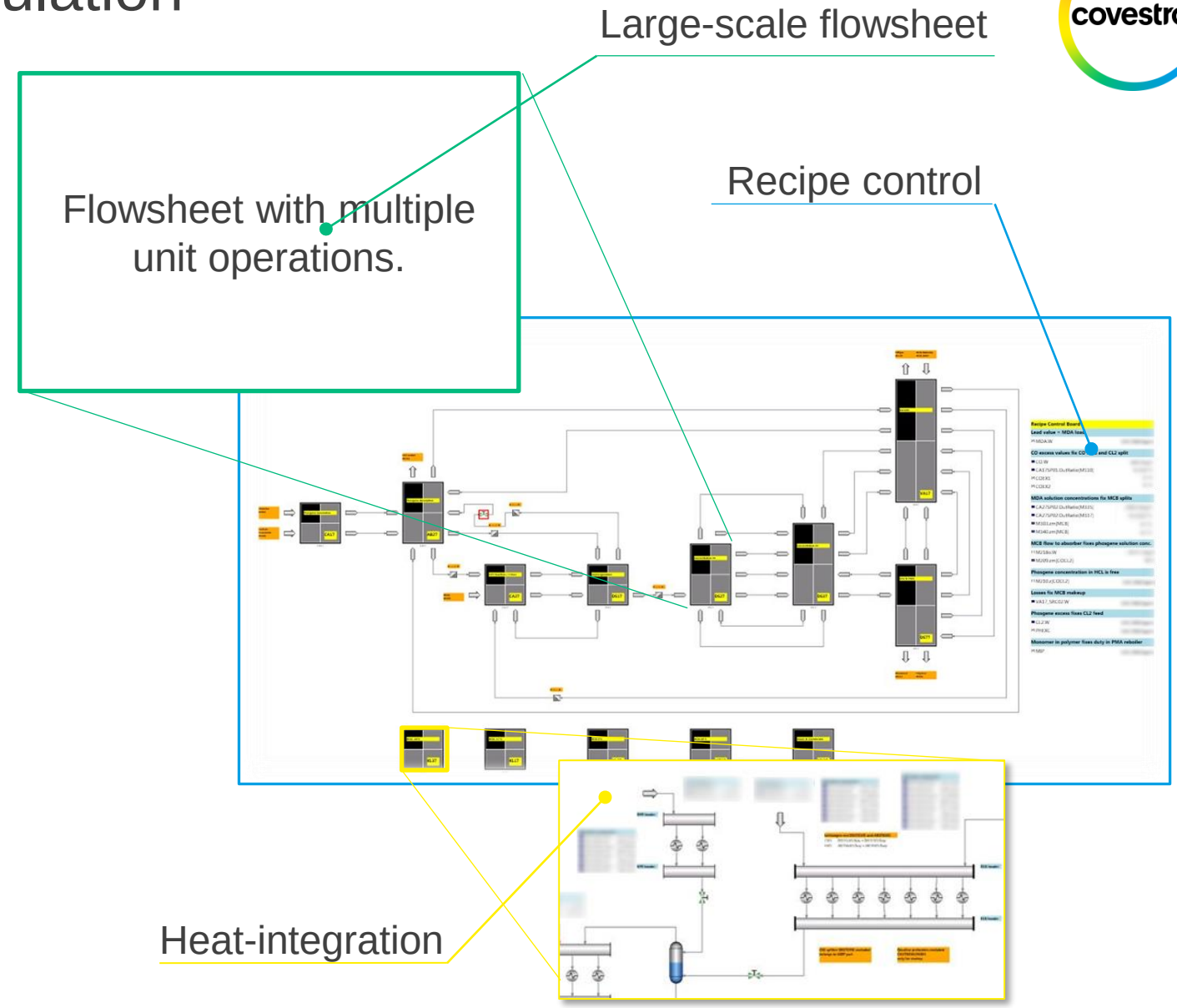
100-200 equilibrium stages

100k+ equations and variables

Many recycles and design specs

**Sucess story:**

- vs. Other: Better convergence
- vs. VtPlan: Better usability



# Robust Vapor Liquid-Liquid Equilibrium

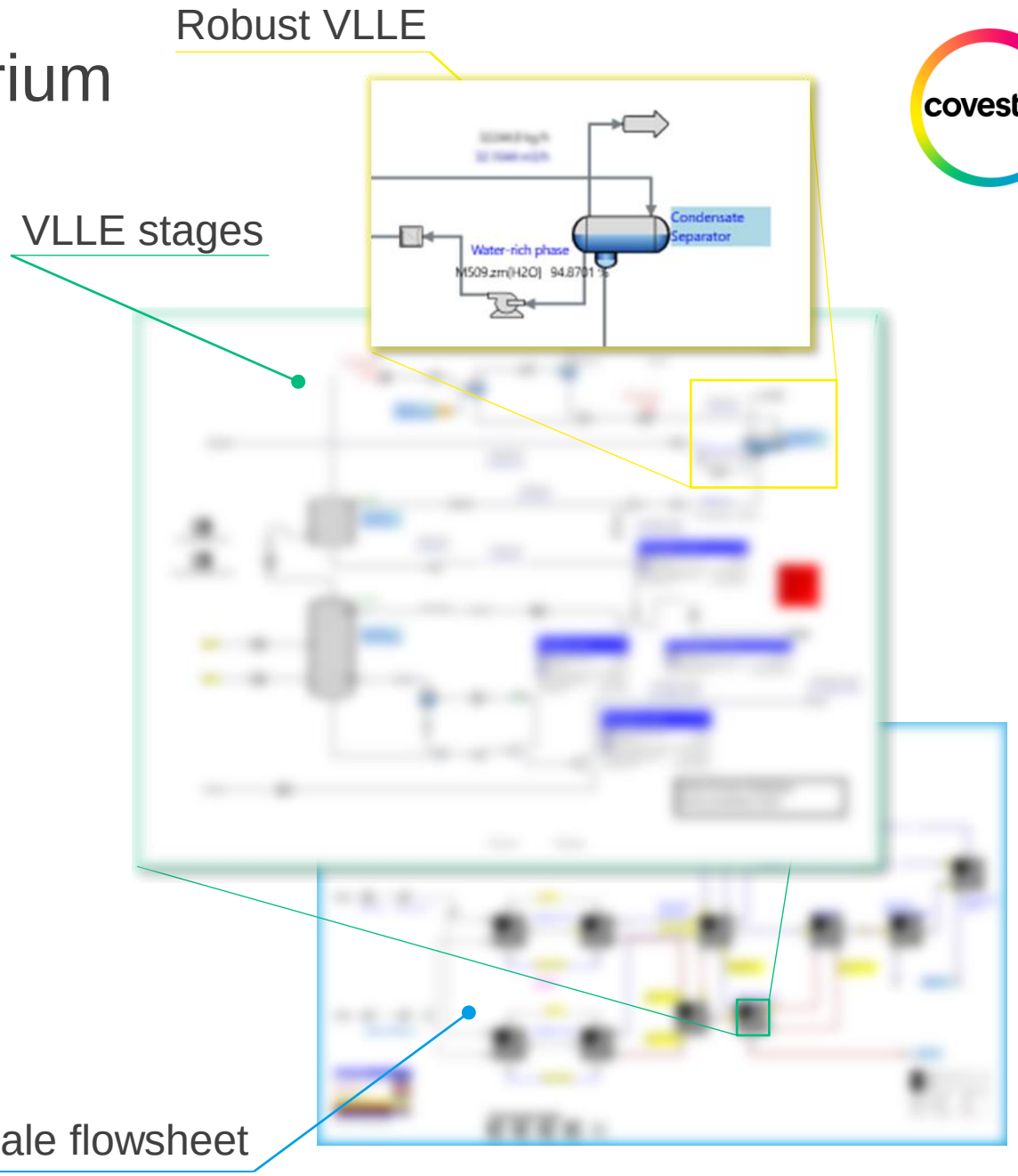
## Showcase: Aniline Process

**Facts:**

- VLLE difficult: Embedded sub-problem (e.g., minimization of Gibbs enthalpy) needs solving
- No good convergence of flowsheet with other simulator involving VLLE
- Initially, performance in APS was poor
- Intensive, hand in hand debugging with Aveva

**Success Story:**

- Issues with VLLE resolved in Jan 2021
- Never-before seen convergence for Aniline flowsheet (seconds!)



# Custom Modeling

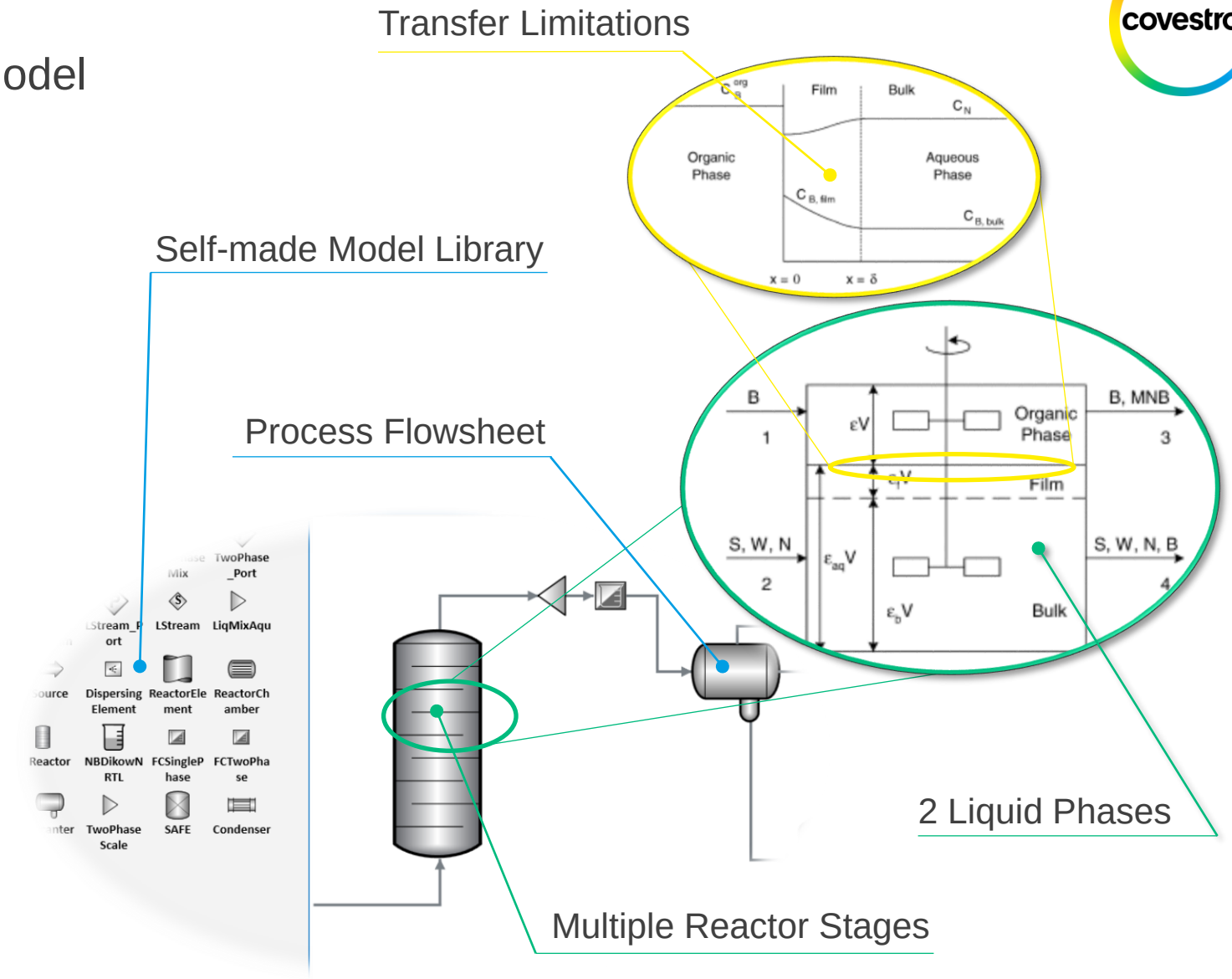
## Showcase: Nitrobenzene Process Model

**Facts:**

- Hard-to-read custom model migrated from other simulator
- Custom model of mass transfer limitations + electrolyte equilibrium
- 200+ self-written equations
- Total 60k + equations

**Success story:**

- Highly improved readability
- Better usability + extendibility



# Miscellaneous

- **Python interface:**
  - Completely flexible interaction with simulation possible
  - Automation promises huge productivity gains

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

- **Detherm / DPP**
  - Open interfaces allow integration best-in-class tools
  - Common thermodynamic backbone based on Detherm / DPP → consistent workflow and source of information

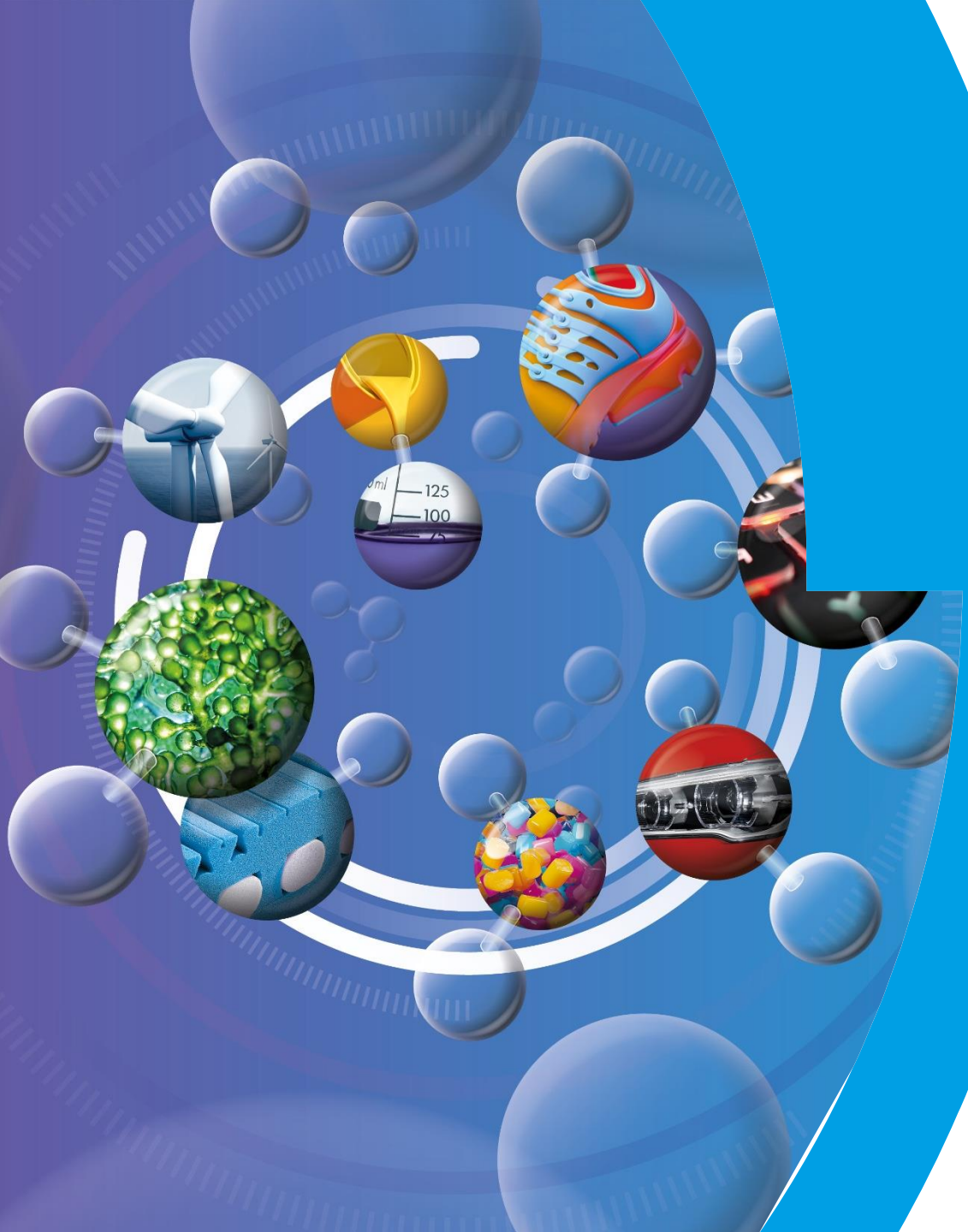
# Conclusion

**Lessons learned:**

- 5 years from selection to final migration manageable, but ambitious
- Rolling out software that is still being developed has huge potential, but there are unforeseeable delays
- Migrating models is labor intensive, but beneficial for Know-How transfer
- Close collaboration was (and still is) helpful

**Perspective:**

- We see high potential in modern software architecture, because development process is faster
- Clean and unified user experience
- Looking forward to updated thermodynamic interface




# Thank you for your attention!

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