Hafnium Labs

Predicting Chemistry

CAPE-OPEN virtual conference

October 2020

Q-props – a system for managing physical property uncertainty in process simulation

1. Intro to Hafnium Labs and Q-props
2. Embedding Julia in CAPE-OPEN through COBIA
3. Demonstrations of how we use CAPE-OPEN to:
    a) Check physical properties of existing process simulations
    b) Perform simplified sensitivity analysis
4. Next steps

Intro to Hafnium Labs and Q-props

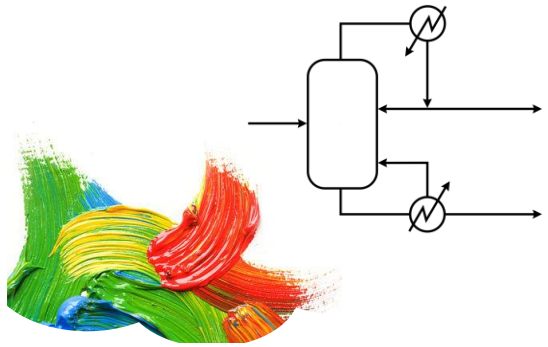
What we do

Hafnium Labs solves one of the biggest challenges in chemical R&D:
Obtaining ***reliable*** physical property data ***fast***

Our Q-props software creates a new standard for property prediction to help digitalize R&D and enable:

FASTER DEVELOPMENT
with less experimentation

SMARTER DESIGN
with data-driven decisions



BREAKTHROUGH DISCOVERIES
with 'infinite' design spaces

Our team

9 full-time: 7 scientific developers (PhDs), 1 full-stack developer, 1 business

Bjørn Maribo-Mogensen

CTO

Properties expert at Linde Eng.

PhD (EFCE Award ‘15)

Darren Rowland

Electrolyte expert

JESS[1] team

PhD & postdoc (MU, UWA)

Rasmus Lundsgaard

Quantum chemistry & MD

PhD & postdoc (DTU)

Diego Sandoval

Flash algos & thermo-dynamics

PhD & postdoc (DTU)

Martin Hangaard Hansen

AI & data science

Catalysis

PhD & postdoc (Stanford)

Jon Christensen

CEO, bus dev

Manager at BCG

MSc ChemEng

Niels Kristian Madsen

Quantum chemistry and HPC

MidasCpp developer

PhD (AU)

Sakse Dalum

Julia-lang expert

Nanoscale biophysics modeling

PhD (KU)

Christian Gehrs Kuhre

Full-stack developer

Cloud computing

MSc SW develpmt.

Collaboration projects

Tine Maja Frimann
Postdoc, DTU, protein phys. property prediction

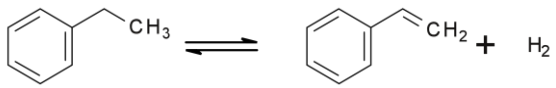
TBA (starting soon)
PhD, DTU, multi-phase electrolyte modeling

1. JESS: Joint Expert Speciation System, software for thermodynamic modelling of chemical speciation in complex aqueous environments and the largest electronic source of thermodynamic information about aqueous systems.

Why are physical properties important to get right?

- Example -

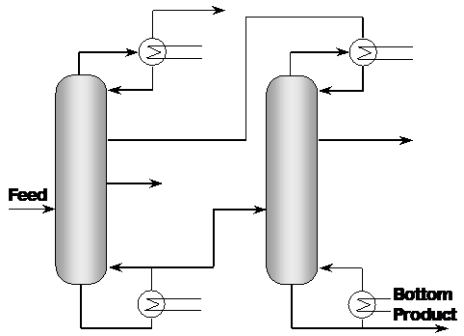
Styrene (S) is produced from ethylbenzene (EB) …



Ethylbenzene
T_{boil} = 136°C

Styrene
T_{boil} = 145°C

Separated by distillation:



… 3 different simulators give vastly different separations

Bottom product styrene concentration:

- Simulator 1: **90%**
- Simulator 2: **81%**
- Simulator 3: **71%**

→ To get same purity would require very different column heights

Same thermodynamic model (SRK) but <u>each simulator uses different physical property data</u>

The problems go way beyond simple examples

Errors propagate with size of system and no. of recycles

You can get the mass balance right, yet get the energy balance wrong

Solids, electrolytes and reactions are notoriously difficult to get right

- But can cause the most costly errors (failures/shutdown)

→ Uncertainty propagation lets you **rationalize** about your design factor

Wrong physical properties can ruin a digital design

*Example from R. Dohrn, O. Pfohl, Fluid Phase Equilibria, **2002**, 194-197, 15-29*

Why are physical properties hard to get right?

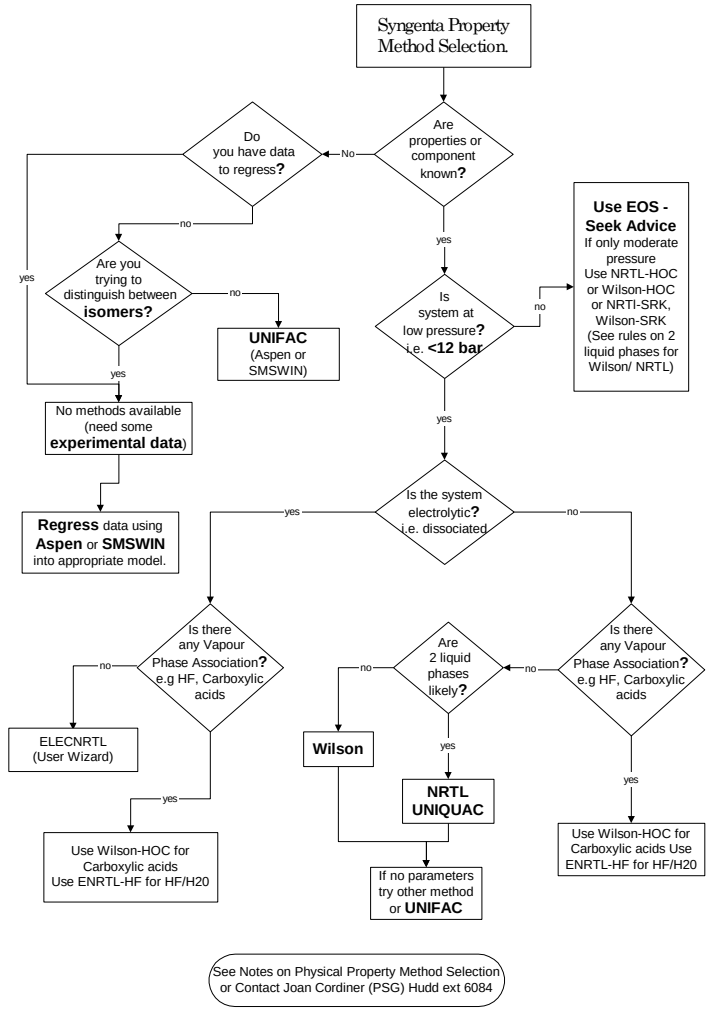
Infinitely many molecules, mixtures, temperatures, pressures **vs.** *Experimentation slow and expensive*

Thermodynamic models are parameterized against available data and can then be used for process design

There are many models available, however, …

- … there is no good way of knowing if a model has been parameterized against ***sufficient*** and ***reliable*** data
- … it is difficult for the user to know which model will work best (see opposite)

Thermodynamic model selection: state-of-art



Syngenta, Computer Aided Property Estimation for Process and Product Design, Elsevier, 2004

Physical properties for process simulation are unreliable

Off-the-shelves thermodynamics is unreliable

Process simulators have implemented “industry-standard” thermodynamics – e.g. SRK, NRTL

Models must be parameterized against reliable data, which is scarce

- Only ~2200 pure compounds included in DIPPR database
- Need binary data as well…

→ **Anything non-standard requires expert attention**

Most models do not account for reactions or electrolytes

Leading to well-known problems

The thermodynamic model does not reflect the true chemistry

The model is applied in a range of conditions outside the fitted values

The thermodynamic model is missing or has incorrect values for parameters

Problem: Errors that are not caught in this phase can impact the detailed design and ultimately become very expensive

How do we deal with these problems today?

Many companies have spent decades implementing and improving their own models

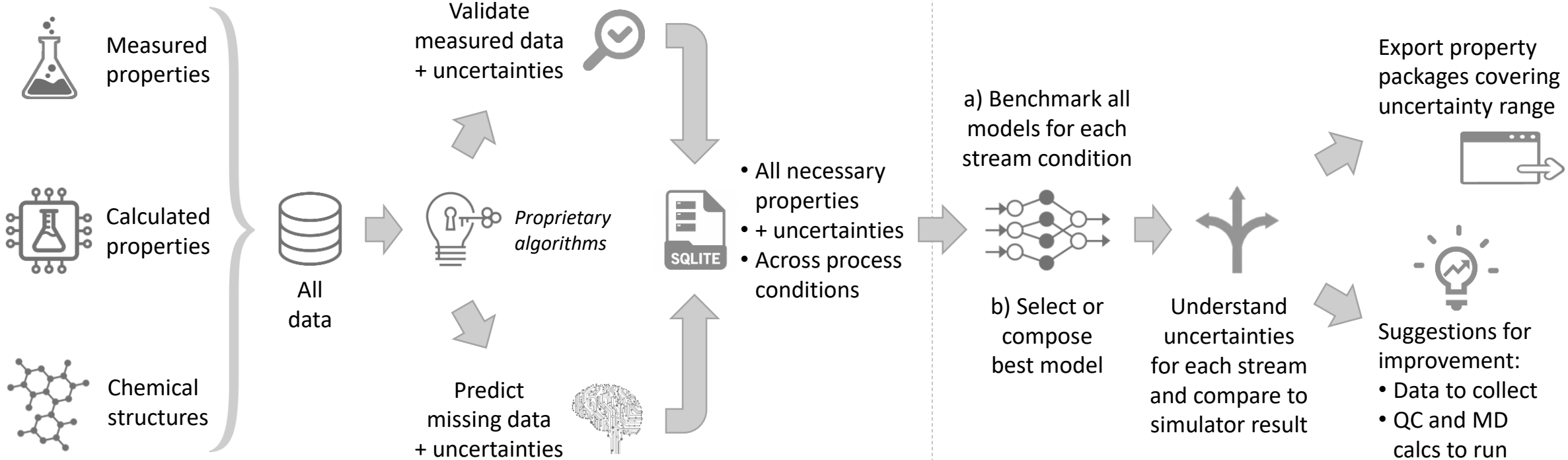
Use of scenarios e.g. low/high/edge loading to assess operation ranges

Off-line calculations through e.g. Excel-sheets and downstream corrections are routinely used

Still, models are often wrong, and it’s hard to know when or by how much…

We have developed Q-props to make it easier to get physical properties right and to understand impact of uncertainties

1. Get all data in one place | **2. For each simulation, build database of best possible property data *with* uncertainties** | **3. Identify best model and understand its uncertainties** | **4. Export or improve**



'Infinite' database of reliable reference properties

(pure compound and binary/ternary mixture data)

Best property model for simulation and impact of model uncertainty

Q-props integrates with process simulation end-to-end

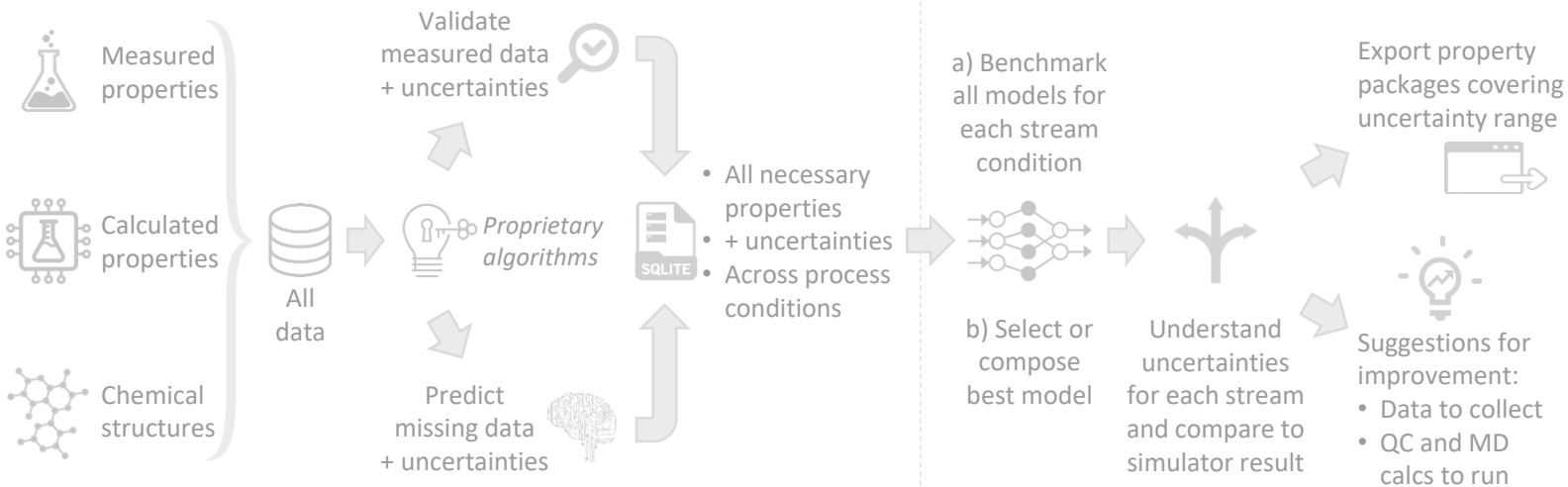
0. Import | **1. Get all data in one place** | **2. Build database of best possible property data *with* uncertainties** | **3. Identify best model and its uncertainties** | **4. Export or improve** | **5. Run simulations**

CAPE-OPEN unit operation imports:

1. Compounds
2. Conditions
3. Simulator physical property predictions (for comparison inside Q-props)

Input loaded into Q-props

→ Q-props runs steps 1-4 automatically



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Best property model for simulation and impact of model uncertainty

Q-props

Run scenarios

Exported packages can be loaded into process simulator to assess impact of physical property uncertainties on process simulation results

Replace property engine

Packages from Q-props can be used for single streams or entire flowsheet

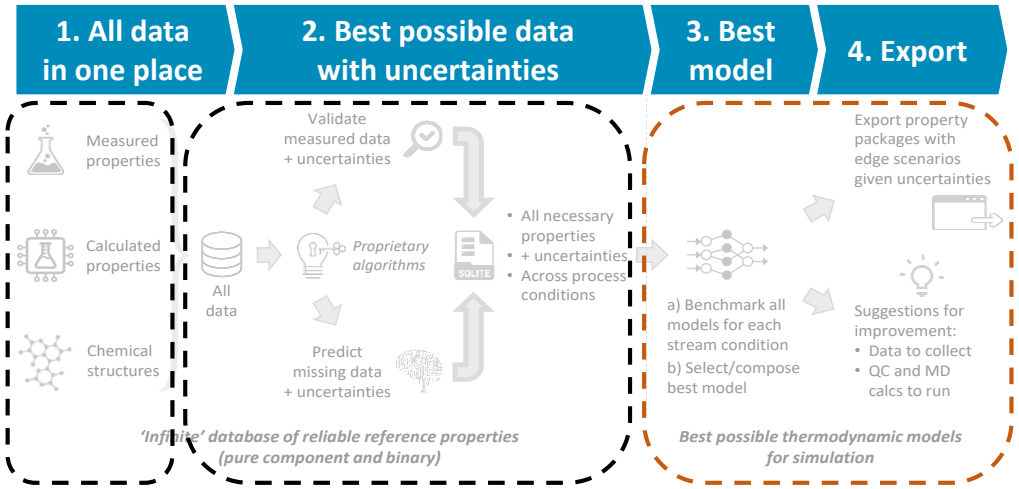
Three Q-props use cases that are enabled by our process simulator interfaces

What we hear from process simulation users	Q-props tools that address the problem
! *Process simulation errors from using wrong physical properties are critical to identify, but options are limited*	**Flowsheet checker** Automated property check of all streams in your process: Gives reliable 2nd opinion, highlights potential problems and suggests data to collect ✓
! *Knowing which property uncertainties affect process and equipment design is hard – often leading to over-design*	**Uncertainty deep-dive tool** Quantified uncertainties for each stream property and transparency on experimental data and models behind each prediction ✓
! *Improving thermodynamic models is time consuming, requires expertise, and models might still be used outside validity range*	**Thermodynamics plug-in** A plug-in to run Q-props thermodynamics in your process simulator – fitted to process conditions ✓

Embedding Julia in CAPE-OPEN

We have built core Q-props components using the Julia programming language

Julia is core to Q-props modeling engine



3rd party, open source | **SQL, C++** | **Julia**

Other languages

- C#/.NET Core for ETL workflows
- Python for automation and Jupyter notebooks
- HTML/Javascript for frontends (Jupyter)

Julia goodies for developers

Julia can be used for both prototypes and production
→ Viable alternative to FORTRAN and C++ but also Python and MATLAB

Built-in package-manager for dependency management in large projects

- Eases maintenance and extensibility
- Internal package repository

Julia is stable (currently at version 1.5)

- More than 3000 packages available on Github

Nice features for thermodynamics modeling

- Support for unicode names enables standard symbols in applied thermodynamics, e.g. β, γ, ω, σ, ϕ, Γ
- Excellent support for unit of measurement, automatic/algorithmic differentiation etc.

Overall, we have good experiences with Julia

Our experiences

Julia **is** fast – when code is written "right"

- Make sure to avoid allocations
- Ensure use of concrete types

Julia can be secured and deployed as executables/dlls (PackageCompiler.jl)

- Doesn't fully protect code by default

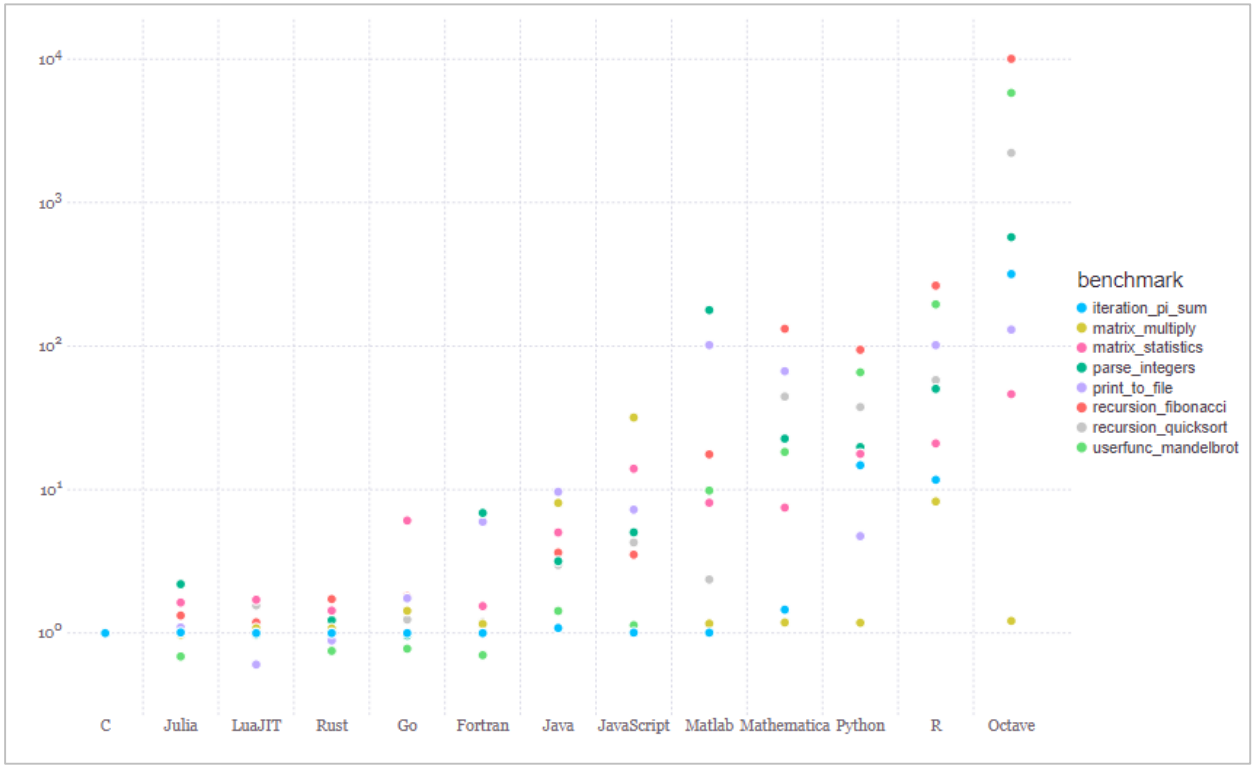
Julia has excellent integration with Python (v2 & v3)

- Easy to write high-performance code in Julia and other parts in Python

Julia is especially strong in combining scientific models and machine learning (SciML)

- **(DEMO)**

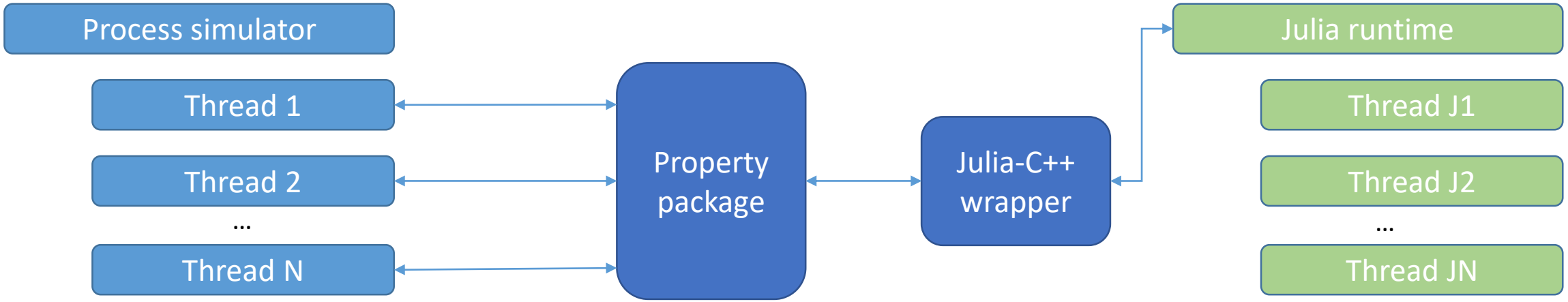
Julia is fast



Integrating Julia with CAPE-OPEN

We used COBIA v/1.0 to implement unit operation and property package wrappers (v 1.1/1.2)

- COBIA acts as a wrapper for COM (COMBIA).
- Julia C API **must** be called from a single thread
    - C++ acts as wrapper for synchronizing calls to Julia via std::future

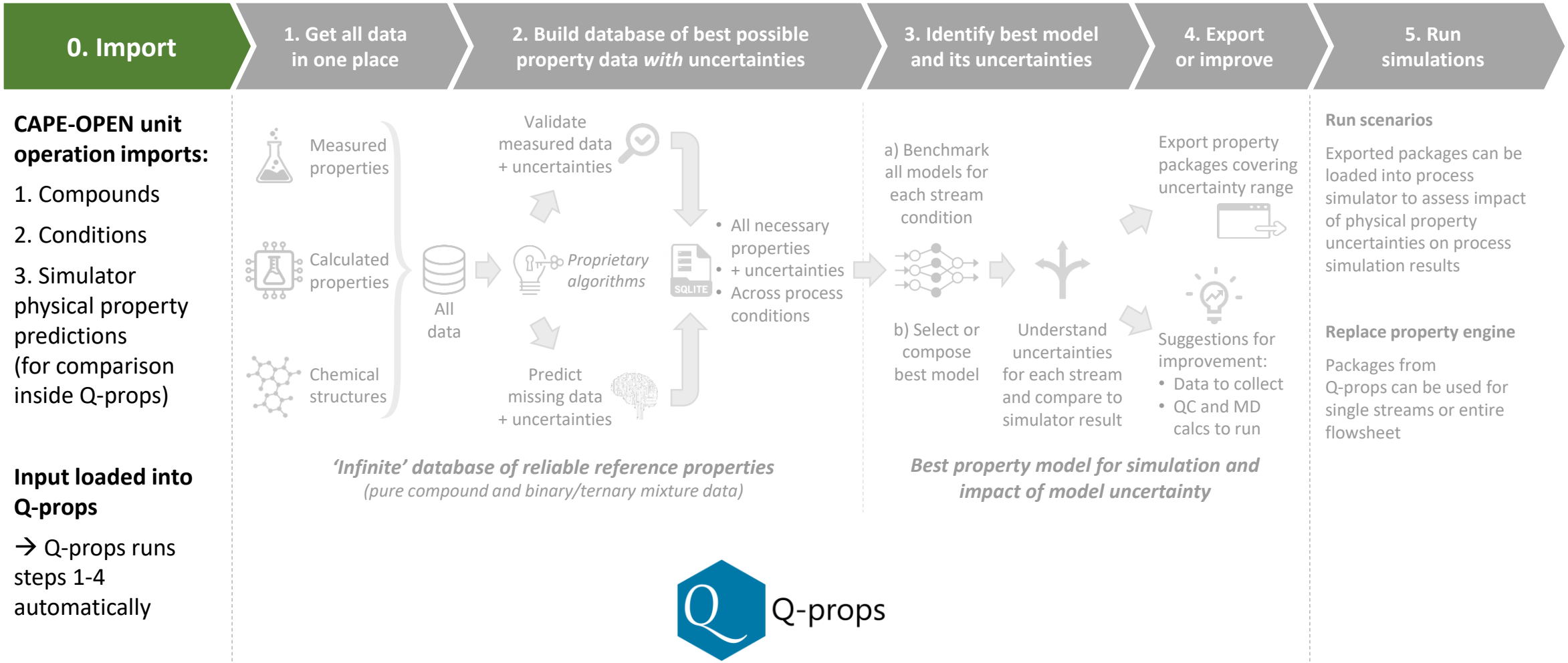


Things to watch out for:

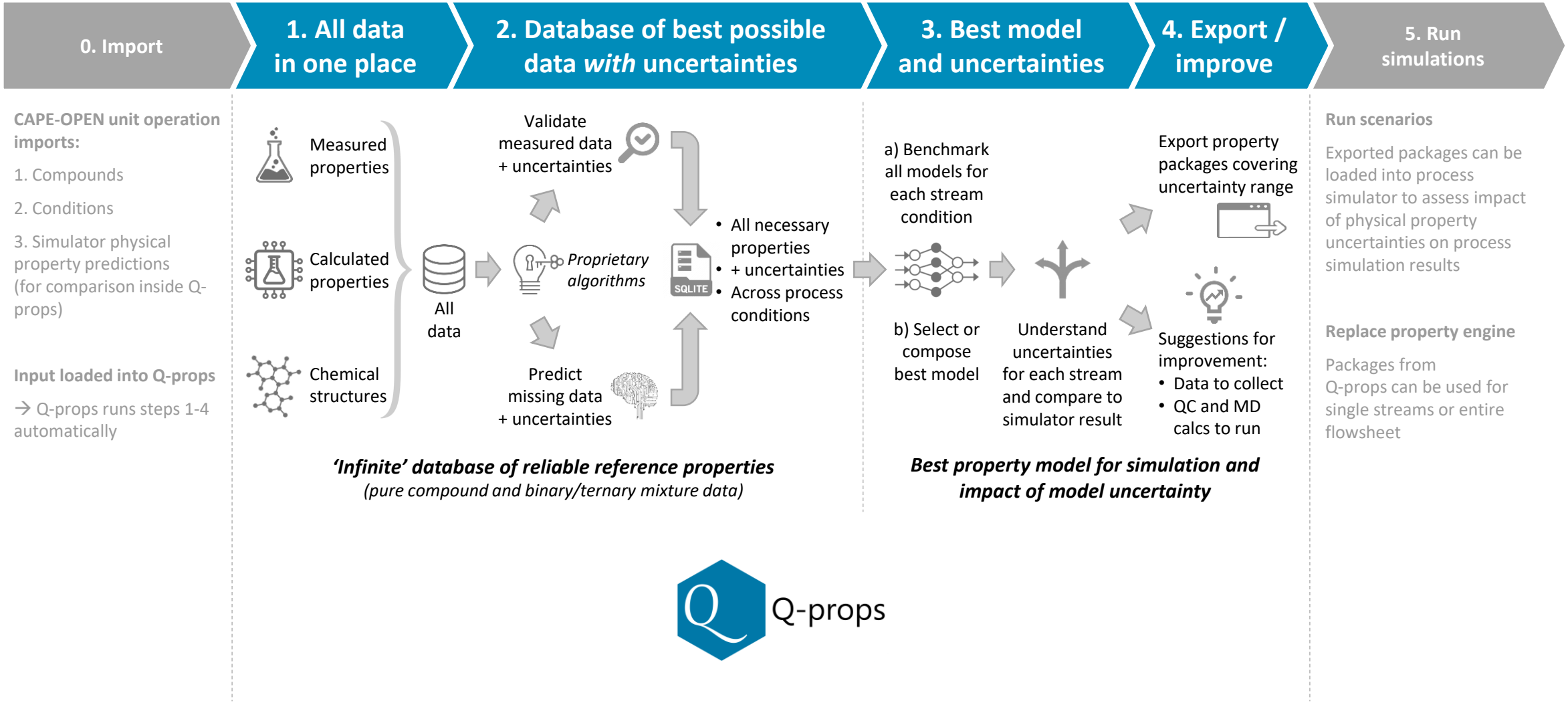
- Julia uses UTF-8 but CAPE-OPEN uses wide strings (16-bit)
- Use e.g. std::wstring_convert<std::codecvt_utf8_utf16<char16_t>>

Demonstrations

We start from the process simulator



The Q-props workflow runs



Q-props

After Q-props workflow has run we can open the flowsheet checker

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To understand drivers of model uncertainties we use the deep-dive tool

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Plug-in makes it easy to use Q-props thermodynamics inside simulators

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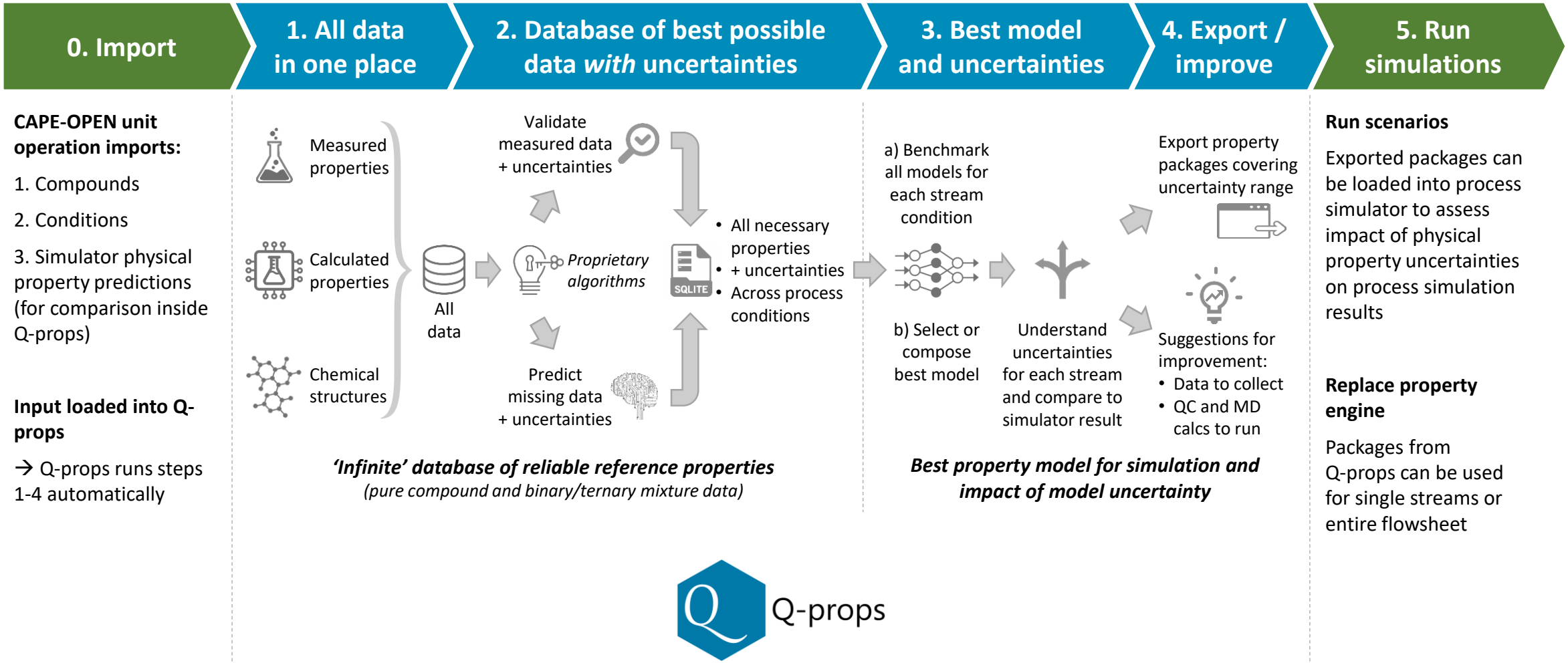
Recap: Demonstration shows how Q-props integrates with process simulation end-to-end



Next steps

Use the Flowsheet monitoring interface to import all streams to Q-props at once

Save cached variables to stream if supported by simulator to speed up subsequent flashes

Use the new CAPE-OPEN interface for reactive mixtures

Q-props timeline

We are about to start beta-testing of Q-props

Reach out if you're interested in learning more

Thank you

Hafnium Labs

Predicting Chemistry