

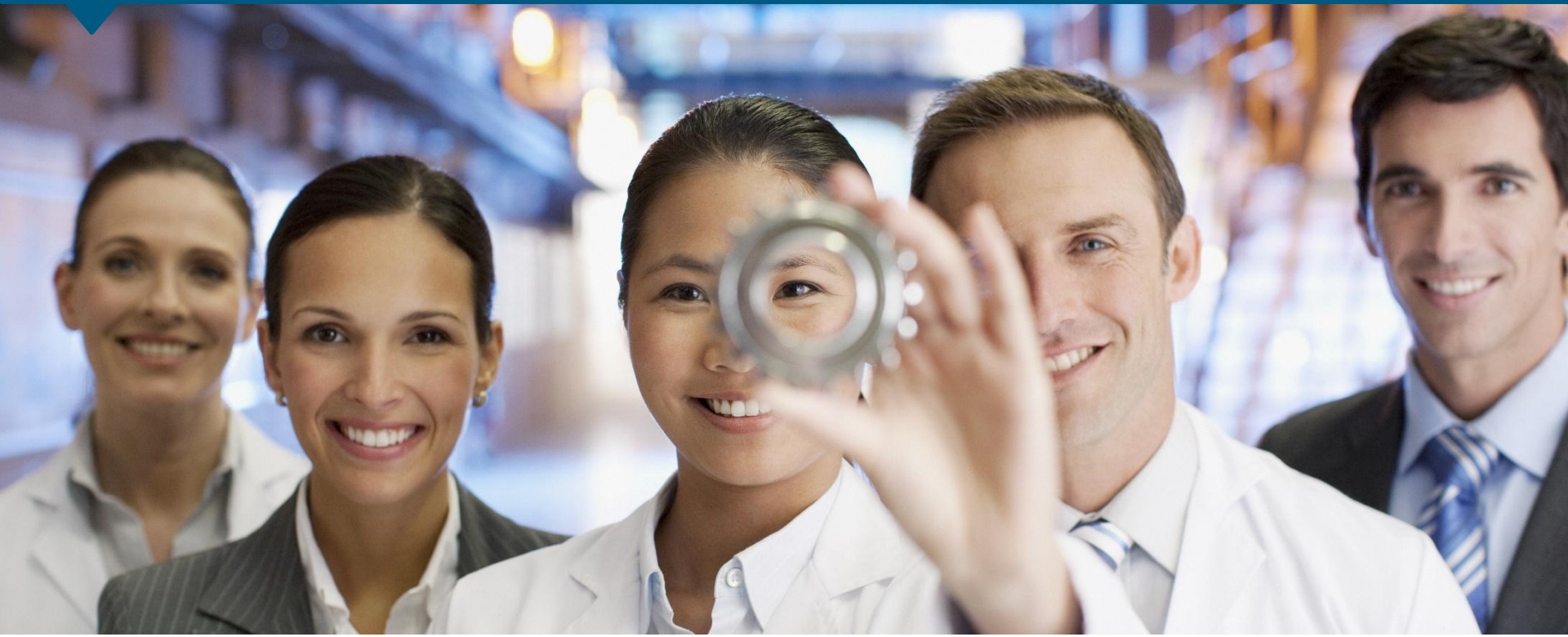
DECHEMA

DECHEMA DETHERM & DPP

Overview on DECHEMA‘s Thermophysical Property Database DETHERM + DPP software incl. new interface to AVEVA Process Simulation

Dr.-Ing. Ulrich Westhaus

“Science and Industry in dialogue“



DECHEMA

Gesellschaft für Chemische Technik
und Biotechnologie e.V.

7 Focal Topics at 1 Glance



DECHEMA
Gesellschaft für Chemische Technik und Biotechnologie e.V.

Our Services for You

Research and project coordination



dechema.de/research

Databases



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Event Management



dechema.de/eventmanagement

DECHEMA
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Facts and Figures at a Glance

Over **5,800** individual members

650 companies

More than **1,000** honorary experts

Around **100** events annually

120 working groups and committees

Over **10,000** conference participants

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3 Organisations under 1 Roof!





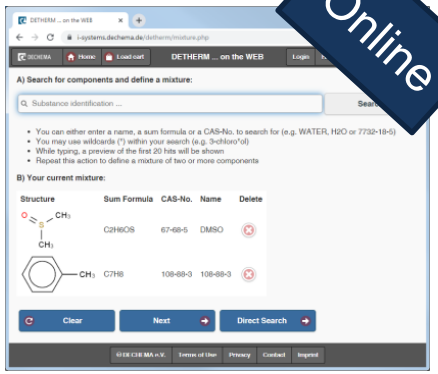
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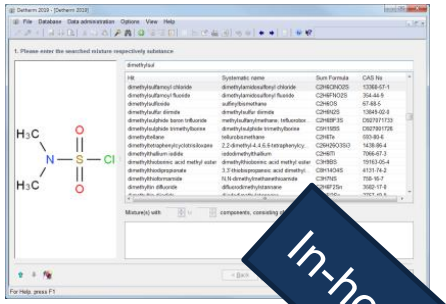
DETHERM – DECHEMA Thermophysical Property Database

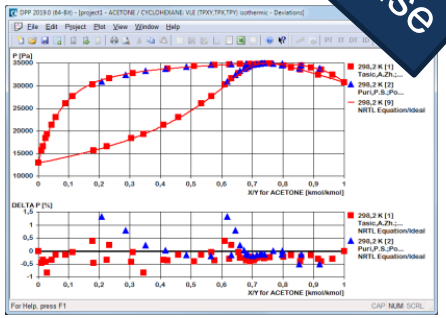
- World's largest factual database for raw thermophysical property data
- Established 1979 and updated yearly (average growth 8% per year)
- Currently **11,9** million data sets for
  - **76,000** pure substances
  - **253,000** mixtures
- Access options: in-house installation or online
  - Inhouse access options: Client-Server, Web-Access, REST-API
- Active collaborations
  - Data producers: DDBST GmbH, DIPPR, Wiley

  - Interfaces to simulation software vendors: AspenTech, Aveva, KBC, ProSim

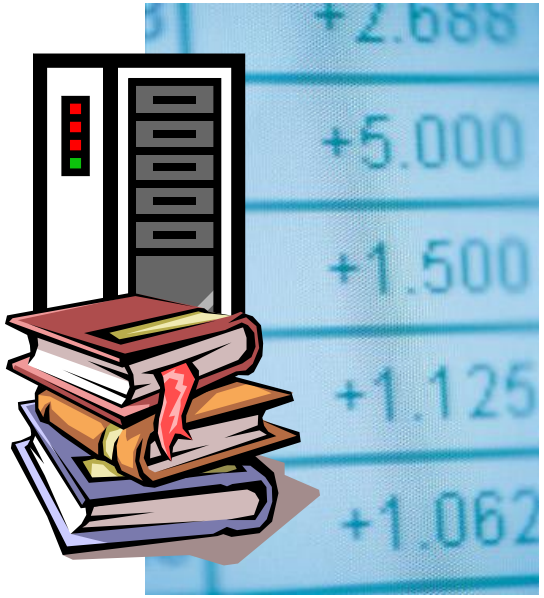
- Reference customers (in-house solution): BASF, Bayer, Lanxess, Covestro, Total, BP Chemicals, Novartis, AirLiquide, and others …







Data Preparation Package DPP: Connecting 2 worlds



Measured data (discrete values) DETHERM



DECHEMA Data Preparation Package (DPP)



Simulator (equation orientated, model based) AVEVA, …

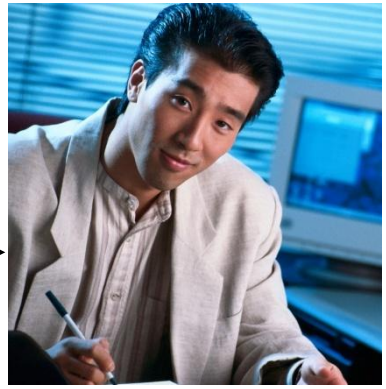
Never forget: The reliability of a (process) simulation is substantially based on the precision of the thermodynamic models used ...

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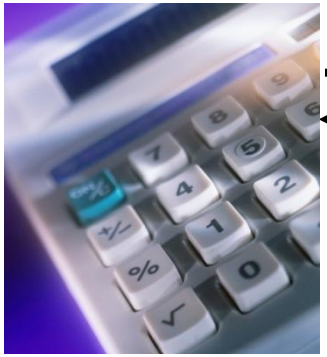
DPP: The Architecture

Thermodynamic Modules

- Aspen Properties
- AVEVA
- IK-CAPE
- Simulis
- Multiflash



End User



Calc.

DPP GUI & CORE

Thermo Interface	Graphics subsystem
Optimizer	Neutral File & COM-Interface

Simulators

- Aspen
- AVEVA
- ProSim
- Multiflash



Model Parameters

Raw Data



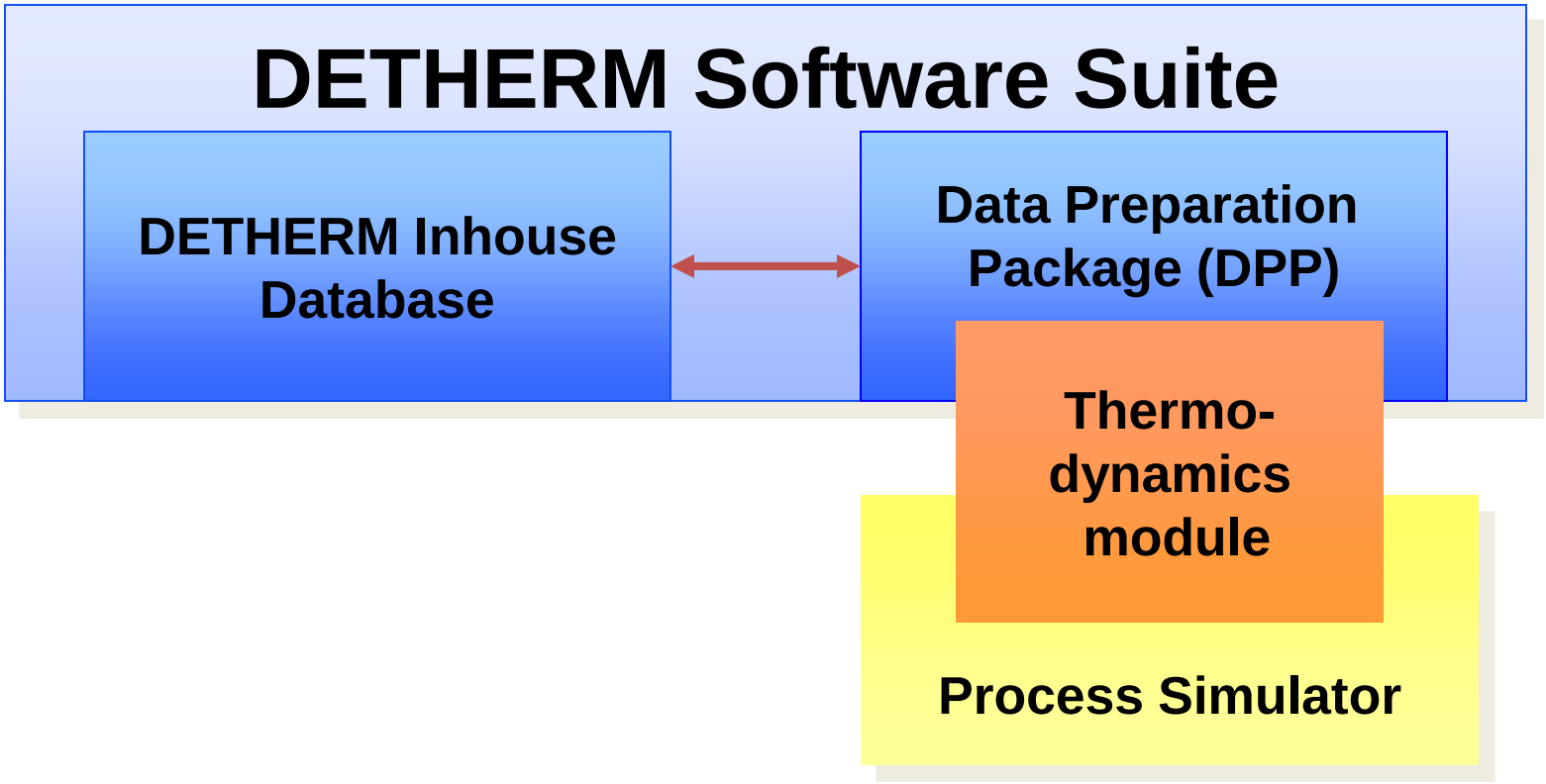
Databases

- DETHERM
- DIPPR
- NIST
- ...

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DPP and DETHERM

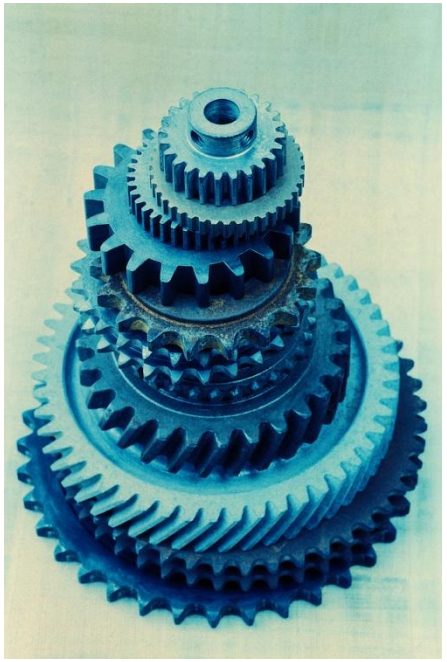
- DPP regression tool couples database with simulator.



The Optimizer

… is the core element of DPP

- Simultaneous correlation
  - of different data types / systems
  - with different error functions
  - e.g. VLE + LLE + HE + γ^{∞} + Azeotrops
- Model parameter transformation
  - 1:1
  - Different ranges -> equal ranges
  - Bounded -> Unbounded
- Mathematical constraints on parameters possible
- Combination with Maximum Likelihood Algorithm (ML) possible

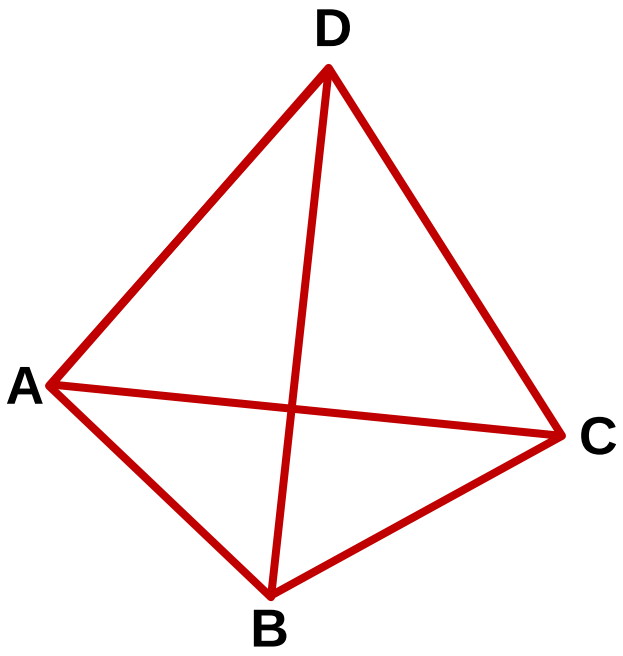


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Sub-System Regression

- N-Component System: Simultaneous Regression using all systems with
  - n
  - n-1
  - n-2
  - ...

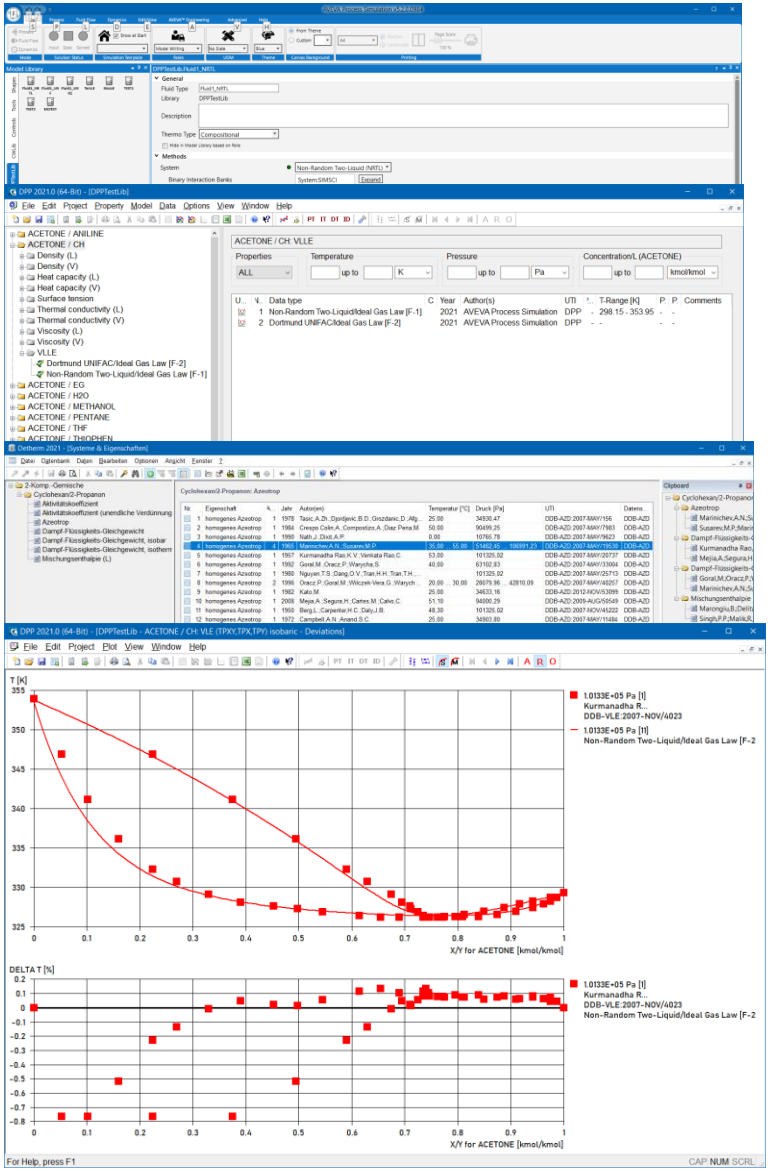
  components and data
- Also pure system could be included



4-Component System

Workflow using Aveva

1. Setup models within AVEVA Process Simulation
2. Start DPP + load prepared AVEVA model library
3. Load or enter data
   - DETHERM database
   - IKC Files
   - Direct entry (copy from Excel)
4. Perform data regression
5. Save results
   - AVEVA library
   - DETHERM database



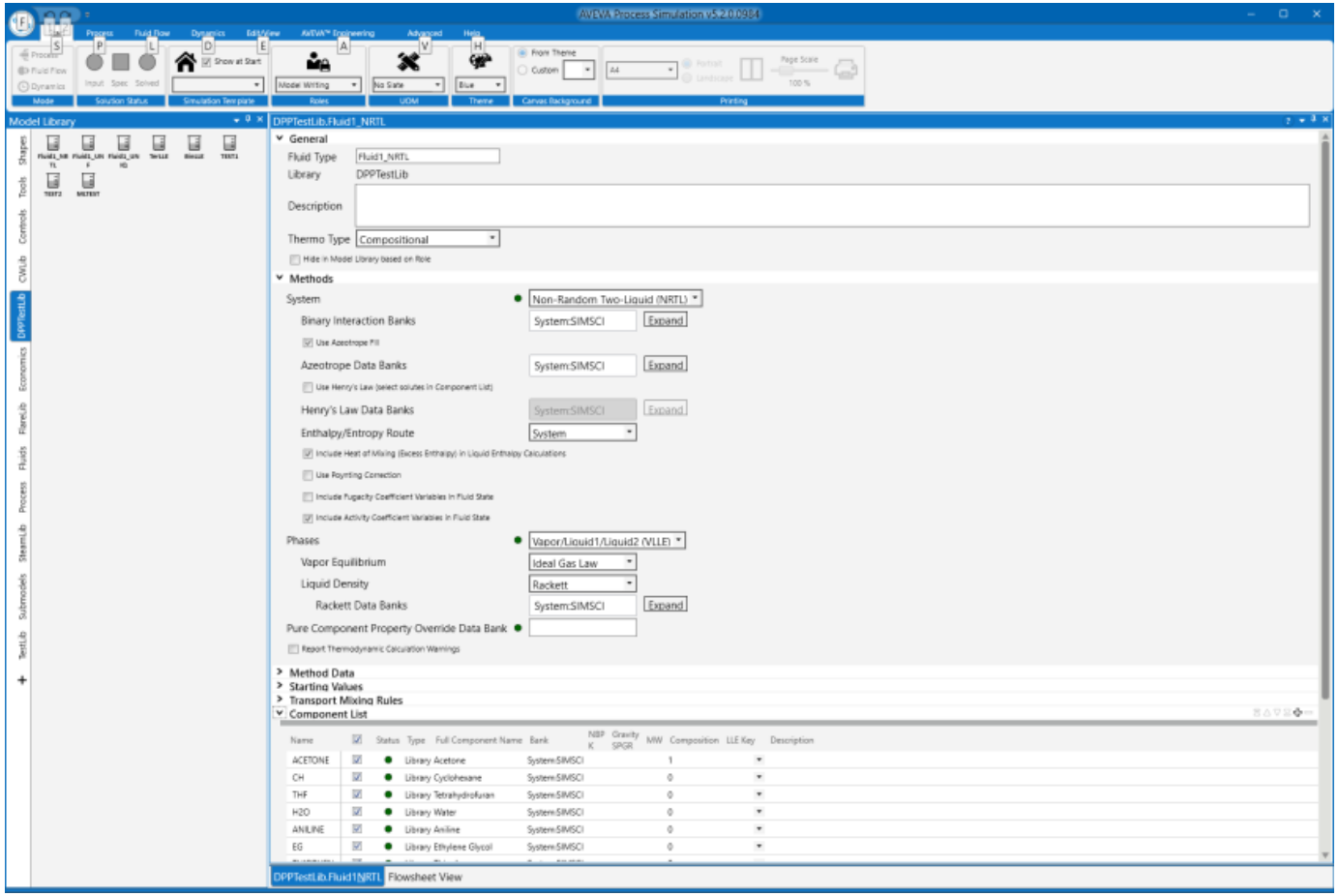
Currently known restrictions (for AVEVA interface)

- Not all models are currently open for regression
  - AVEVA 5.3 includes:
    NRTL, UNIQUAC, Wilson
- No simultaneous reactions



Live demonstration

VLLE of Water / Aniline using NRTL



THANK YOU VERY MUCH FOR YOUR ATTENTION …

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