Use of the THEREDA database in ChemApp for Potash Process Modelling

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Overview

- What is a Process Model?
- Thermodynamic Engines in SysCAD
- THEREDA database in ChemApp
- Model Validation
- Application to muriate of potash to sulphate of potash conversion process
- Summary

What is a Process Model?

- Digital twin of your process
- A valuable tool for evaluating what-if scenarios
- Useful for comparing relative benefits of different operating modes or circuit designs
- A comparative tool, useful for comparing relative benefits
- Does not always *exactly* match your process
- Should always trend with your process

What Constitutes a “Good” Model?

- Appropriate level of detail
- Clear defendable assumptions
- Proper documentation
- No “fudge” factors
- Validation against plant or test data
- Responds appropriately to changes in input
- Can be used to evaluate large numbers of scenarios

SysCAD Model Life Cycle

- Process Flow Diagrams (PFD's)
- Mass & Energy Balance Validation
- Process Design Criteria (PDC)
- Trade-Off / Tabletop Study

FEASIBILITY STUDY

- Equipment Size & Cost Analysis
- Process Control Blueprint
- Alternative Analysis
- HAZOP Validation

ENGINEERING DESIGN

COMMISSIONING

- Troubleshooting
- Process Control Validation
- Nameplate Capacity Validation

PLANT OPERATION

- **DIGITAL TWIN**
- Analytics and Decision Support
- Production/Reagent Accounting
- Energy and Carbon Emission Management
- Improvement and Optimization

PLANT MAINTENANCE

- Asset Utilisation & Planning
- Predictive Maintenance
- Prioritisation of Work Orders

PLANT EXPANSION

- Cost-Benefit Analysis
- EIS/EA Support

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What is a Thermodynamic Calculation Engine (TCE)?

- Highly specialized third-party software used to perform complex equilibrium chemistry calculations
- Provides information on phase equilibrium, solution properties (pH, density, enthalpy, osmotic pressure, etc.)
- In SysCAD, TCE capabilities range from low temperature aqueous systems to molten metals, eutectics, slags, and gas mixtures
- Currently supported:
  - ChemApp
  - OLI
  - AQSol
  - PHREEQC

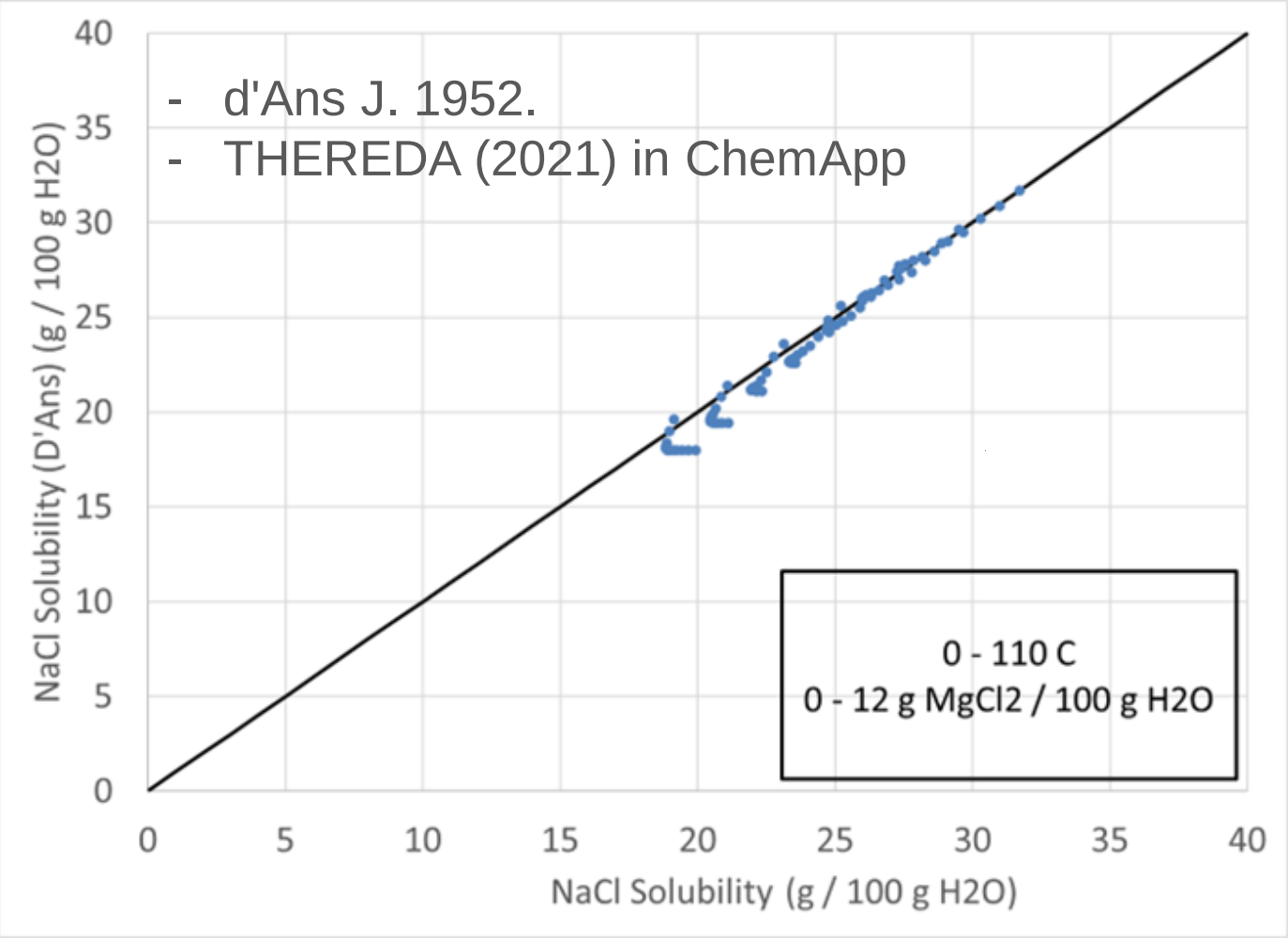
SysCAD Implementation of Thermodynamic Engines

- The approach taken allows maximum flexibility for the user
- Detailed thermodynamics can be applied *as needed*, while traditional SysCAD mass and energy balances can be used elsewhere
- Multiple Thermodynamic Engines can each use multiple chemistry models on a single flowsheet
- SysCAD has implemented parallel processing (multithreading) for all engines, enhancing solution speed for large projects
- Many user-friendly features are available to maximize utilization of these powerful chemistry analysis tools

THEREDA Database in ChemApp

- Contains aqueous speciation and phase solubility data
- Pitzer model parameters for many ion interactions
- Cations: Al^{+3}, Am^{+3}, Ca^{+2}, Cm^{+3}, Cs^{+}, K^{+}, Mg^{+2}, Na^{+}, Nd^{+3}, Np^{+4}, Pb^{+2}, Pu^{+4}, Si^{+4}, Sr^{+}, Tc^{+4} , Tc^{+7}, Th^{+4}, UO_2^{+2}, U^{+4}, Se^{+6}, Se^{+4}
- Anions: CO_3^{-2}, OH^{-}, PO_4^{-3}, SO_4^{-2}, Cl^{-}
- Suitable for use in sulphate of potash and muriate of potash applications, among others

Muriate of Potash Validation



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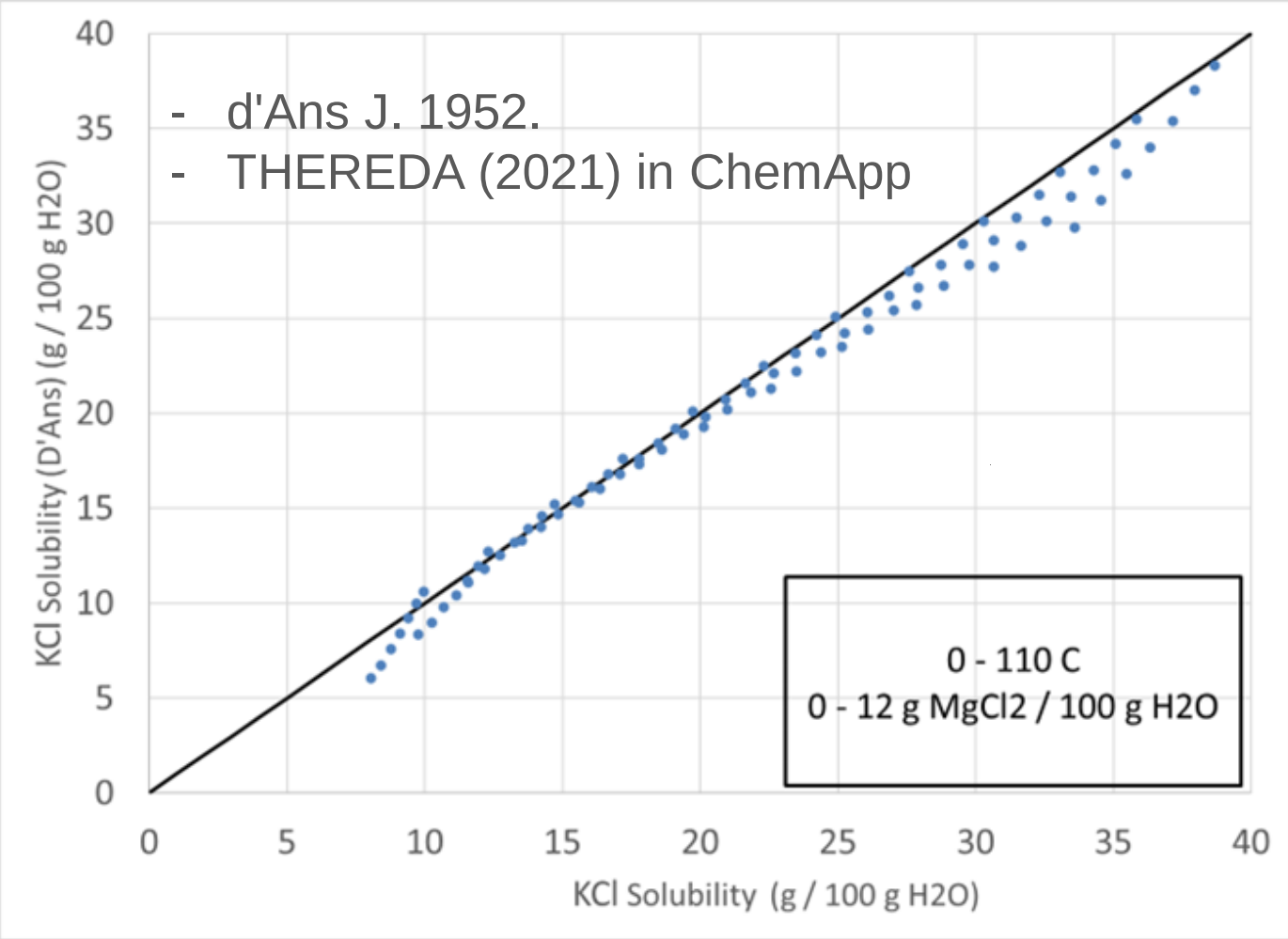
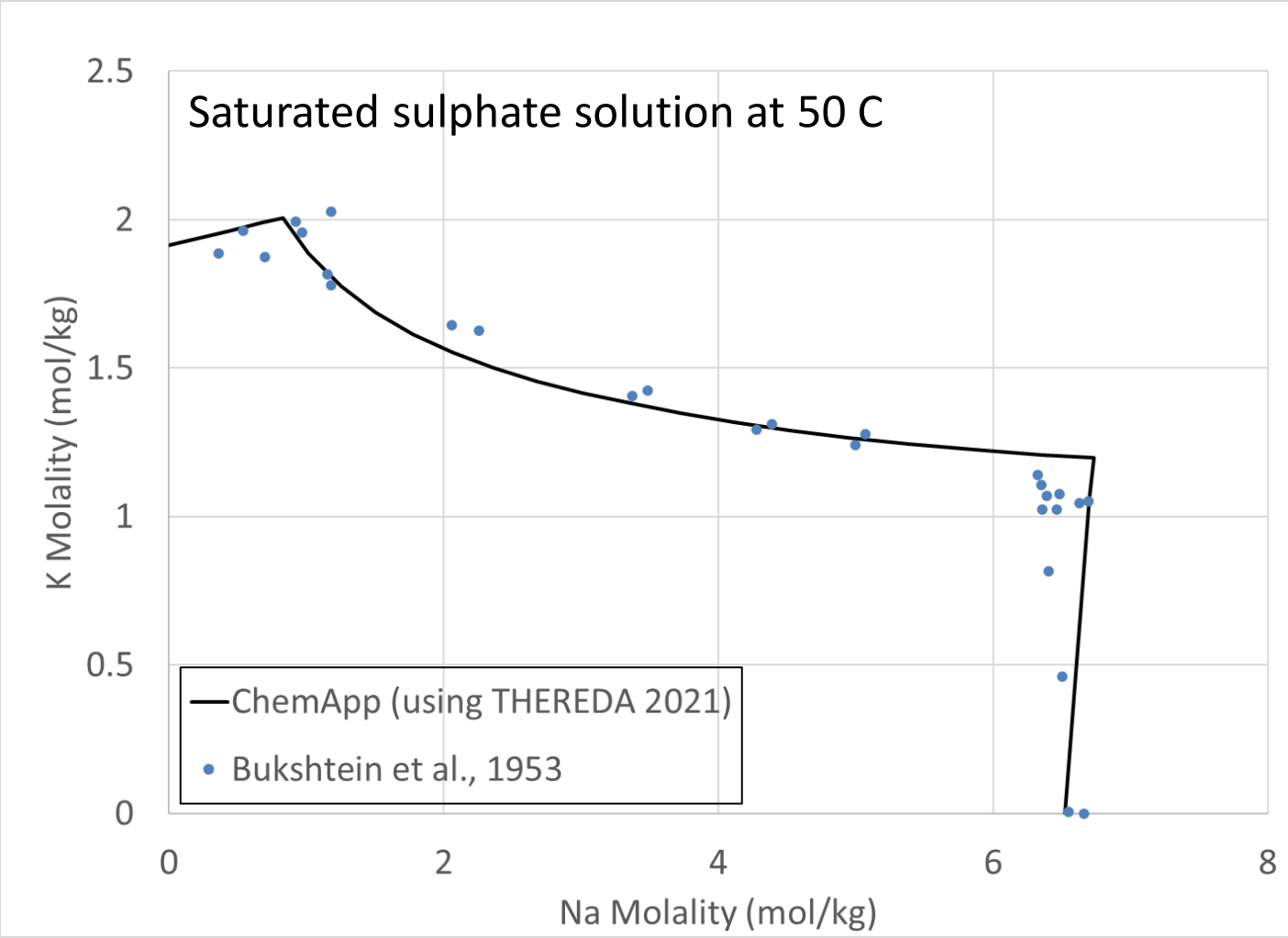
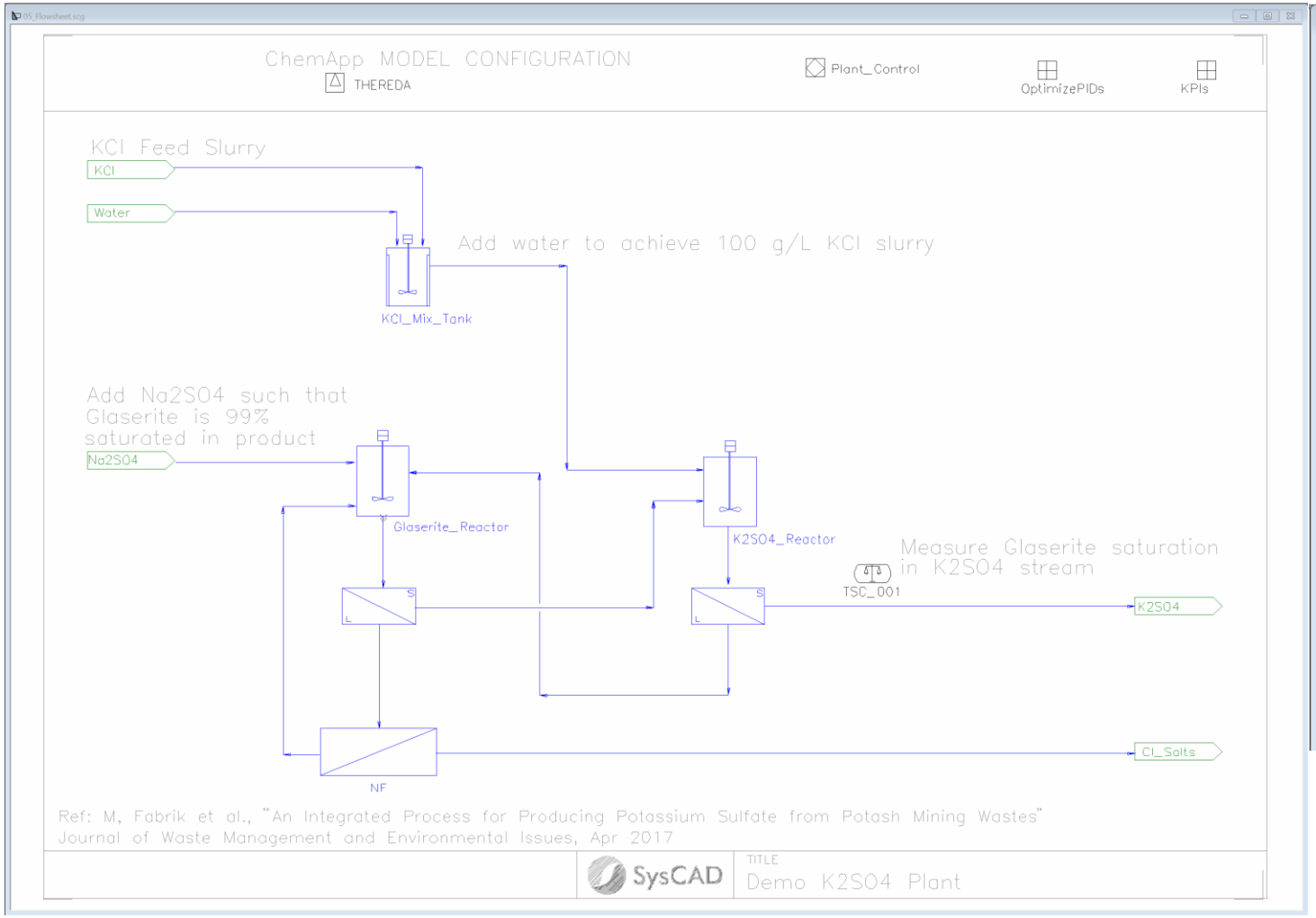
Muriate of Potash Validation

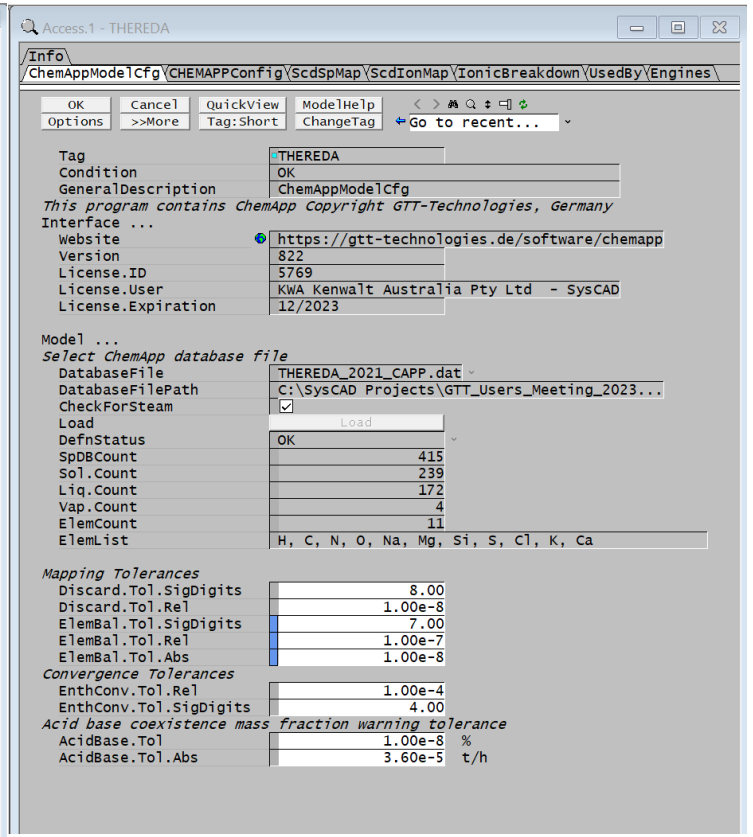


Sulphate of Potash Validation



Application to Sulphate of Potash





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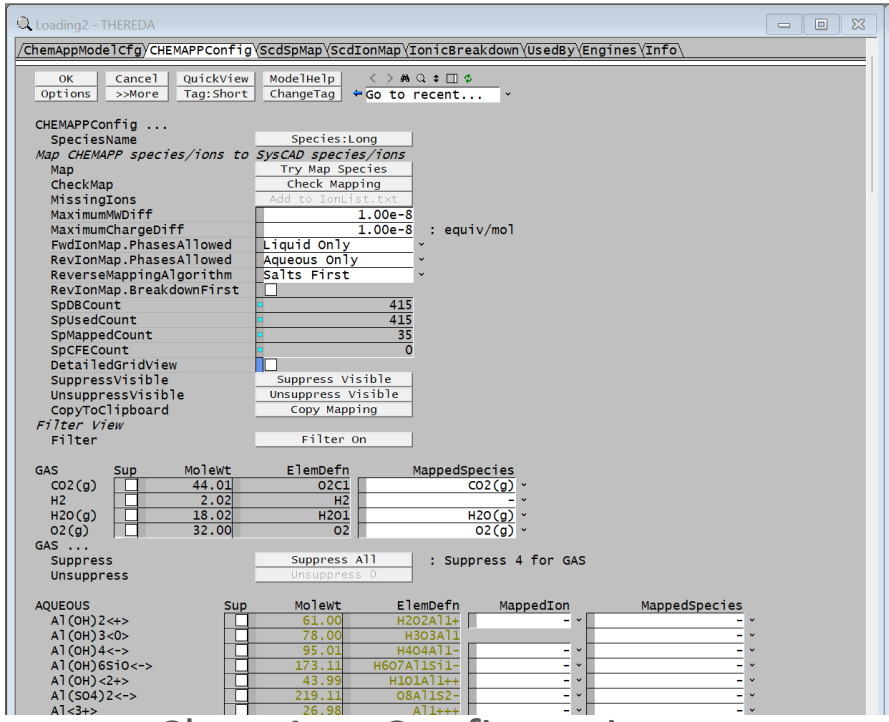
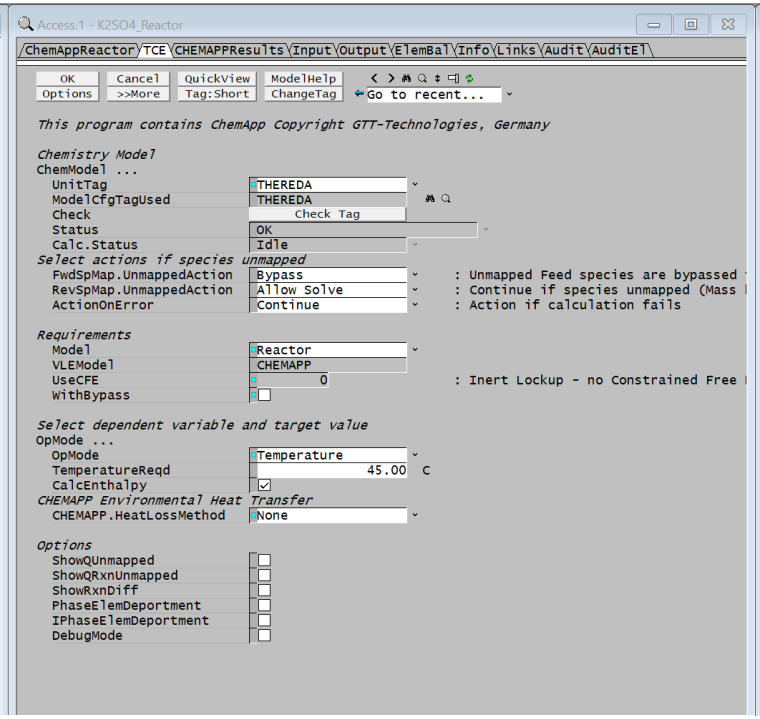
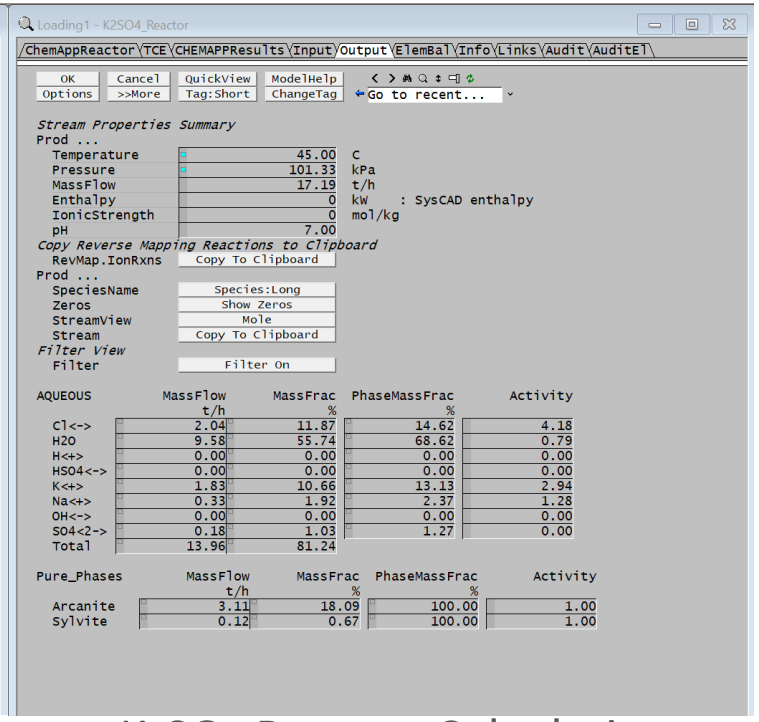
Application to Sulphate of Potash



ChemApp Configuration



K_2SO_4 Reactor



K_2SO_4 Reactor Calculation

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Heat Balance

- Stream enthalpy is calculated from hybrid approach:
  - Phase equilibrium calculated by THEREDA in ChemApp at T, P
  - Std. State enthalpy and heat capacity for each constituent is defined in the SysCAD database
  - Mapping algorithms correlate ChemApp species to SysCAD species
- Hybrid approach enables detailed heat balance simulations for full plant models with ChemApp (and THEREDA)
- Thermochemistry data can be inputted from many sources

Example Operating Conditions

Slurry feed rate (t/h)	7.9
Feed slurry KCl concentration (%)	50
Mixed slurry KCl concentration (g/L)	100
NF sulphate loss	5%
NF chloride removal	95%
SL separation slurry mass fraction	50%
Operating temperature (C)	25

Simulation Results

	Base Case	Operating T = 35 C	Operating T = 45 C
Production rate (t/y)	30,200	29,400	27,250
Na2SO4 consumption (dry basis) (t/y)	26,400	25,300	23,500
Recovery (%)	98.0	96.0	90.5
KCl Utilization (%)	74.6	72.5	67.2

Conclusions

- THEREDA with ChemApp in SysCAD allows calculation of complex brine chemistries
- Excellent tool for computing equilibrium compositions as part of mass balance
- Thermochemical data can be integrated in SysCAD for heat balance

Conclusions, cont.

- High accuracy phase equilibrium for Muriate and Sulphate of Potash brines can be computed
- Incorporates Pitzer's equations making it applicable to high ionic strength solutions
- Significant data for solution impurities in brine systems

Acknowledgements

- THEREDA Database development team
- GTT Technologies

Thank you!

Questions?

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