BatchColumn use of CAPE-OPEN thermodynamics

CAPE-OPEN thermodynamics in dynamic simulations

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ProSim

Software & Services In Process Simulation

Summary

- Introduction
- Model description
- Presentation of the BatchColumn example
- Results comparison between property packages
- Conclusions
- Improvements

Introduction

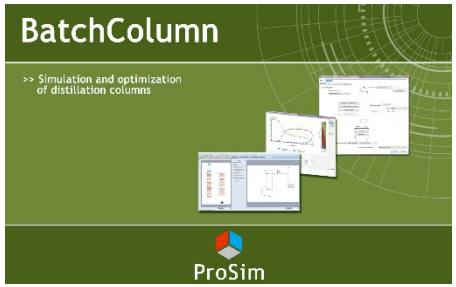
- Distillation columns operating in batch
  - Complex operation to model
    - Dynamic nature of the operation
    - Discontinuities
    - Stiffness
- Mathematical model
  - System of Ordinary Differential Equations + Algebraic equations
  - Intensive use of thermodynamic (enthalpy, density, …) and phase equilibria properties (K-values)
- Simulation success
  - Strongly linked to a good representation of the thermodynamic and phase equilibria properties and their derivatives with respect to the temperature, pressure and number of moles.

Introduction

- Software involved:

BatchColumn

- ProSim software dedicated to the modeling and the simulation of batch distillation columns.
- Thermo server: Simulis Thermodynamics
  - Proprietary (native) interface
  - CAPE-OPEN specifications 1.0 and 1.1
  - Thermodynamic “Socket”

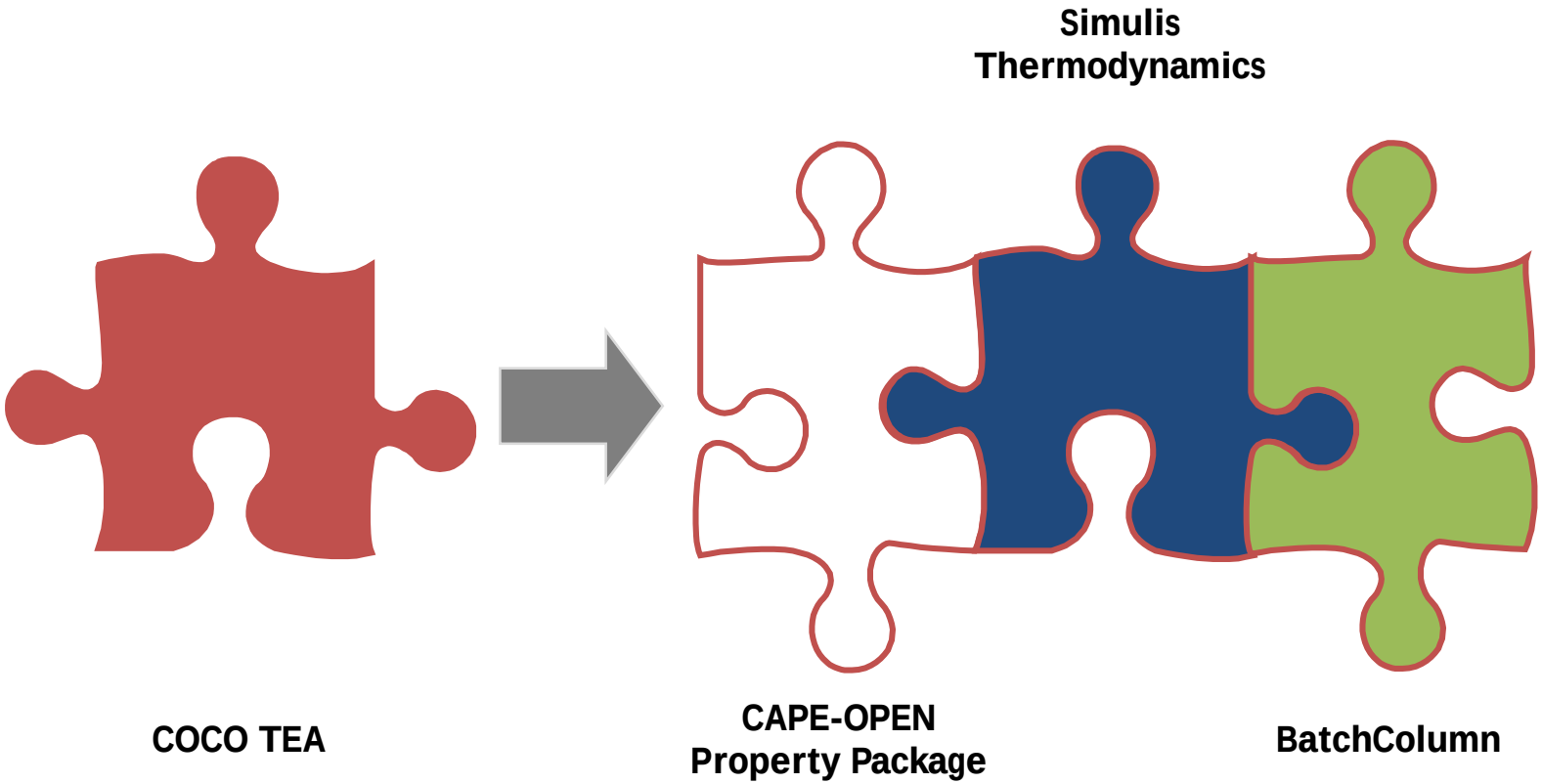


COCO-TEA

- AmsterChem thermo server
  - CAPE-OPEN specifications 1.0 and 1.1
  - Thermodynamic “Plug“

Introduction

- Thermodynamic Plug/Socket :

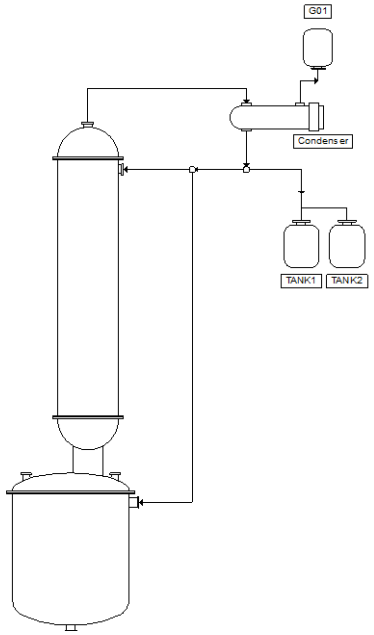


Model description

- BatchColumn model
  - Theoretical stage approach
  - Writing of mass and energy balances on each stage
    - Overall material balance,
    - Partial material balance,
    - Energy balance,
    - Thermodynamic equilibria,
    - Enthalpy model,
    - Holdup model,
    - Pressure drop model
  - Main properties required:
    - Enthalpies (L, V)
    - K-values
    - Density
  - Mix of differential and algebraic equations solved by a modified version of LSODI solver from ODEPACK (rootfinding capability and tridiagonal block banded matrix algorithm).

BatchColumn example

- Water, Toluene, Acetonitrile and Methanol separation
  - Column with 30 theoretical stages (incl. boiler and condenser) and two collection tanks.
  - Liquid hold-up: 150 l at the condenser, 5 l on every stage
  - Operating pressure: 280 mbar (no pressure drop)
  - Reboiler duty: 300 kW
  - No feeds



BatchColumn example

- Water, Toluene, Acetonitrile and Methanol separation
  - Initial load:
    - Water 6.7 kg
    - Toluene 3611.9 kg
    - Acetonitrile 1931.1 kg
    - Methanol 10.0 kg
  - Thermodynamics:
    - Heterogeneous approach,
    - Liquid phase: NRTL activity coefficient model,
    - Vapor phase: Ideal gas,
    - Property packages tested:
      - Simulis
      - COCO-TEA (CAPE-OPEN interfaces 1.0 and 1.1)

BatchColumn example

- Water, Toluene, Acetonitrile and Methanol separation

  - Objectives:
    - Recover of the maximum quantity of the binary Toluene – Acetonitrile at the azeotropic composition.
    - Maximum of pure Toluene

  - Constraints:
    - Toluene – Acetonitrile cut: Methanol content < 0.1% wt.
      Toluene content < 25% wt.
    - Pure Toluene cut: Toluene content > 99.5% wt.
    - Maximum time allowed: 10 h

BatchColumn example

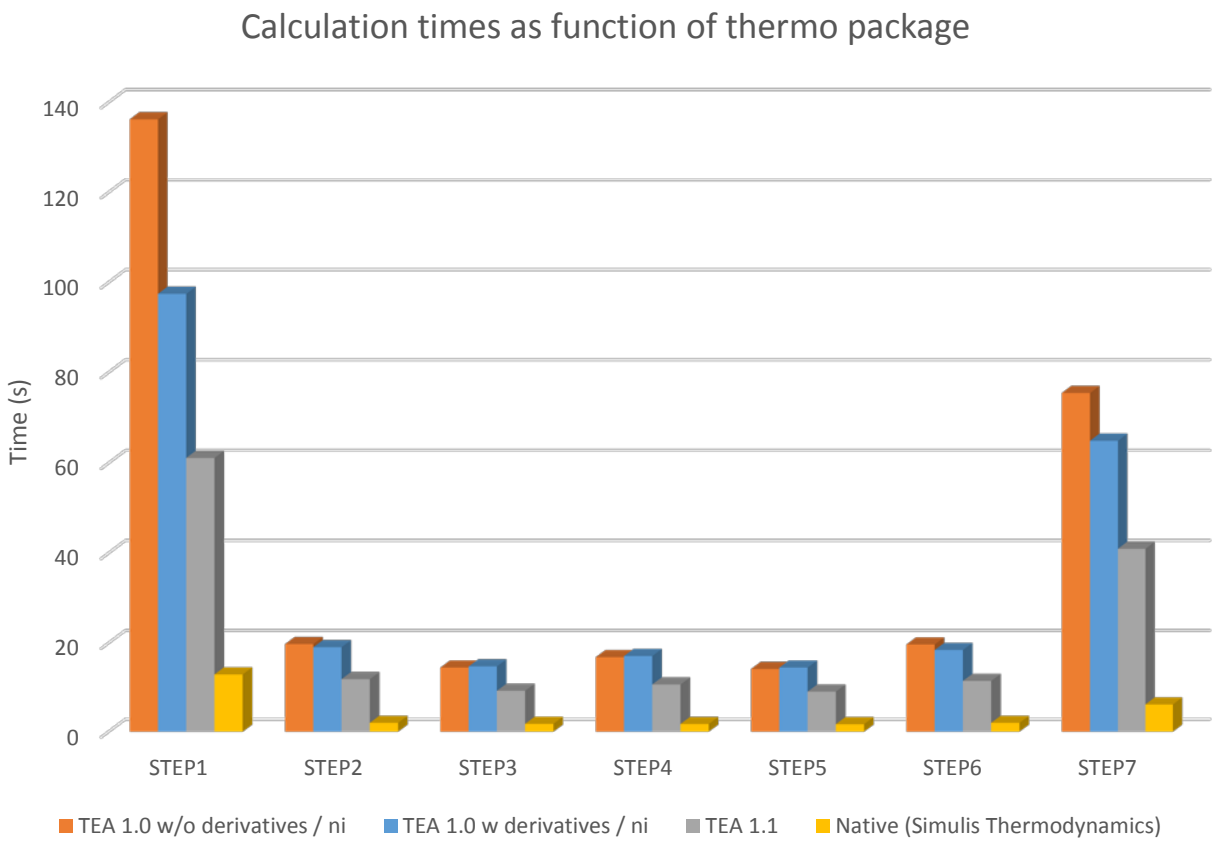
- Water, Toluene, Acetonitrile and Methanol separation
  - Operating mode
    - Step 1: Column filling from a cold state, initial temperature 25°C
    - Step 2: Total reflux during 1 h
    - Step 3: Distillation with reflux ratio = 0.001 until 100 kg is produced in collection tank 1
    - Step 4: Total reflux during 30'
    - Step 5: Distillation with reflux ratio = 0.001 until the distillate temperature reaches 42°C.
    - Step 6: Total reflux during 1 h
    - Step 7: Distillation in collection tank 2 with reflux ratio = 0.001 until the top temperature reaches 65°C.

BatchColumn example

- Calculations summary
  - CAPE-OPEN Property package 1.0
    - Without derivatives of the K-values / T
      - Failure of the simulation
    - Without derivatives of the K-values / ni (property package failed)
      - Success
    - With derivatives of the K-values / ni (numerical derivatives)
      - Success
  - CAPE-OPEN Property package 1.1
    - Success
  - Simulis (native)
    - Success

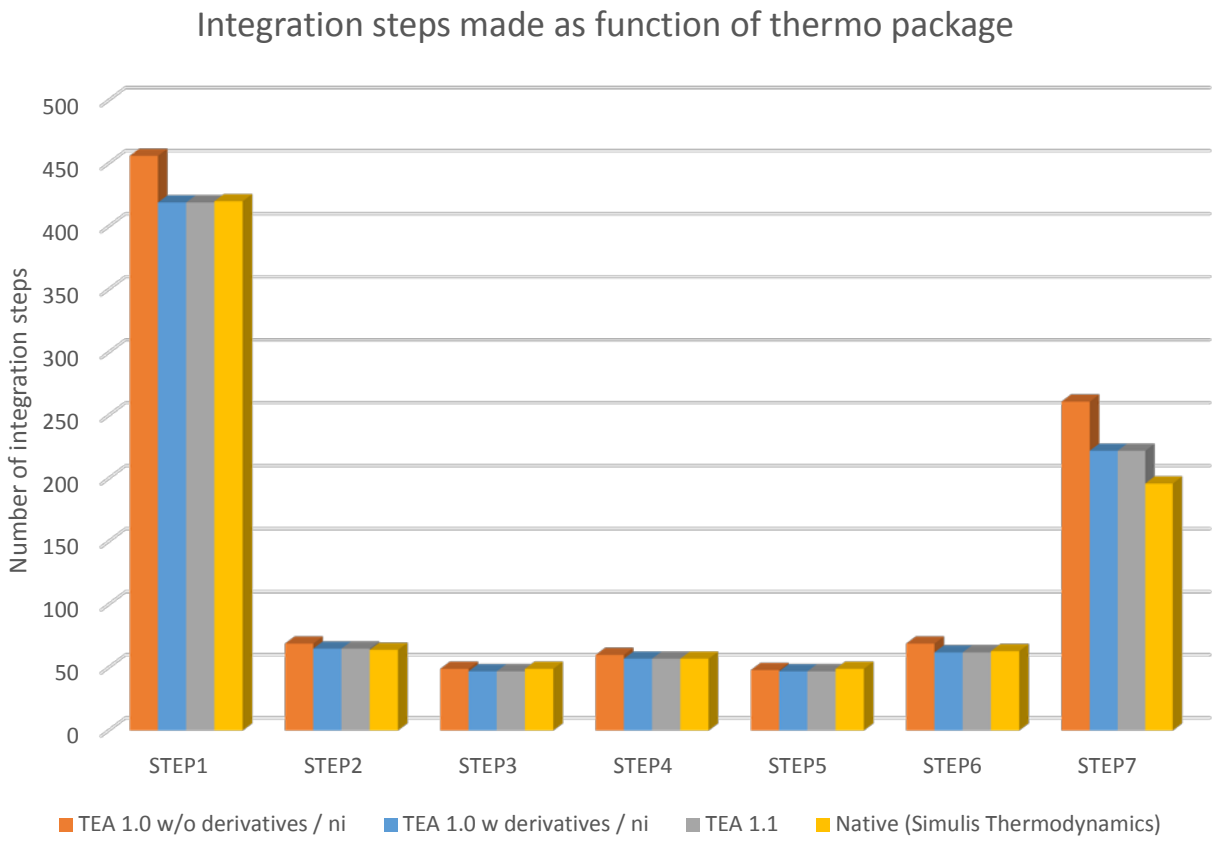
BatchColumn example

- Comparison between native and CAPE-OPEN thermo packages



BatchColumn example

- Comparison between native and CAPE-OPEN thermo packages



Conclusions

- The use of BatchColumn with a CAPE-OPEN property package provided by another supplier (COCO-TEA) has been demonstrated.
- The results show that the success of the simulation is strongly relying on the availability of the derivatives (and their accuracy) of the thermodynamic properties used in the simulation model.
- But, if not available in the property package used, the derivatives can be calculated numerically.
- Whatever the property package used, the results are consistent as long as the property package is correctly configured.

Improvements

- Added the possibility to compute the K-values from the fugacity coefficients when these properties are not provided by the property package (property and derivatives) (CAPE-OPEN socket only)

- Added the calculation of the derivatives of all the properties with respect to:
  - The number of moles
  - The temperature
  - The pressure

  When the property is not available or the calculation as raised an exception or systematically (CAPE-OPEN socket and native).

- Upcoming improvements:
  - Rewriting of the material object implementation to lower the use of units conversions and object creations.

Thank you for your attention…

ProSim

Software & Services In Process Simulation

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