ChemSep
Modeling Separation Processes

Cape Open Overhead in Distillation Modeling

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Harry Kooijman

Jasper van Baten

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Acknowledgements

Michael Gobler – Aspen Tech

CO Warning!

CAPE OPEN
will not succeed
because
run time will be too high

CObservation

- It is reported that 70-90% of simulation time is taken up by physical property calculations.
- CO property calls should have a major impact on run time.
- By how much?

  And does it matter?

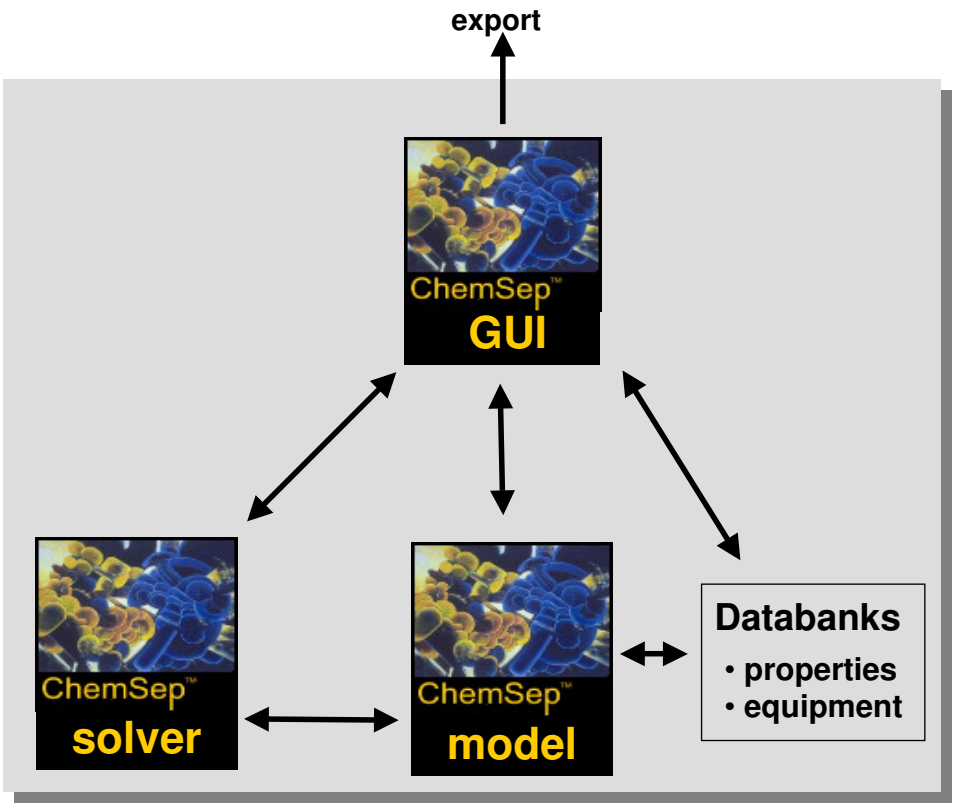
Measuring the Overhead of Cape-Open - Check with different:

- Process Model Environments (PME's)
  - Aspen-Plus
  - COFE (flowsheeter of COCO)
- Process Model Components (PMC's)
  - ChemSep Flash
  - ChemSep Column
- Process Model Libraries (PML's)
  - TEA (properties packager of COCO)
  - Aspen-Plus properties

… and compare with the native application!

- Just another distillation column simulator
- Widely used in academia
- Few commercial users

  (because it did not function with flowsheet simulators)



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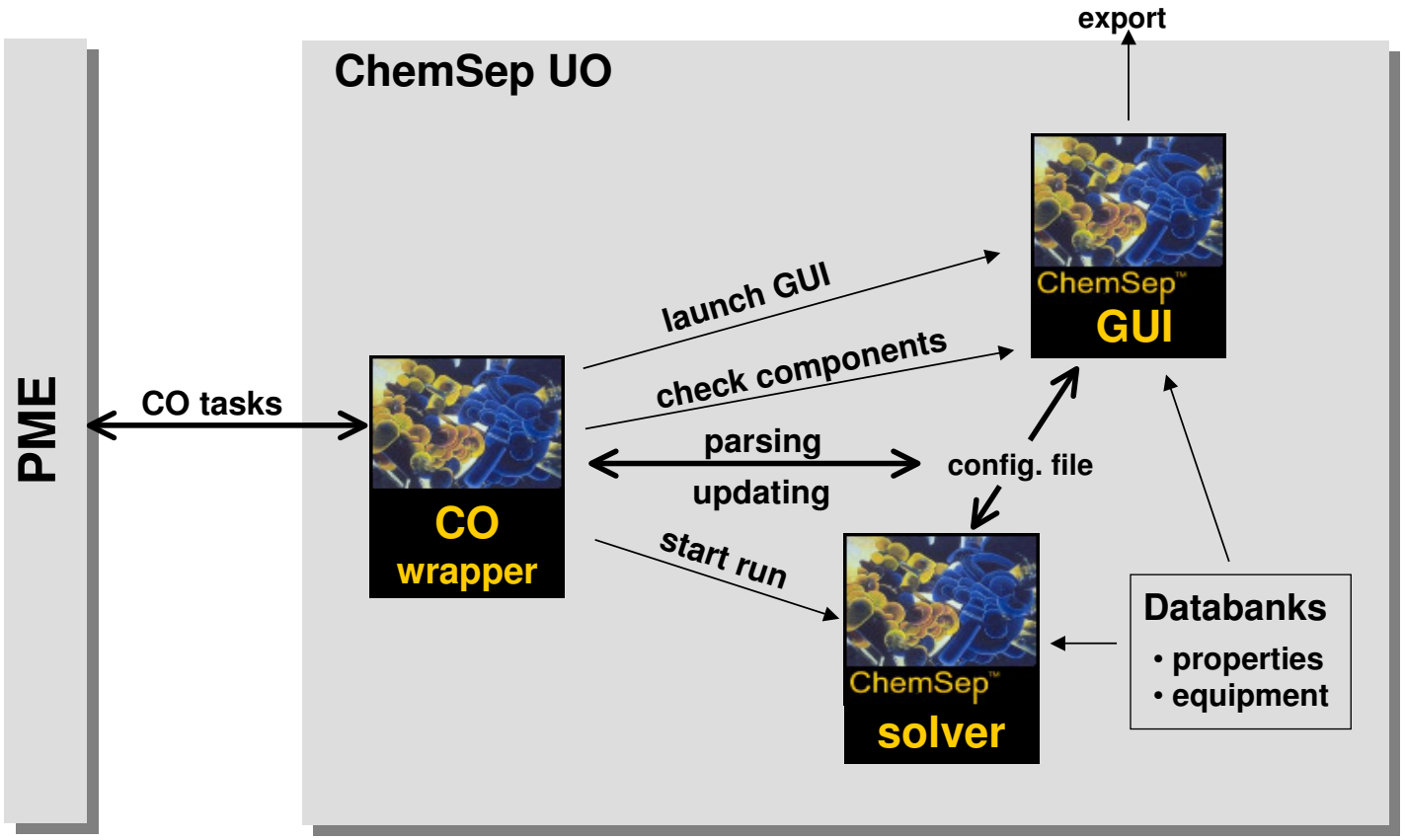
CO ChemSep: Phase I



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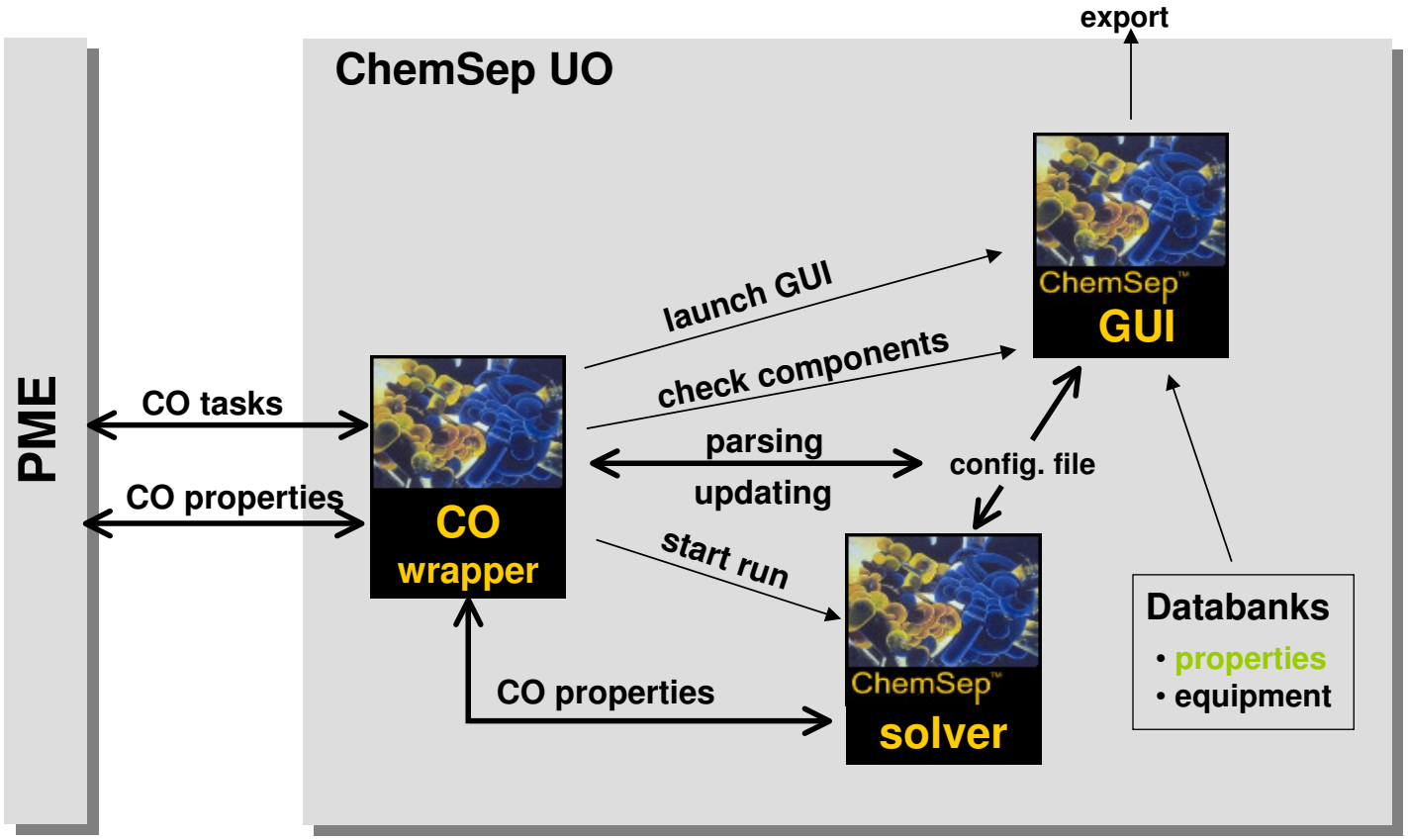
CO ChemSep: Phase II



ChemSep Now?

- More than just a distillation column simulator
- Functions with your favorite flowsheet simulator
  → as long as it is CAPE OPEN compliant
- Tested with:
  Aspen Plus
  HYSYS
  Pro/II
  COCO

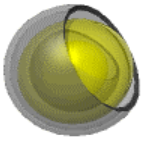
What is COCO?

CAPE-OPEN to CAPE-OPEN (COCO):

Simulation environment (COFE)

Thermodynamic property package (TEA)

Collection of unit operations (COUS)



Reaction package (CORN)

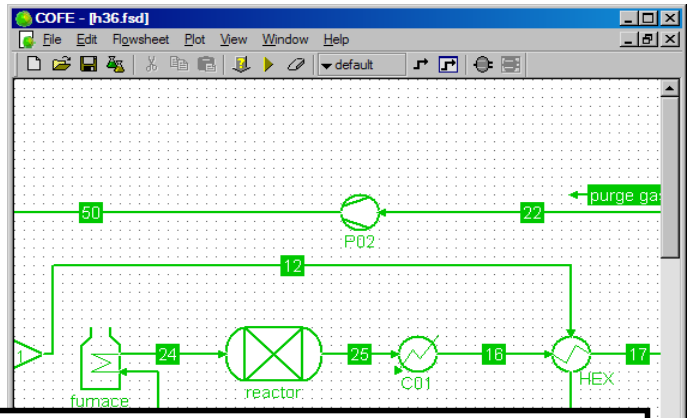
COFE: CAPE-OPEN Flowsheeting Environment

GUI:

- Graphical flowsheet editing
- Compact display of streams
- Quick access to CO objects
- Property graphing & printing
- Extensive help

Flowsheeting:

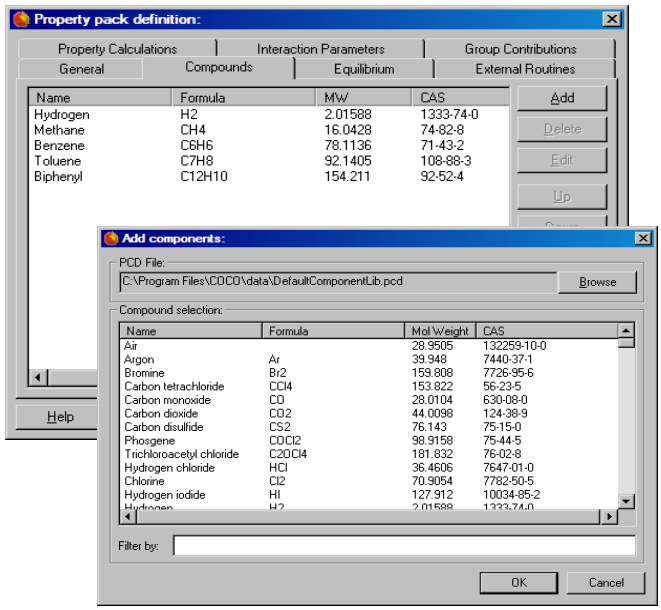
- Steady state
- Solution by tearing algorithm
- Multiple material templates



COCO Programming by
Jasper van Baten
Richard Baur
www.cocosimulator.org

TEA: Thermodynamics for Engineering Applications

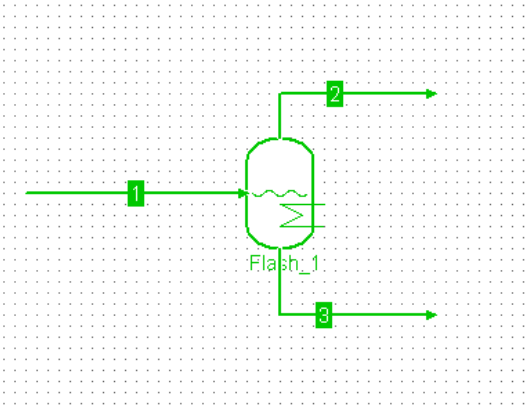
- Pure compound data library (extendible, or use DIPPR)
- 100+ Property calculation methods (> 25 different properties)
- Property derivatives
- Support of external property calculation routines (ICapeThermoCalculationRoutines)

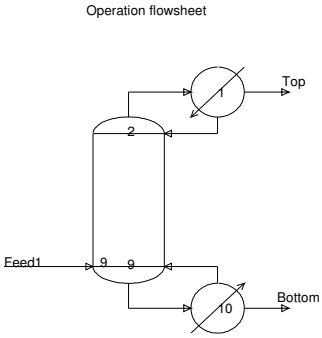


Thermodynamic models and compounds from ChemSep

Test Cases

- PME: COCO and Aspen Plus
- PMC: ChemSep PH Flash and Distillation Column
- Properties: PR EOS in ChemSep or TEA or Aspen Plus
- Feed: up to 200 components





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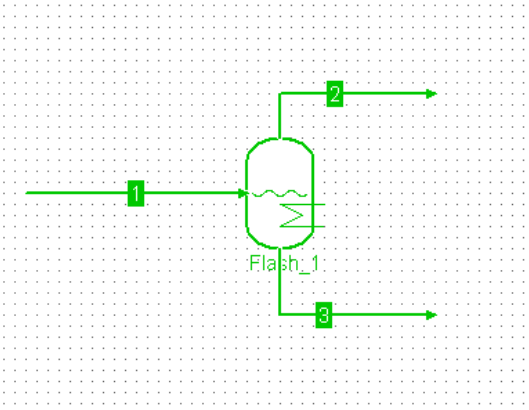
Test Case I

- COFE as PME versus ChemSep native
- PH Flash ChemSep as PMC
- TEA properties
- Crude oil feed
- 33 – 200 pseudo components



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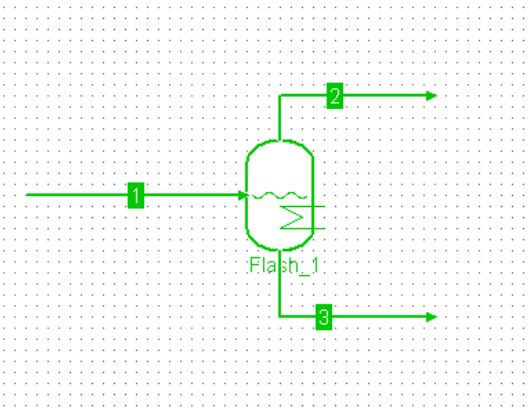

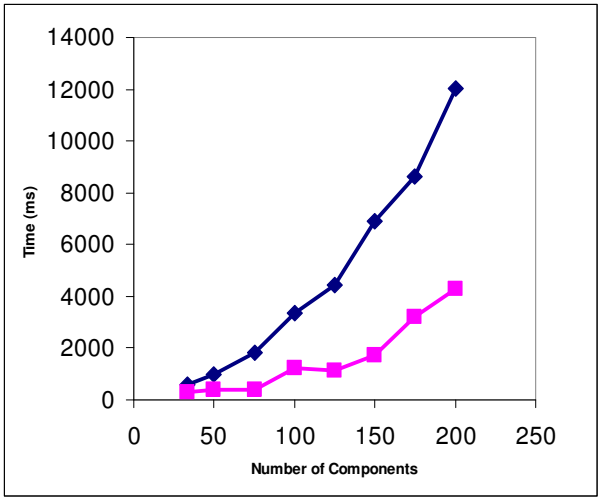

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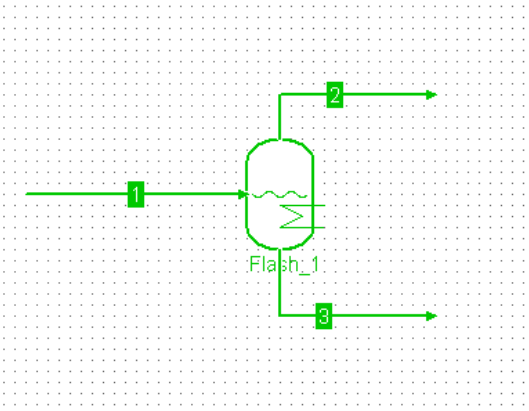

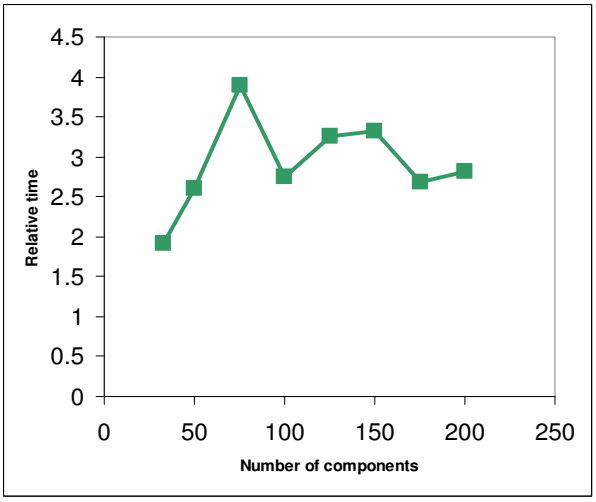

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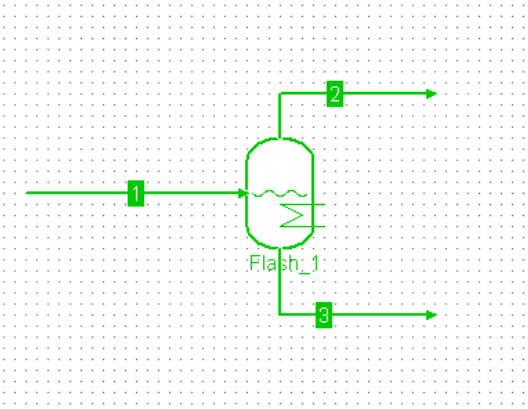
Test Case II

- Aspen Plus as PME versus ChemSep native
- PH Flash ChemSep as PMC
- Aspen Plus properties
- Crude oil feed
- 21 – 88 pseudo components



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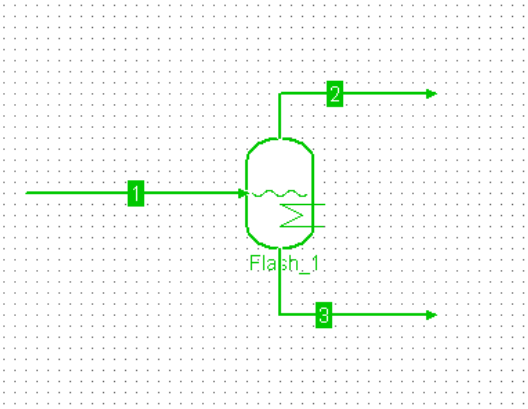

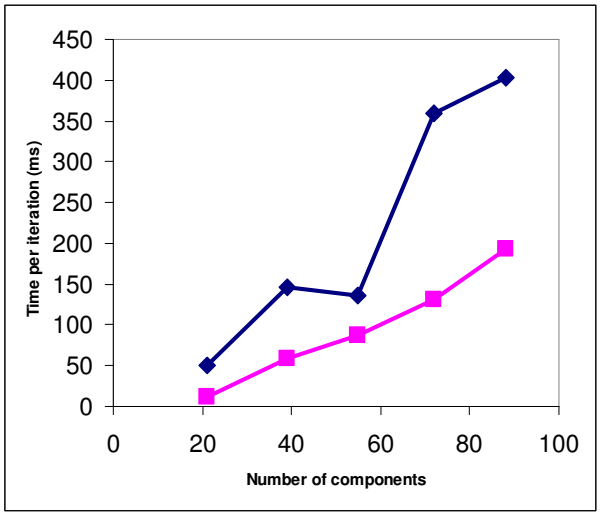

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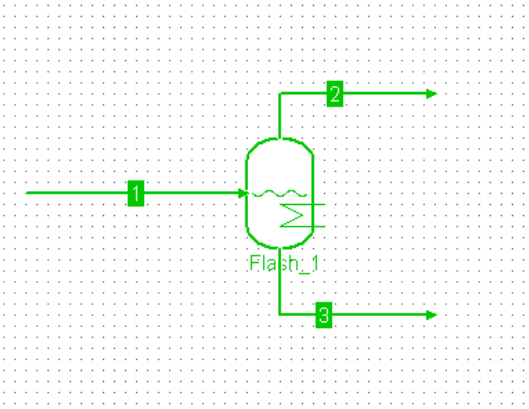

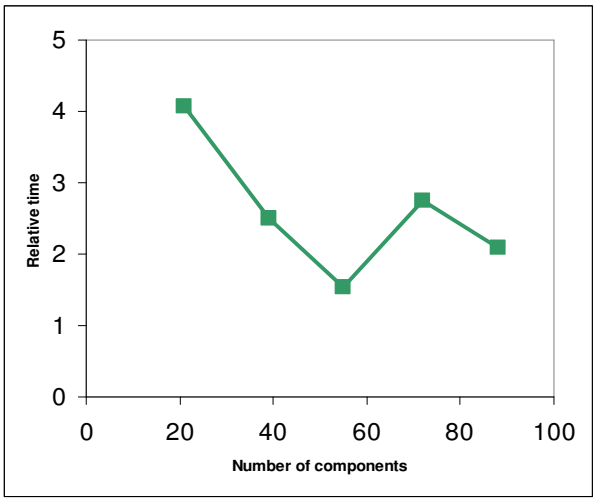

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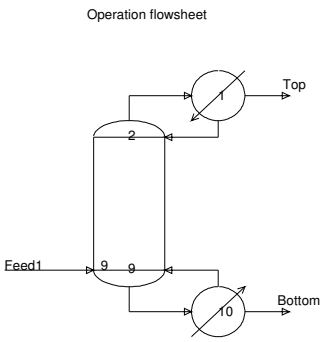
Test Case III

- COFE as PME
- ChemSep as PMC:
  10 stage distillation column
  RR = 1; B = 0.9F
- TEA properties
- Crude oil feed
- 33 – 125 pseudo components

versus

ChemSep native



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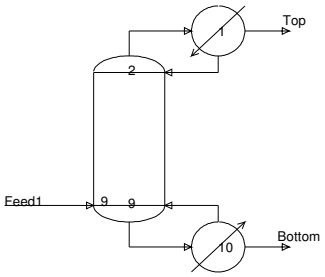
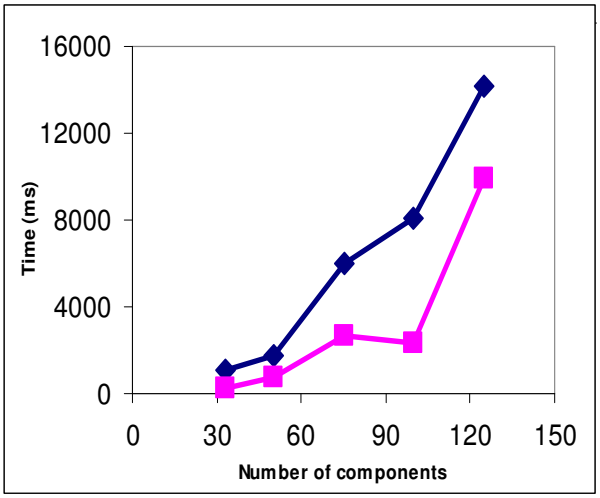
Operation flowsheet





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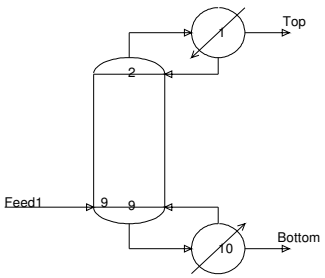

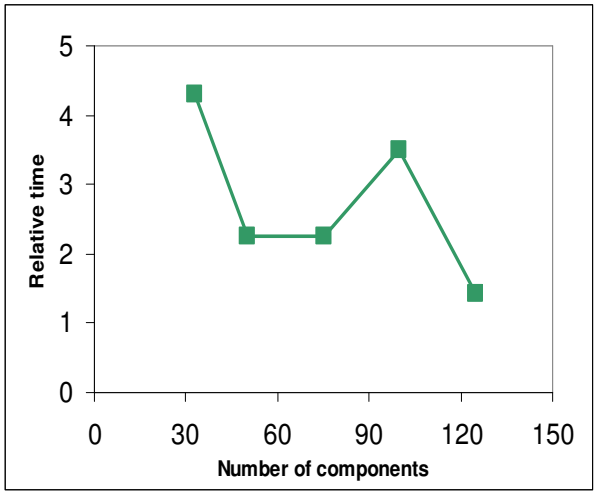

COnclusion

- CO property calls increase simulation run time by a factor of 1.5 to 4.5 in sample PH flash and distillation column calculations with many components

- Is this enough to matter?