SIMULATION SOLUTIONS for bioprocessing and batch industries

Development of CAPE-OPEN interface for integration of thermodynamic properties

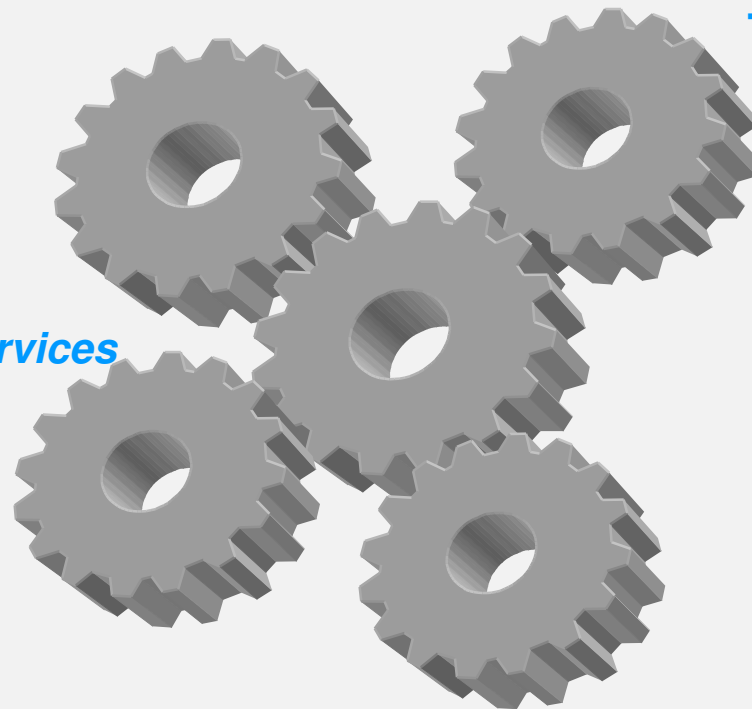## CAPE-OPEN annual meeting, Lyon

Motivation

CO interface implementation is part of a collaborative research project for development of a process simulation software for biotechnical and life science processes

Founding
- *BMBF*

Academic Partner
- *TU Dortmund*

Industrial Partner
- *Bayer Technology Services*
- *Bayer Health Care*
- *Planton*

Software Vendor
- *INOSIM*

Motivation

□ Simulation models require detailed process and material information for proper calculation

    □ Using existing calculation packages for material properties eliminates the effort to make own packages

    □ Pure component and mixture properties are available in existing commercial and in-house database

□ Conclusion: Connect simulation software, property calculation and property database by established and standardized interface

Requirements and Implementation

☐ Requirements
- ☐ User dialogs for CO-package selection
  - ■ Choose available property packages
  - ■ Mapping of internal and external components and phase identifiers for proper communication
- ☐ Access to CO-package within INOSIM Professionals VBA scripting environment
  - ■ Access to Component properties
    - ■ Constant, temperature and pressure dependant
  - ■ Access Material properties
    - ■ For one and two phases
- ☐ Support for CAPE-OPEN Version 1.0 and 1.1
  - ■ e.g. AspenTech still on Version 1.0
- ☐ …

☐ Implementation of Thermo socket in C++

Implementation: e.g. Phase mapping

Phases in INOSIM	Phases in CAPE-OPEN
1	
2	Liquid
3	Vapor
	Solid

- ☐ Mapping has to be unique

- ☐ INOSIM phases that don't exist in CO are supported
  Example: A phase is used to track the composition inside bacterial cells

- ☐ CO phases that don't exist in INOSIM are supported
  Example: CO defines a solid phase that is never used in INOSIM

- ☐ Users need to be aware that unmapped phases may result in inaccurate or invalid results

www.inosim.com

Implementation: e.g. Component Mapping

Components in INOSIM	Compounds in CAPE-OPEN
1	
2	A
3	B
4	B
	C

☐ Ambiguous mapping is allowed for INOSIM components
   Multiple INOSIM Components can be mapped to one CO Component

☐ CO components may be hidden from INOSIM

☐ Users need to be aware that unmapped components may result in inaccurate results

Implementation: e.g. VBA Access

☐ Created VBA objects for CO Access to:

☐ Component properties:

PropertyPackage.ComponentProperty(*component*, *property*, *options*)

PropertyPackage.ComponentPropertyT(*component*, *property*, *temperature*, *options*)

PropertyPackage.ComponentPropertyP(*component*, *property*, *pressure*, *options*)

PropertyPackage.ComponentStringProperty(*component*, *property*)

☐ Material properties:

PropertyPackage.MaterialPhaseProperty(*material*, *phase*, *property*, *options*)

PropertyPackage.MaterialTwoPhaseProperty(*material*, *phase1, phase2*, *property*, *options*)

☐ Equilibrium calculation:

PropertyPackage.CalcEquilibrium(*material*, *spec1, spec2*, *solutionType*)

Testing and Validation

☐ First interface testing during implementation executed with COCO's TEA

- ☐ Thanks for this free testing environment to all contributors (http://www.cocosimulator.org)

☐ Further testing with Aspen Properties

- ☐ There are still issues that need to be investigated

Summary

- ☐ Currently CO for thermodynamic properties mainly used in VBA programming module, but additional usage imaginable

- ☐ CO generates additional benefit in INOSIM by using calculated properties in the simulation and in user dialogs, e.g.:

  - ■ Molar mass, Heat capacity, density, …

- ☐ Application of CO Unit Operations has to be evaluated