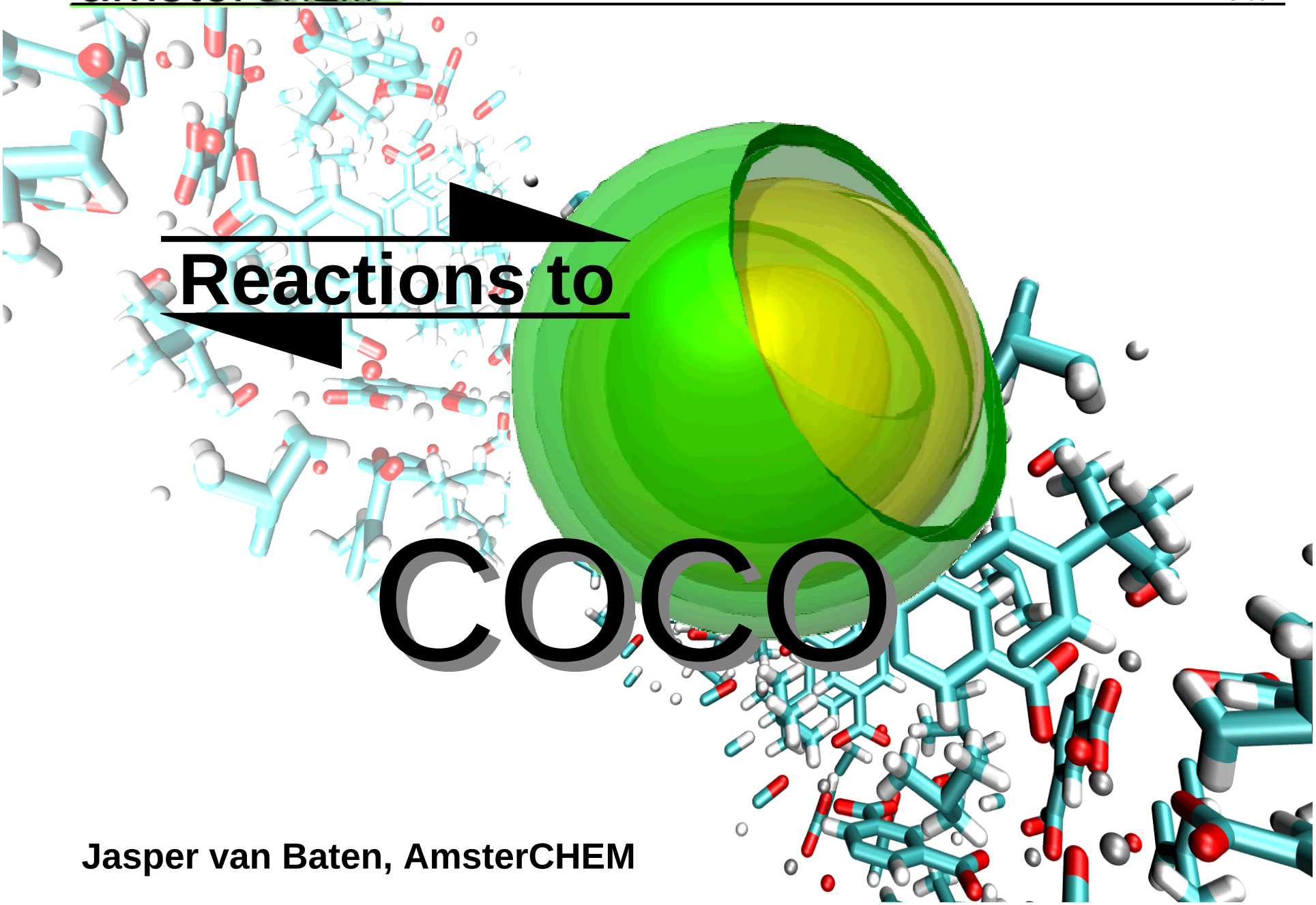


Reactions to COCO

Jasper van Baten, AmsterCHEM

Presentation outline

- Reaction packages in the CAPE-OPEN framework
- Compound identification
- Heat of reaction
- Issues with standard specification
- Reactors supplied by COCO
- Support by COSEs is required

CAPE-OPEN to CAPE-OPEN (COCO):

Simulation environment (COFE)

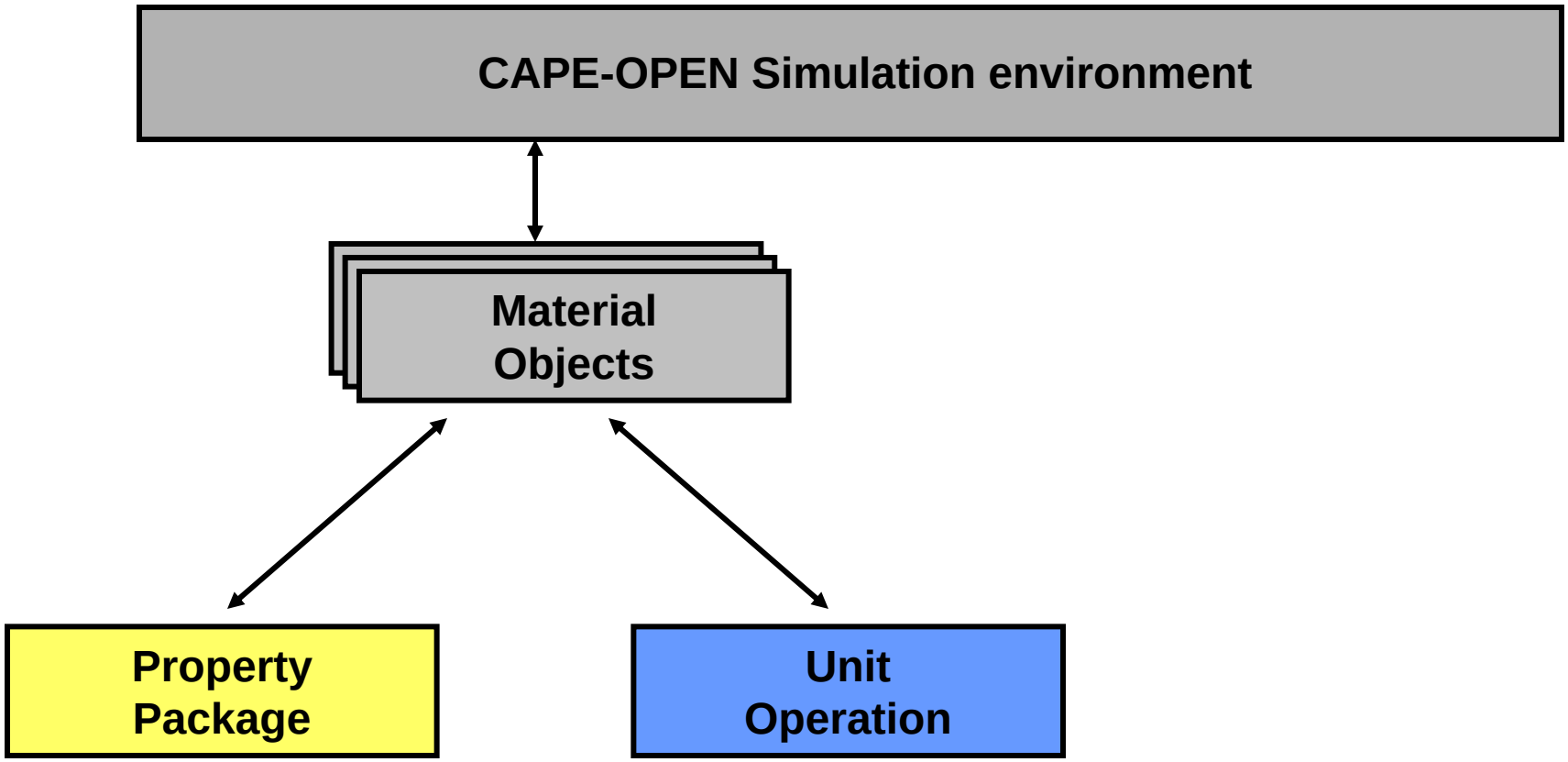
Thermodynamic property package (TEA)

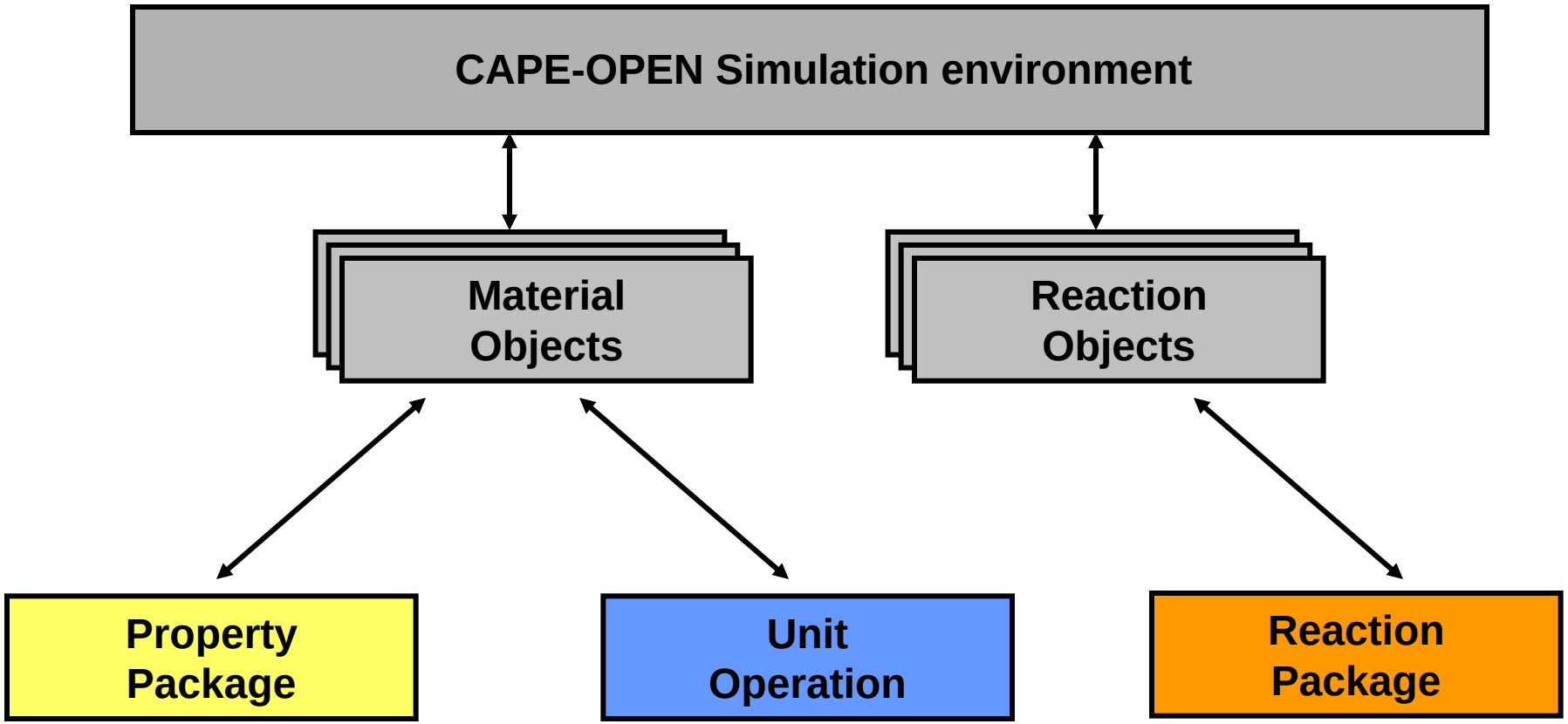
Collection of unit operations (COUSCOUS)

Reaction package (CORN)

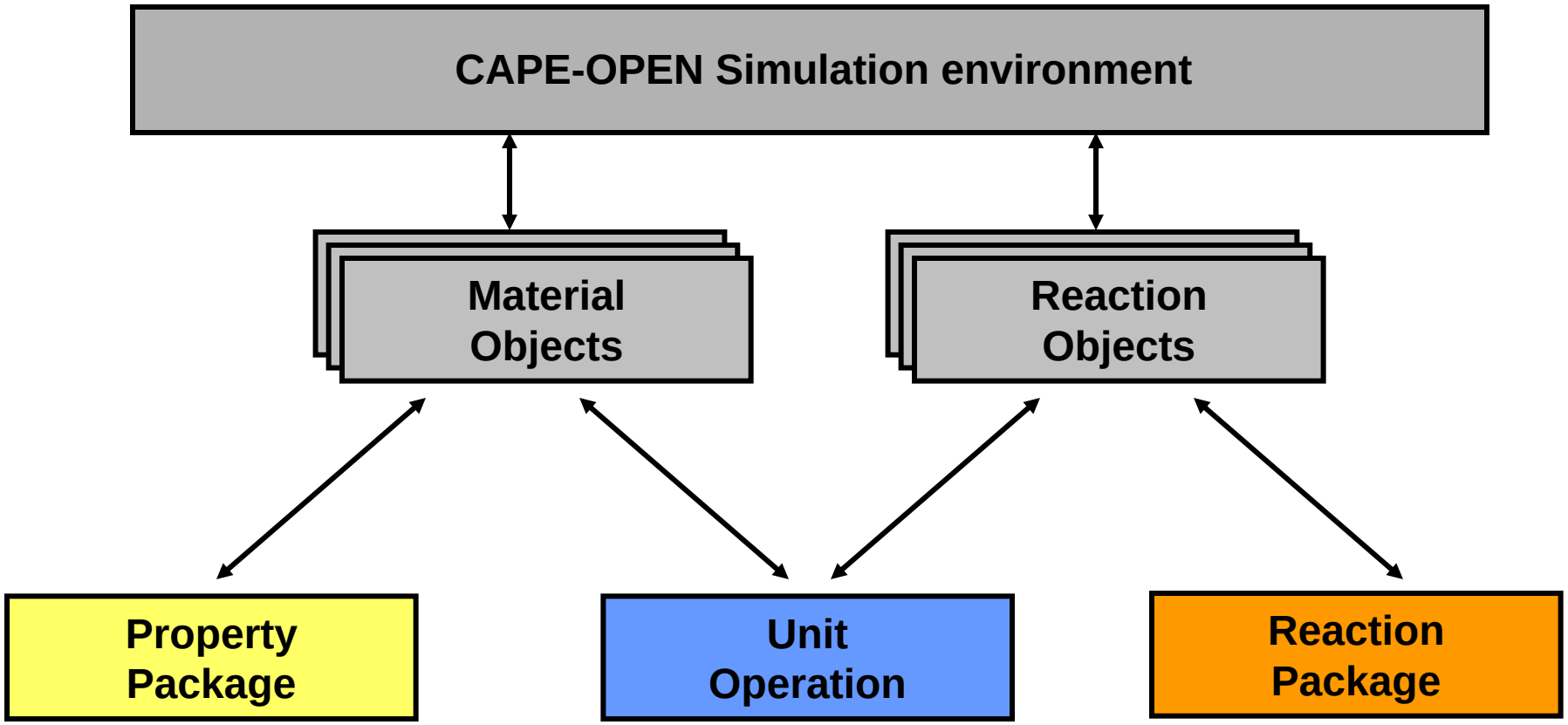
Reaction Packages contain:

- Reactions
- Reaction compounds
- Reaction stoichiometry
- Reaction type:
    - + kinetic or equilibrium
    - + homogeneous or heterogeneous
- Reaction phase
- Reaction rate / equilibrium constant
- Heat of reaction

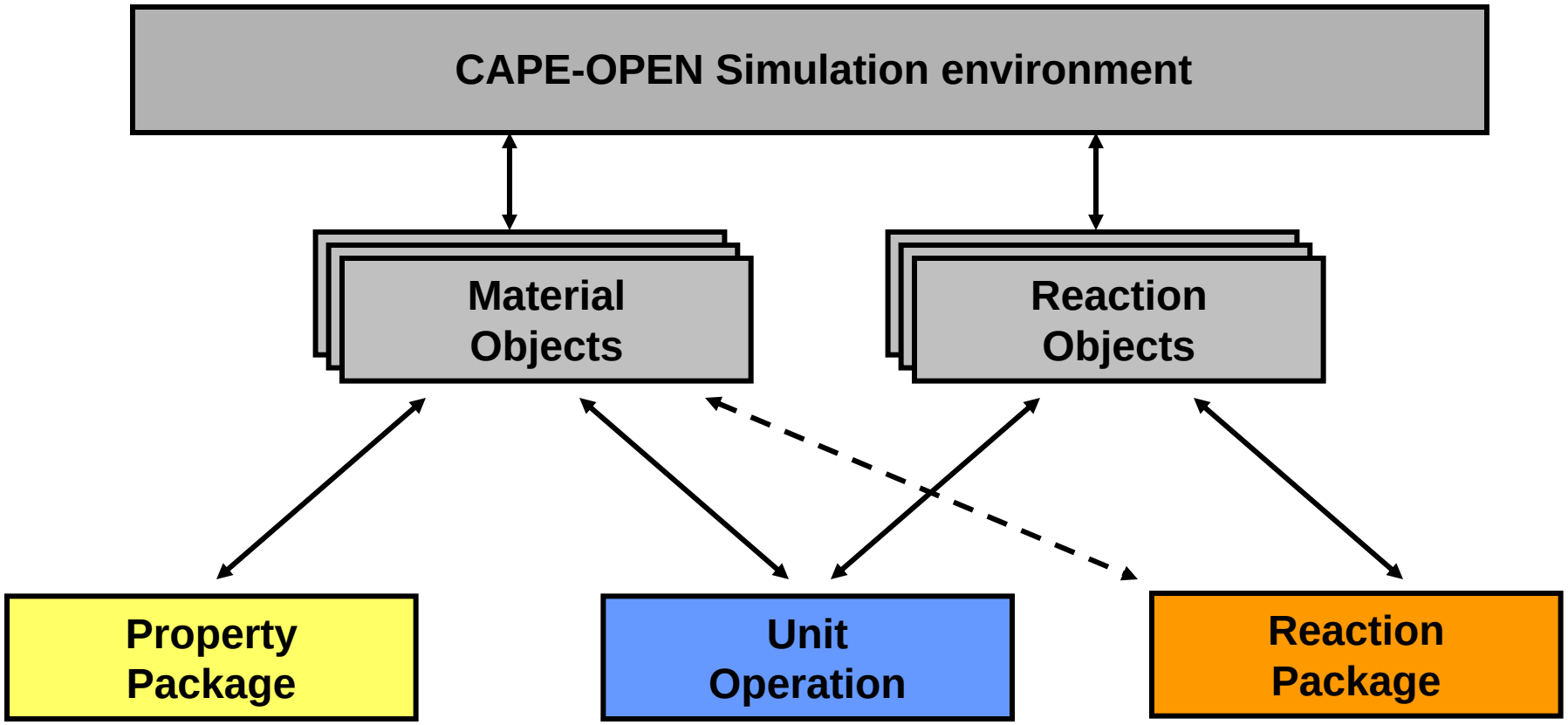

CAPE-OPEN Simulation environment
Material Objects
Property Package
Unit Operation



- Ability to load and maintain reaction packages
- Implementation of reaction object



- Assign reaction package to unit operation



- The unit operation must specify to the reaction package which material object to use

Potential pitfalls: Compound identification

- Property Package exposes: ID, CAS, MW, BP, formula, structure formula, IUPAC name, charge, …
- Reaction Package exposes ID, charge, CAS
- Reaction Package must match compounds
- Unit Operation must match compounds

Advice: Reaction package should adjust its IDs to match Material Object compound IDs

Potential pitfalls: Heat of reaction

- Heat of reaction relates to heat of formation:

$$-\Delta H_r = \sum_i \upsilon_i \left(-H_f^0\right)_i$$

- "Enthalpy" may or may not include heat of formation
- "EnthalpyF" is not widely available (yet), but is sure to include heat of formation
- Balance with EnthalpyF requires flash: e.g. "PHF"

Standard specification issues (I)

- Units of measure should be SI; kmol/h should be mol/s
- Undefined items should be removed or defined: GetBaseReactant, GetPhaseCompounds
- Derivatives are not available
- There is no Validate() method: validation at SetMaterial()
- Kinetic / Equilibrium reaction context: same
- Basis argument should be revised for some calls

Standard specification issues (II)

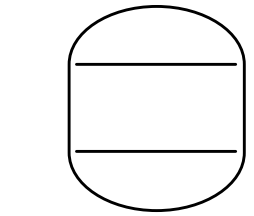
- GetReactionConcBasis:

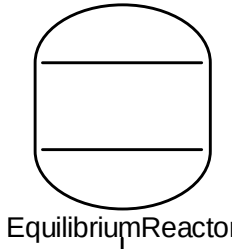
  + should apply to equilibrium – not kinetic – reactions

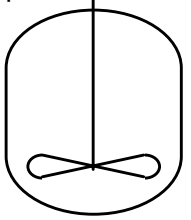
  + additional identifiers: “molarity”, “concentration”, “moleFraction”, “massFraction”

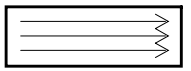
- Reaction specification document is from 2003

Reactors supplied by COUSCOUS:


FixedConversionReactor


EquilibriumReactor


CSTR


PFR

Fixed conversion reactor: specify conversion of reactions (parallel or series)

Equilibrium reactor: combined phase and reaction equilibrium calculation

Continuously stirred tank reactor: mix of equilibrium and kinetic reactions, well mixed

Plug flow reactor: kinetic reactions, one dimensional model

Why use a Reaction Package:

- Uniform way of specification of reactions
- Reusable throughout the document in multiple reactors
- Reusable throughout multiple documents
- Reusable in various simulation environments (…)
- No duplication of data

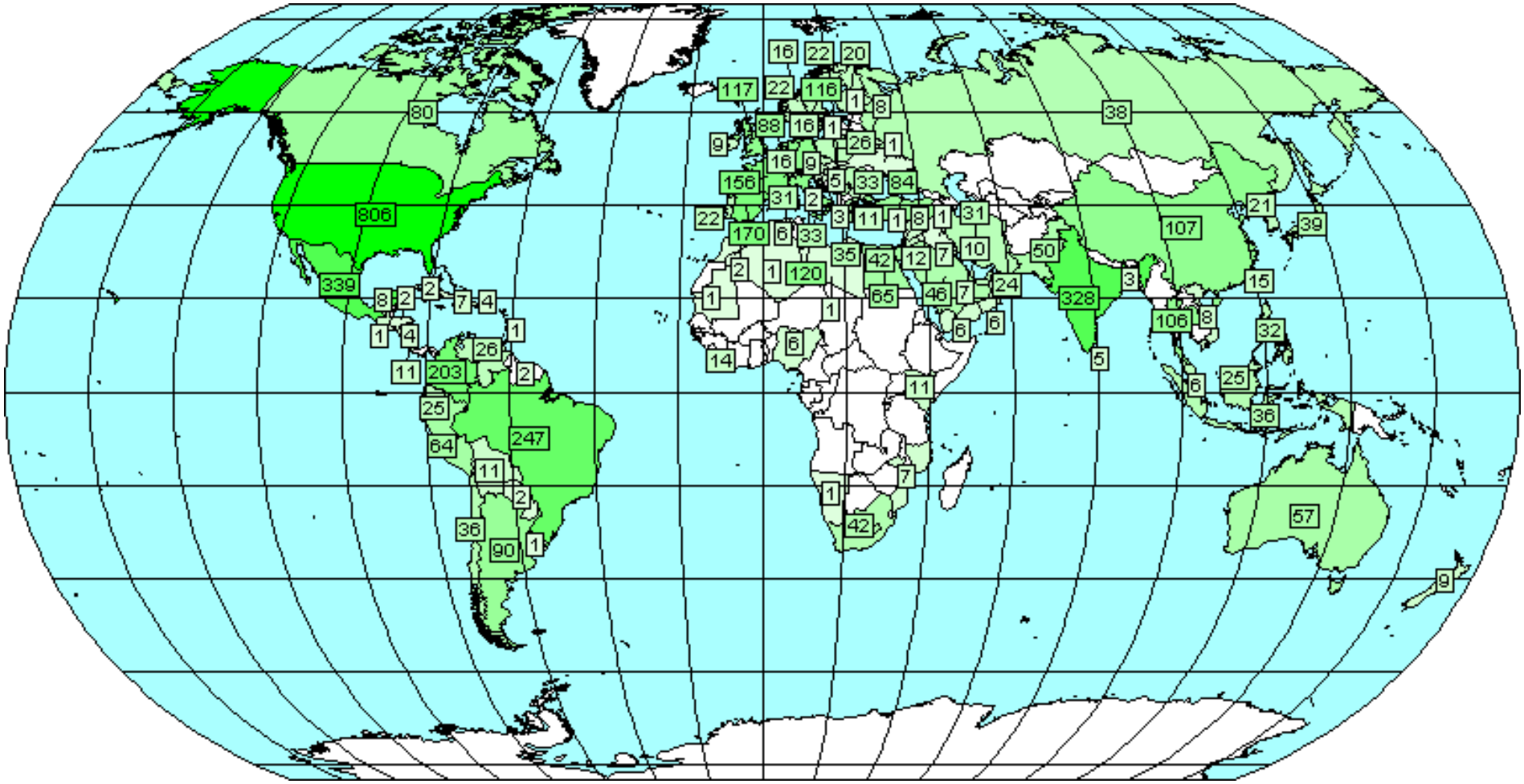
Implement!

- This is an important interface
- None of the major software vendors currently support it
- Support is required at COSE level
- There is a reference implementation

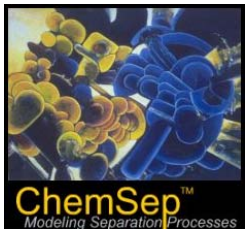
- Download COCO: http://www.cocosimulator.org/
  (or ask for a copy during the workshop)
- Contact amster**CHEM** for CAPE-OPEN consulting
- Interoperability testing program:
  http://www.cocosimulator.org/index_compliancy.html

Acknowledgements:

- Richard Baur
- ChemSep: Ross Taylor, Harry Kooijman
- Cosmo*THERM*: Frank Eckert
- Michel Pons

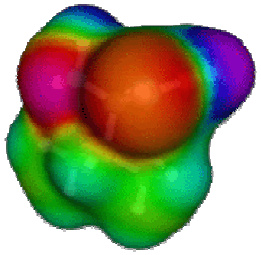


COCO downloads



ChemSep:
ChemSep 6.10

ProSim:
ProSimPlus 2.1
Simulis Thermo 1.2

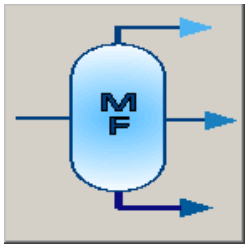


CosmoLogic:
CosmoTherm C21

Simsci-Esscor:
Pro/II 8.1.3

HTRI:
Xchanger Suite 5.0

SolidSim:
SolidSim 1.1



Infochem:
Multiflash 3.7

TUV-NEL:
PPDS v4.1.0.0

PSE:
gPROMS 3.0.3

VMG:
VMG Thermo 5.0