CAPE-OPEN & Global CAPE-OPEN

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Agenda

- CAPE OPEN description
- CAPE OPEN opportunities
- CAPE OPEN open access simulators
  - COCO
  - DWSIM

CAPE-OPEN: where everything started ..

- Cape Open project
  - Partially funded by EU Brite-EURAM programme
  - Consortium structure
    - 7 operating companies
    - 4 process software companies
    - 3 universities
- Global Cape Open project
  - Undertaken under the international Intelligent Manufacturing Systems (IMS) programme
    - European Union (including Norway)
    - Japan
    - USA
    - Canada
  - Partially funded by the EU and the Japanese government

Consulting partner simsci

What is CAPE-OPEN

- **CAPE**:
  - Computer Applications in Production and Engineering (source: about.com)
  - Computer-Aided Process Engineering (source: CO-LaN leaflet)
- **OPEN**:
  - Freely available standard specification
- The CAPE-OPEN standard is the de facto **standard for interfacing** process modelling software components for use in the design and operation of chemical processes.
- It is based on recognized software technologies (**COM and CORBA)**
- The **CO standard** is open, multiplatform, uniform and free of charge.
- It is described in a **formal documentation set**
  - unit operations, physical properties and numerical solvers, (…).
- It enables components **supplied by third parties**,
  - physical property packages or unit operation models,
  - to be used in "plug and play" mode in commercial process modelling software tools.

(Note: implementations restricted to COM at Windows OS)

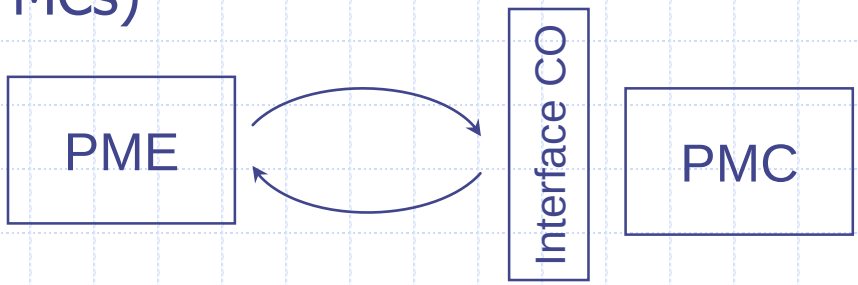
What is CAPE-OPEN today?

- CAPE-OPEN Laboratories Network http://www.colan.org/
  - 44 Software vendors
  - 24 Academic institutions
  - 2 Administrations
  - 7 Other members

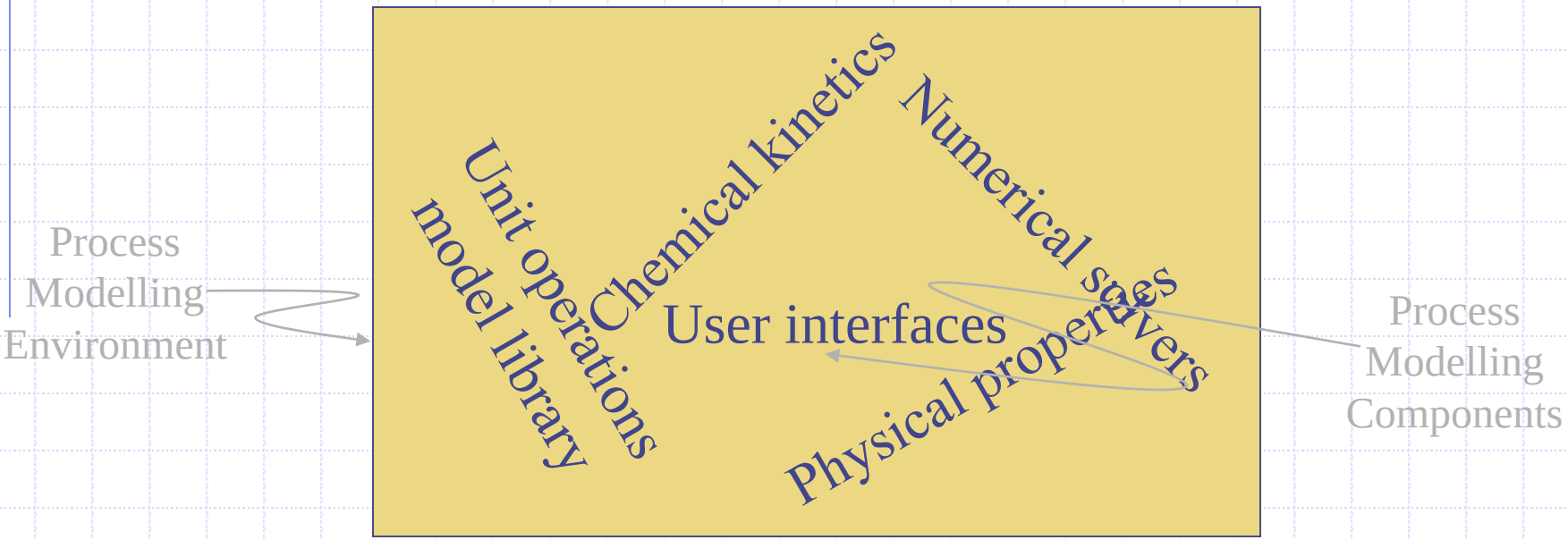
- Air Liquide
- BASF AG
- BP
- DOW Chemical Company
- IFP
- Shell Global Solutions
- TOTAL
- AKZO-Nobel

CAPE-OPEN vision

- Complete interoperability between
  - Process Modelling Environments
  - Process Modelling Components...
  - from diverse sources…
  - written in diverse computer languages…
  - implemented on diverse computer platforms...
- Process Modelling Components (PMCs)
  - well-defined pieces of software
  - wide range of applications
    - physical properties
    - unit operation modules
    - numerical solvers
- Process Modelling Environments (PMEs)
  - support construction of process model
    - from first-principles and/or library of unit operation models
  - support a number of model-based applications
    - simulation, optimisation, …
  - may make use of one or more PMCs

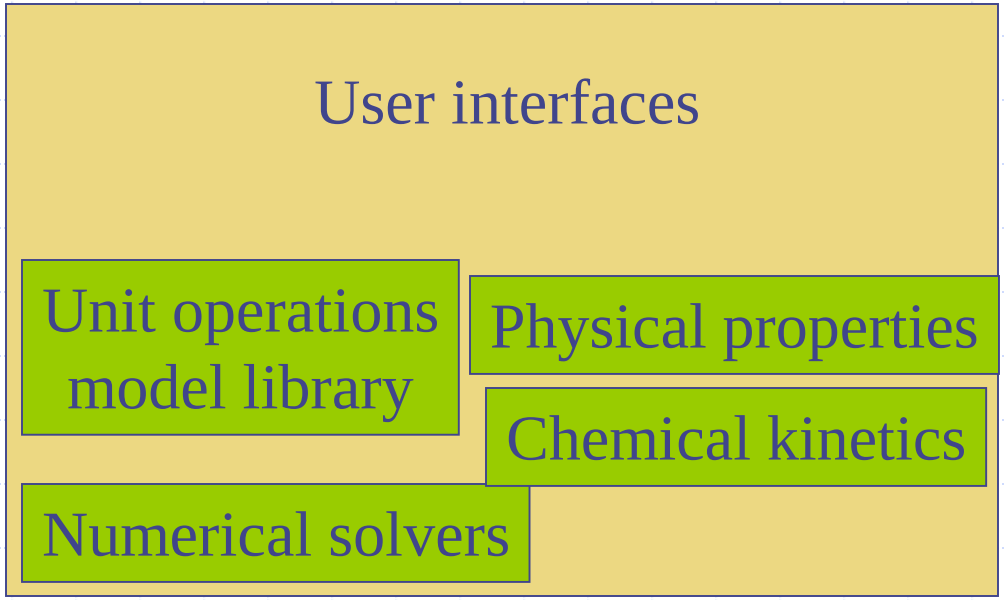


Where does one begin ?

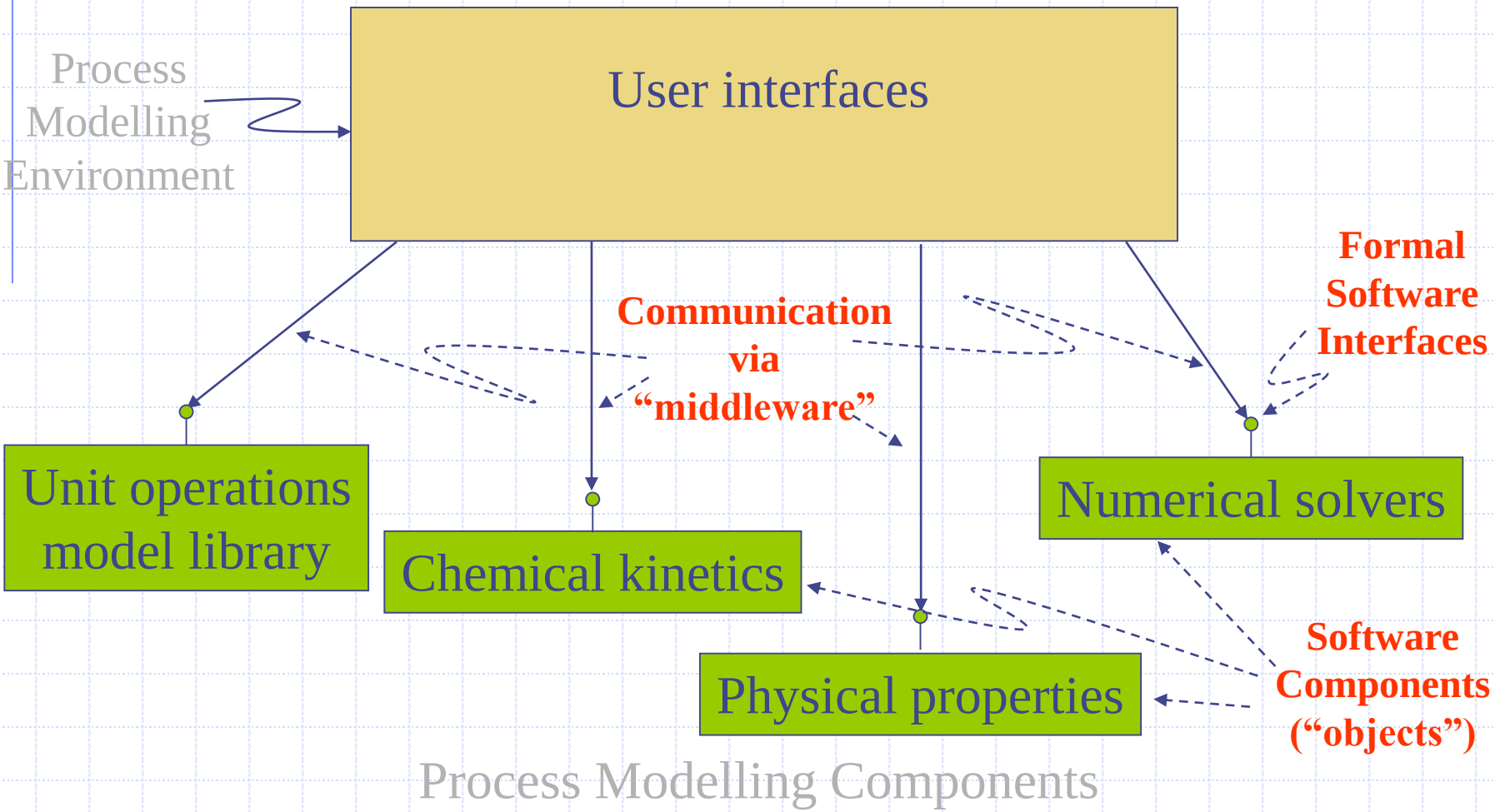


- Many interacting components…
- …all tightly coupled with each other
- Component boundaries not always clearly delineated

Clarify boundaries between key components…



...and break tool into one PME & multiple PMCs



CAPE-OPEN objectives & scope

OBJECTIVES

- To deliver the **power of component software** and open standard interfaces in computer-aided process engineering
- Identify **major classes of PMCs** and define general software interfaces for them
- **Develop & test prototype** software demonstrating PMC use & benefits
- **Promote** understanding, acceptance & adoption of open software architectures
  - industry
  - process engineering software companies
  - academic community

SCOPE

- Primarily focused on **process modeling** software tools
  - but technology has applicability to other areas (e.g. supply chain optimization)
- Both "**modular" and "equation-orientated**" process modeling tools
- **Focus on components** for
  - building the process model
    - unit operations models, physical properties, chemical kinetics
  - carrying out various activities with the process model
    - simulation, optimization, parameter estimation

CAPE Open has defined interfaces for…

- Physical property computations
  - conventional materials & electrolytes
- Physical property databanks
- Chemical kinetics computations
  - non-equilibrium & equilibrium reactions
- Numerical solvers
  - solution of systems of equations
    - linear algebraic, nonlinear algebraic, differential algebraic, partial differential-algebraic
  - solution of optimization problems
    - LP, NLP, MILP, MINLP
  - solution of parameter estimation
- Unit operation modules
  - primarily for modular steady-state modeling tools

Opportunities for ...

- **End-users** of process engineering software
- Niche software component **providers**
- **System integrators**
- **Suppliers** of Process Modeling Environments

Opportunities: end-users of process engineering software

- A wide variety of PMCs to choose from
  - use "best-of-class" components
  - not confined to whatever PME providers can supply
- Combine variety of tools to carry out complex tasks
  - e.g. use gPROMS to model a complex reactor…
  - …then insert reactor model into HYSYS within existing steady-state plant model
- Ensure consistency across tools
  - e.g. use same physical properties software for
    - steady-state simulation in ASPEN+
    - dynamic optimization in gPROMS
- BUT… support issues need to be addressed
  - who to call when things do not work ?

Opportunities: niche software component providers

- Develop CAPE-OPEN compliant PMCs
  - that can work seamlessly within any CAPE-OPEN compliant PME
- Maximise market size
  - e.g. the same physical properties PMC can be used by ASPEN+, HYSYS or gPROMS users
- Particular opportunities for developing countries with strong/emerging software industry
  - PMCs have relatively narrow function
    - usually simpler than PMEs
    - pricing more easily related to end-user benefit & competition
  - minimise required infrastructure
    - distribute over the WWW

Opportunities: system integrators

- Build new software by combining existing components
  - e.g. advanced plant automation environments
- Minimise amount of "bespoke" code that has to be developed
- Minimise time & effort required to bring new products to market

Opportunities: suppliers of Process Modelling Environments

- Similar benefits to system integrators
- A changing & confusing world
  - maintaining control of the central environments

    BUT…
  - losing monopoly of components used in these environments
- Several implications not yet fully worked out
  - competition ?
  - pricing ?
  - support ?

Results of CAPE-OPEN Standard

- **global acceptance** as a standard for communication between simulation software components in process engineering
- **availability of software components** offered by leading vendors, research institutes, and specialized suppliers which will enable the process industries
- open **new markets** for suppliers of CAPE components.
- **major breakthrough** as compared to the current state-of-the-art, which is that of no integration at all.

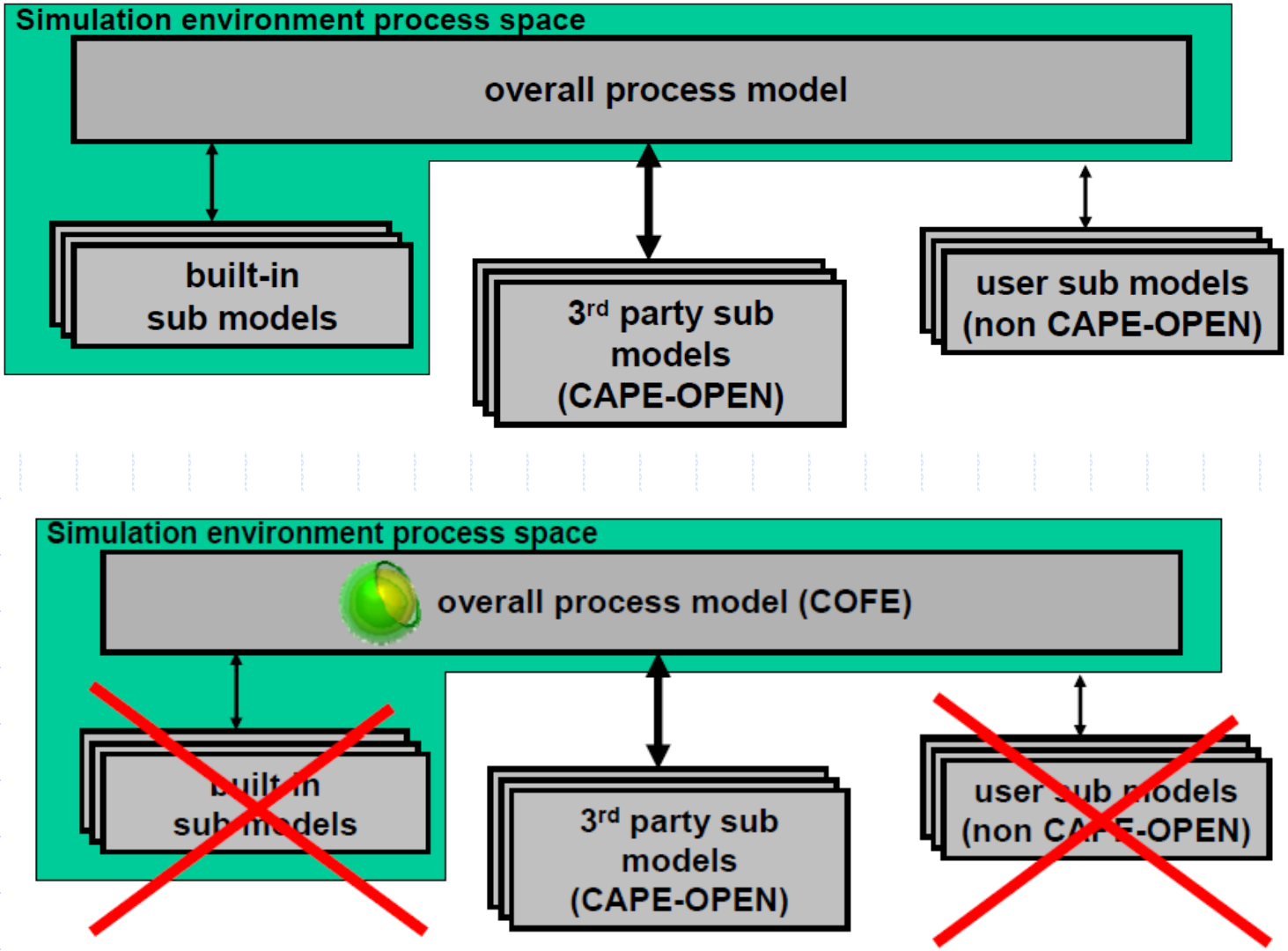
COCO-COFE a cape Open process simulator

What is COCO?

CAPE-OPEN to CAPE-OPEN is a free-of-charge CAPE-OPEN compliant steady-state simulation environment

- COFE: CAPE-OPEN Flow-sheeting Environment
- TEA: ThermoDynamics for Engeering Applications
- COUSCOUS: CAPE-OPEN Unit-operations (Simple)
- CORN: CAPE-OPEN Reaction Numerics

COCO-COFE a cape Open process simulator



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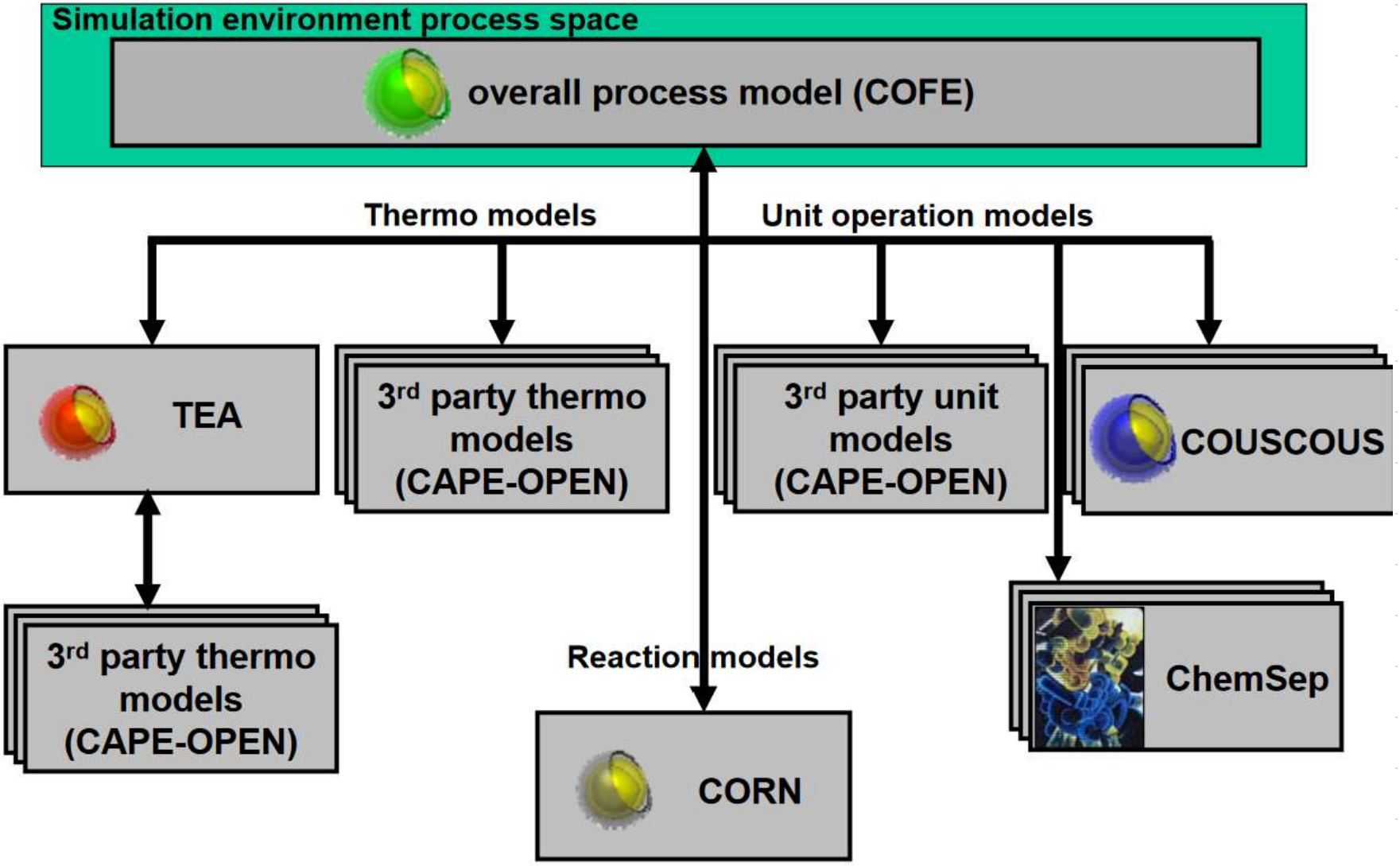


Steps to simulate a process in COFE …

- **Define the components**

  Start→ All Programs → COCO → Configure TEA → TEA Thermo → Create Template → Compounds → Add

- **Define the thermodynamic method**

  Start→ All Programs → COCO → Configure TEA → TEA Thermo → Property Pack Definition → Interaction Parameters

- **Define the reaction pack**

  Start→ All Programs → COCO → CORN → Create Template → Compounds (add the compounds) → Reactions (define the stoechiometry, the reaction rate, the heat of reaction, the phase of the reaction)

… steps to simulate a process in COFE …

- **Open COFE**

  Start→ All Programs → COCO → COFE

- **Import the thermodynamic method and the components**

  Start→ All Programs → COCO → COFE → Flow-sheet Configuration → Property Packs → TEA (CAPE_OPEN 1.0) → Add your own thermodynamic pack

- **Import the reaction pack**

  Start→ All Programs → COCO → COFE → Flow-sheet Configuration → Reaction Packs → CORN Reaction Pack Manager → Add your own reaction pack

… steps to simulate a process in COFE.

- **Build the flow-sheet**

  insert the unit operation

  connect the streams

  define the input streams

OBS 1. Define first the unit of measure and after that the values of the input streams, otherwise, COFE makes automatically the conversion of the units of measure

OBS 2. Once the user defines the units of measure for the first stream these will be kept for all the other streams of the simulation

- **Run the simulation**
- **Analyze the results**

COCO-COFE pros & coms

pro

- The simulator is useful to simulate simple processes
- It is not difficult to use it, even if the user interface is not so users friendly as those of other simulators
- The main thermodynamic methods are implemented in TEA (PR, SRK, RK, UNIQUAC, NRTL, virial EOS, van Laar, Wilson)
- Possibility to use the groups contributions methods for estimating some properties
- The main UO are implemented using the CO Methodology
- The user can create his own UO (using the version 1.0 of the Wizard which is compatible with COCO) or can develop his own thermodynamic methods

cons

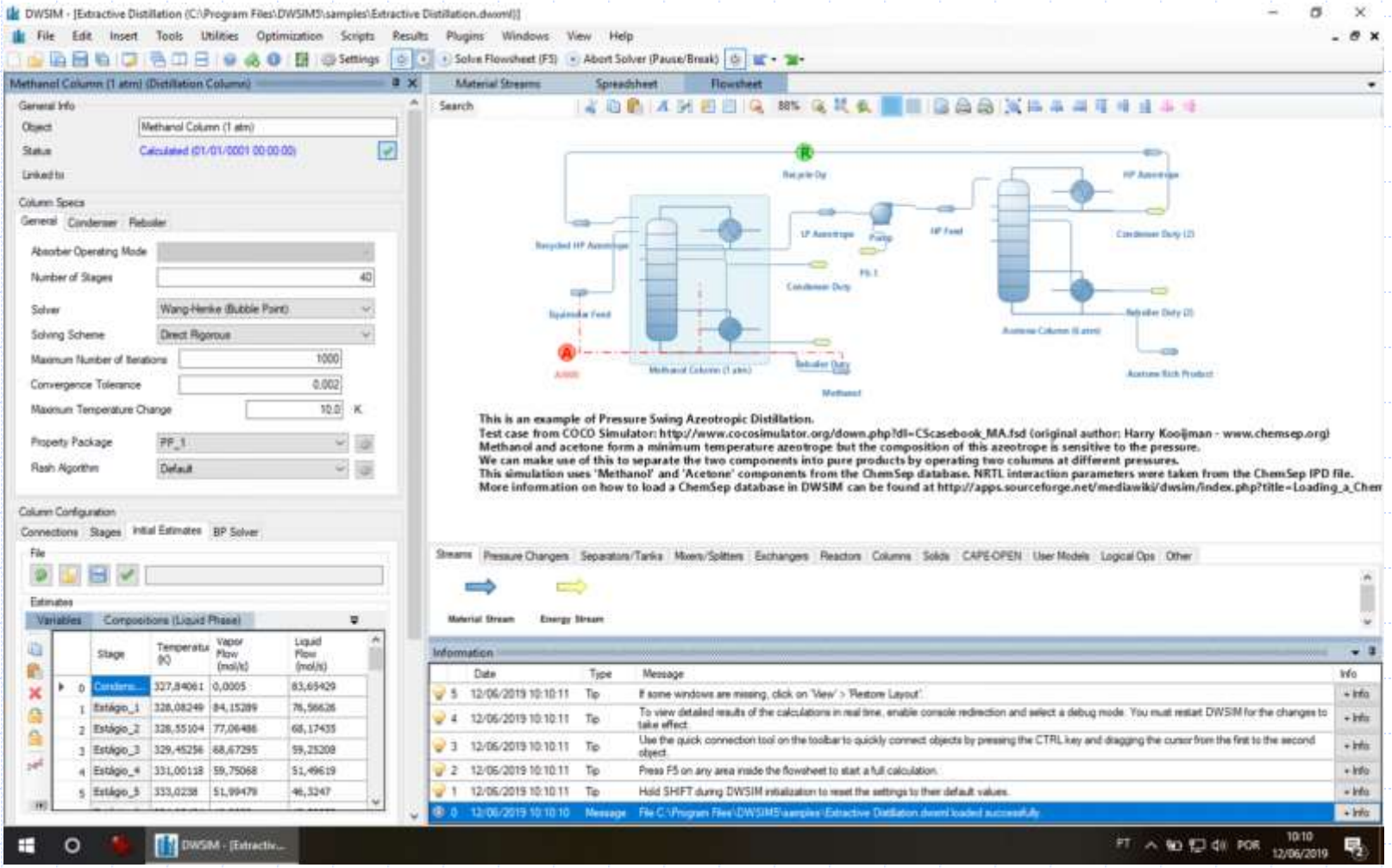
- ...limited for complex processes
- The database containing the chemical substances is not very big (around 200 compounds)
- ...time consuming

How to get it

www.cocosimulator.org

DWSIM

- How to get it:
  http://dwsim.inforside.com.br/wiki/index.php?title=DWSIM



A final remark

The road towards open architectures in process engineering software is irreversible

...and CAPE-OPEN has already taken us more than ever before down this road