Towards CAPE-OPEN 2.0

Michel Pons,

CO-LaN Chief Technology Officer

CO-LaN contractor / France

www.colan.org

Goals

❑ A response to Mark STIJNMAN's presentation at CO 2019

❑ My views: not revised/approved by CO-LaN MB

❑ Mark addressed:
  - Changes in the computing landscape
  - Changes in the process simulation landscape
  - Pain points in the current standard:
    • Thermodynamics
    • Unit operations

CAPE-OPEN 2.0

- ❑ Scoping version of CAPE-OPEN not often done
  - ■ Made for CAPE-OPEN 1.0 (released in 2003) as part of scoping of Global CAPE-OPEN project (before mid 1999)
  - ■ Never a question (unfortunately?) for CAPE-OPEN 1.1
- ❑ CO-LaN known for slow progress on interface specification
  - ■ No different from most Standard Development Organizations
  - ■ With less resources involved than most SDOs
- ❑ Aiming too high calls for dissatisfaction
- ❑ Aiming too low makes goal unattractive
- ❑ Need for a time horizon
  - ■ Is October 2025 the right evidence for CAPE-OPEN 2.0?
  - ■ End of CO-LaN duration if not extended

www.colan.org

Changes in the computing landscape

❑ "*Present is mostly single-threaded / future is multi-threaded*"

  ■ Single-thread is indeed common: architecture of the 90s

  ■ When multi-threaded, most often it is not "many" threads.

  ■ Some side effects of different threads used by separate components (Windows handle) resolved in COBIA Phase 2

    • Specified in CAPE-OPEN 1.2 in ICapeUtilities::Edit

❑ Multi-threading <u>is</u> addressed by COBIA

  ■ Threading model/rules have been developed by M&T SIG within Phase 2

    • Need still to be refined in Phase 3

    • Not necessarily an impact on CAPE-OPEN 2.0 specifications

Changes in the computing landscape

❑ "*Future of process simulation is cloudy*"

▪ Present becomes progressively to get cloudy

- ProSim, AVEVA, ANSYS, COMSOL, etc.. are present on the cloud
- For evaluation purposes as well as daily calculations
- User subroutines, plug-ins like CAPE-OPEN not always part of cloud
  – Solution to possible license issues not yet defined

❑ Additional CAPE-OPEN interface specifications or technical solution for CAPE-OPEN implementation to be developed?

▪ If business case, can be considered as within scope of COBIA Phase 3 (still under definition) and hence towards CO 2.0

www.colan.org

Business case

- ❑ Organization X makes available on the cloud Unit Operation A (PMC) to its customers for use in any PME (desktop or cloud)
  - ■ No download of CAPE-OPEN PMC allowed by organization X
  - ■ Generalization of case used in Virtual Plant Demonstration Model (VPDM) Project presented at CAPE-OPEN 2006 Annual Meeting by PSE Ltd
    - • *aimed to support "arms-length" inter-organisational collaborative modelling, allowing companies to make their models available in a strictly controlled manner to collaborating organisations, with which they may potentially be competitors in different contexts.*

- ❑ The above business case led to a demonstration project *only*
- ❑ What would make it more important today?

www.colan.org

Way forward on cloud issues?

❑ **End-user organizations/ software vendors**
  ▪ Develop relevant business cases
  ▪ Manifest intent to use solution once preliminary design available
    ▪ No use of a solution which is not implemented

❑ **Possible consequences**
  ▪ Additional delays in COBIA Phase 3 deliverables
  ▪ Additional budget for COBIA Phase 3
  ▪ Increase attractiveness of CAPE-OPEN
  ▪ But would performance not be a big issue?

www.colan.org

CO·LaN

Dynamics and equation-oriented modeling

❑ "*More dynamic and equation-oriented modelling in future than currently*": yes

❑ Equation-oriented modeling
  - ▪ Considered from the start in CAPE-OPEN (end of 90s)
    - As part of the Numerical interface specifications
      - – Given same importance as Thermo and UNIT packages
  - ▪ Conceptual design by Imperial College (*PSE Ltd*)
    - "Equation Set Object" to encapsulate systems of equations
    - Numerical solvers to encapsulate solvers of many kinds
  - ▪ Implemented (with sometimes some adaptations)
    - In one commercial tool: gPROMS
    - In academic tools: EMSO, CheOps, Diana

CAPE-OPEN numerical interfaces

❑ Out of scope of COBIA Phase 2
- Consequently out of CAPE-OPEN 1.2
- Will they be in scope of COBIA Phase 3
  - And consequently of CAPE-OPEN 2.0?

❑ Current reasoning within M&T SIG on COBIA
- There is no Numerical SIG to take care of Numerical interface specifications: no maintenance
- There is almost no implementation in commercial tools
- No business case exists for maintaining Numerical interface specifications within CAPE-OPEN standard

www.colan.org

CO LaN

CO-LaN past activities on numerical interfaces

- ❑ NUMR interfaces included in original Tester Suite
  - ▪ Reason: Tester Suite needs to cover the entire spectrum of CAPE-OPEN
- ❑ Mixing equation-oriented and sequential approaches
  - ▪ Black box models / classic Unit models in EO PMEs
  - ▪ Partly in current CAPE-OPEN Unit Operation interface specification: never implemented? (maybe in Aspentech Mixer VB example!)
    - • Needs to be extended to be completely functional
  - ▪ Proposal made by PSE Ltd to CO-LaN Full Members (10 yrs ago)
    - • No follow-up, for budgetary reasons mostly
  - ▪ Unclear if design contained in project proposal can be re-used
    - • Copyright held by PSE Ltd
- ❑ Lack of business case and of financial resources for further activities?
- ❑ Lack of Numerical Special Interest Group to maintain sustain interest in Numerical interface specifications?

www.colan.org

CO·LaN

Creation of a Numerical Special Interest Group?

❑ Creation attempted at very beginning of CO-LaN
- ▪ Not successful

❑ Potential for a Numerical SIG
- ▪ Expertise exists in academics/software vendors/end-users
  - ▪ Carnegie Mellon University / Federal University of Rio de Janeiro
  - ▪ PSE Ltd / Aspentech / AVEVA
  - ▪ BASF / Linde Engineering / Shell

❑ W/o a Numerical SIG, no numerical interfaces in CO 2.0

www.colan.org

Dynamics and equation-oriented modeling

❑ "*More dynamic simulation in future than currently*": yes

❑ In CAPE-OPEN, two approaches to dynamic simulation

- ■ Interface specification for dynamic unit operations
  - Designed with Operator Training Simulation in mind
  - Prototyped in INDISS Plus (RSI/CORYS) and in PMCs at IFPEN
    - – But nowdays "*no impact on CORYS current business*"
  - Not implemented in any other commercial/academic tools
  - No business case?
  - Design to be revised?

- ■ Interface specification for Differential Algebraic Equations
  - Implemented in academic tools
  - Not implemented in commercial tools
  - No business case?
  - Design to be revised? Go back to need for a Numerical SIG.

www.colan.org

Interface specification for dynamic unit operations

- ❑ Activity located within UNIT Special Interest Group
    - ■ Extension to the Unit Operation interface specification
        - • No real constraint w.r.t. inclusion in CAPE-OPEN 2.0
    - ■ Nobody currently within UNIT SIG from original design team
    - ■ Is this the interface specification which is needed?
    - ■ Where is the expertise, out of CORYS/IFPEN in CO-LaN?
        - • Kongsberg: K-Spice® multipurpose dynamic simulator
        - • Sim Infosystems: ProSimulator OTS system
        - • ?

- ❑ Is there a business case for changing UNIT SIG charter to include work on this specification?

www.colan.org

CO·LaN

Pain points in thermodynamic PMC lifecycle

❑ "*No way to create an empty Property Package*"

❑ Property Package Manager exists
  ■ But its functionality is too reduced

❑ Current proposal (see Thermo SIG) to address issues
  ■ Manager interface specification
    • Carries functionality defined for Chemical Reaction Package Managers in Chemical Reactions interface specification
      – Editing, saving/loading, preset management, etc…
    • Common to Property Package Managers, to Chemical Reaction Package Managers, to ?
    • Is meant to be part of CAPE-OPEN 1.X and further

www.colan.org

Pain points with multithreading and thermodynamics

- ❑ "*Property Packages are inherently unsafe for multi-threading*"
  - ▪ Property Package calculations are progressively made threadsafe
    - See KBC presentation: "extension of threadsafe models"
    - Underlying legacy software often an issue slowly resolved
- ❑ Mark points Material Object as root cause of pain points
  - ▪ MO used as a data container to store calculation results
- ❑ Solution proposed by Mark
  - ▪ Make a Property Package a stateless object
  - ▪ No move of data in and out of MO by Property Package
  - ▪ Move part of complexity to Package Manager
    - This part underway by specifying Manager interface
    - But Mark requests more e.g. in terms of compound subsets

www.colan.org

Pain points with multithreading and thermodynamics

❑ Mark advocates major changes in design of Thermodynamic and Physical Properties interface specification

- ▪ Current specification widely implemented
- ▪ New solution needs to be fully specified
  - • Much time needed, since would be a major revision
  - • Could be reason for success/failure of CAPE-OPEN 2.0.
- ▪ Who would be willing to implement new solution?
  - • In parallel or to replace current solution
  - • Software vendors often showed reluctance to change
    - – Heavy development and maintenance costs

❑ Need to hear from software vendors

- ▪ Any interface design has benefits and flaws

www.colan.org

CO·LaN

Other priorities on thermodynamics

❑ Inclusion of revised Chemical Reactions interface specification in Thermodynamics and Physical Properties interface specification
  ▪ A single (reactive and non-reactive) phase equilibrium interface

❑ Distributed properties support: needed for solids for instance
  ▪ TUHH made a proposal and implemented interface in SolidSim
  ▪ Design to be reviewed (any intellectual property issue with Aspentech?)

❑ Semantics of Property Package parameters
  ▪ No naming convention makes identification of parameters difficult

❑ Support for multiple point calculations in one call
  ▪ Came up as a use case for multi-cell unit operation models

www.colan.org

CO·LaN

Pain points on Unit Operations

- ❑ *"Need some way to support "classic" unit operations in an equation-oriented environment"*
    - ▪ See part above on blackbox UOs in EO PMEs
    - ▪ Solution proposed by PSE Ltd
- ❑ Actionable for CAPE-OPEN 2.0

- ❑ *"Real-time display of current conditions"*
    - ▪ A complete use case is needed
    - ▪ Possible implementations: ChemSep, HTRI?

www.colan.org

CO·LaN

Other points on Unit Operations

- ❑ CAPE-OPEN looked upon as a reference
- ❑ At CAPE-OPEN 2019: CFIHOS / DEXPI communications
- ❑ Discussions initiated with DEXPI
  - ■ Linking a data model and an interface model
  - ■ Possible modifications to identification of Unit Operations
    - ■ But not only
    - ■ More than an extension: CAPE-OPEN 2.0
- ❑ Analysis
  - ■ Challenge: new domain to be mastered
  - ■ Benefits: access to new stakeholders
  - ■ Risks: expectations of other SDOs not met

www.colan.org

What could be CAPE-OPEN 2.0 in 2025?

- ❑ Thermodynamics (already under development)
  - ■ Close integration between chemical reactions and thermodynamics
  - ■ Manager interface offering enhanced functionality
    - • Compared to Property Package Managers
- ❑ Unit Operations (preliminary design but need of business cases)
  - ■ Black-box modeling support
- ❑ Equation-oriented and dynamic simulation
  - ■ Strong basis exists that could be ported to CAPE-OPEN 2.0
  - ■ Needs a Numerical SIG to make it happen
- ❑ Opening to digital twin aspects
- ❑ Software engineering aspects
  - ■ Multi-threading / cloud: technical scope of COBIA Phase 3

www.colan.org

CO·LaN

Questions?

Thank you for your attention!

www.colan.org

CO·LaN