UNIT SIG report

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CAPE-OPEN 2025 Annual Meeting

October 31, 2025

Outline

Report period: October 2024 till September 2025

- ❑ Charter and scope
- ❑ Members
- ❑ Summary of activities 2024/2025
- ❑ Objectives for 2025/2026

Charter

- Maintain and publish the standard
- Respond to issues raised by developers and users
- Prioritize registered issues and give recommendations on solutions
- Promote and support the use of the CAPE-OPEN interface for Unit Operations

Scope of UNIT Special Interest Group

- Unit Operation interface specification
  - *Well Established*
- Unit Operation Derivatives
  - *Early stage of development*
- Petroleum Fractions interface specification
  - *Early stages of production*
- Dynamic Unit Operation interface specification
  - *Documents ready for final review pending business case*

- Support to compliance testing and certification
  - On implementations of interfaces within scope

Unit SIG Members

- Members:
  - Krishna Murthy Penukonda (AVEVA Solutions)
  - Jasper van Baten (AmsterCHEM)
  - Cesar Pernalete (University of Ghent)
  - Michael Hlavinka (Bryan Research & Engineering)
  - Richard Baur (Shell Global Solutions)
  - Harry Kooijman (Shell Global Solutions)
  - Kyle Abrahams (CO-LaN)
- To Join the SIG, contact the SIG Leader
- Monthly Teams meetings

Unit SIG Leadership is Changing

Krishna Murthy Penukonda (2013 - 2025)

We are please to announce that César Pernalete (University of Ghent) will take over as the new SIG leader from November 2025

Summary of activities for 2024/2025

- Petroleum Fractions interfaces now available
  - COBIA release Feb 2025
  - COM IDL release June 2023
  - Commitment to prototypes in the coming year

- Unit Operation Derivatives
  - Worked with the Thermo SIG to develop Flash Derivatives
  - A draft has been made as an appendix to the Unit Operation Specification
  - Will be release for RFC pending internal reviews

Unit Operation Derivatives

- Motivation
  - Equation Oriented (EO) specifications were never adopted and incomplete
  - Without EO specifications, EO simulators must perturb (which is inaccurate and computationally expensive)
  - Compromise: Unit derivatives of all outputs with respect to all inputs (Ports and Parameters)
  - Not equivalent to EO: Unit gets solved at each iteration
  - This is more accurate and faster than perturbation

- Requirements
  - Agree on degrees of freedom
  - Who is responsible for the degrees of freedom?
  - Flash derivatives need to be defined by Thermo SIG

Summary of activities for 2024/2025

- **Errata & Clarifications:**
  - Addressed inconsistencies between the Unit Operation specifications and the ICapeUtility specifications.
  - Developed errata for workflow completion when deleting units and error handling within unit operations.

- **Testing Specifications:**
  - Significant progress was made on the ICapeUnit testing specifications, including defining tests for validation statuses and port configurations.
  - A substantial part of Unit testing is completed with Thermo Specification testing. This information has already been prepared by the Thermo SIG. (Thermo Progress Report)
  - A new document specifically for testing unit ports was initiated to align with the testing approach taken by other SIGs like Thermo SIG.
  - The focus is on PMC testing. PME testing will be done at a later stage (Timeline for certification releases).

Summary of activities for 2024/2025

❑ Configuration Discussions:

- Discussed the configuration of test categories, including whether thermodynamic configurations should be shared across tests.
- Concluded that while port connections depend on thermodynamics, specific values should be defined within the unit tests.

❑ Meetings:

- The SIG held regular monthly meetings, during which these activities were discussed and developed further.
- Collaborated with the M&T SIG on aligning approaches to testing and specifications, especially around collections in unit operations.

Objectives for 2025/2026

- Support development of tests of Unit Operations
  - List of tests prepared by CTO
    - with help from some UNIT SIG members
  - Review of list of tests
  - Errata & Clarifications expected to support test rationale
    - Malcom's presentation on PMC testing
    - Presentation on Common source documentation

- Unit Operation Derivatives
  - Define further high-level design
  - Obtain feedback on major decisions from community

Objectives for 2025/2026

- **Improve Documentation and Clarity:**
  - Continue refining the language and structure of the documentation to improve clarity, especially around test configurations and the integration of thermodynamics.
  - (Common Document Format)

- **Collaborative Development:**
  - Testing is completed with the Certification Testing Working Group
  - Testing and Unit Derivates with Thermo SIG
  - Documentation and Tooling with the M&T SIG
  - Integrate feedback from the community and ensure that major decisions are supported by a broad consensus within the CAPE-OPEN community.