

# **UNIT SIG report**

**Krishna Murthy Penukonda  
CAPE-OPEN 2017 Annual Meeting  
Sunbury-on-Thames, UK  
October 13 , 2017**

# Outline

- **Report period: October 2016 till September 2017**
- **Key responsibilities**
- **Members**
- **Update on Petroleum Fractions specification**
- **Objectives for 2017/2018**

# 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**

# Unit SIG Members

- **Members:**
  - **Krishna Murthy Penukonda (Schneider Electric)**
  - **Michel Pons (CO-LaN)**
  - **Jasper van Baten (AmsterCHEM)**
  - **Michael Hlavinka (Bryan Research & Engineering)**
  - **Richard Szczepanski (KBC Advanced Technologies)**
- **Join? Contact Krishna Murthy Penukonda**
- **Monthly phone meetings**
  - **Follow them on website. Subscribe to RSS feed.**

# Objectives for 2016/17

- **Petro Fractions**
  - **Submit specification for Request For Comments**
  - **Publish Petroleum Fractions specification**
  - **Produce an IDL against the textual specification**
- **Continue to maintain Unit specification and E&C**
- **Prepare for COBIA**
- **Dynamic unit / Equation-oriented**
  - **on hold until business cases justify action**

# Update on Petroleum Fractions specification

- **Scope section: October to December 2016**
  - **Flowsheet simulation sub-section restructured and simplified**
    - Defining “characterization properties” and “characterized properties” in glossary (terms used in subsection dealing with flowsheet simulation).
    - *Inlet is described by a given set of pseudo-compound properties; outlet is determined by the ‘dynamically’ revised pseudo-compound properties.* This represents an ideal whereby all properties of each pseudo-compound (basic and petroleum), other than boiling point, are updated by the reactor algorithm. Such a solution introduces the concept of stream-dependent, modifiable (compound-) properties.

# Update on Petroleum Fractions specification

- **Textual Requirements section: Jan-Feb 2017**
  - **Re-arrangement of the section on textual requirements**
    - by splitting between general requirements, requirements on interaction between a Unit Operation and a PME, requirements on interaction between a PME and a Property Package.
    - By making sure to stress out the differences between pseudo compounds and real compounds in terms of properties, and possible change of their values.
    - Additional requirement introduced: Petroleum Properties can not be set for real Compounds
    - Initially products are populated with same pseudo properties as those on feed. Unit *can* change these.

# Update on Petroleum Fractions specification

- **List of petroleum bulk and compound properties**
  - **Started on March 28, 2017 (version 5.29)**
    - Possible need, in order to avoid confusion, to name differently a property when it is a Petroleum Property and when it is a Compound Constant (e.g. critical temperature): prefix “petro”
    - Properties referring to elemental contents were given a generic name, e.g. petro**C**Content, petro**Ni**Content
    - Provide a table of Properties and bases that includes the references defining each of the Petroleum Properties, e.g. measurement method
  - **March 31, 2017:**  
property table revision provided by KBCAT



# Update on Petroleum Fractions specification

- **List of petroleum bulk and compound properties (continued): since April 2017**
  - **April 25, 2017**
    - Went through the table modified by KBCAT, leading to more questions
  - **May 30, 2017**
    - More on the table.
  - **June 27, 2017**
    - More work on table, trying to figure out how to organize it and fill it with consistent information.

# Objectives for 2016/17: in progress

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# Conclusion

- **Progress on Petroleum Fractions interface specification**
  - **But not yet complete**
  - **External input is welcome**
- **Objectives 2017/2018: same as 2016/2017**
- **Need to compromise on property list:**
  - **Short list with e.g. just Mono-aromatics, or**
  - **Long list with many different mono-aromatic definitions**