

# Thermo SIG Progress Report 2020

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# Thermo SIG Annual Report: Charter

## Task:

**Develop, maintain and promote Thermodynamic and Physical Properties interface specifications**

## Key Responsibilities:

- **Maintain and manage existing interface specifications**
- **Assess expansions of interface specifications**
- **Manage the development of expansions**
- **Help organizations to develop implementations**

# Thermo SIG Annual Report: Active contributors

- Sergej Blagov
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- Bjørn Maribo-Mogensen
- Richard Szczepanski
- BASF (co-leader)
- CO-LaN
- Shell Global Solutions
- AmsterCHEM (co-leader)
- Hafnium Labs
- KBC Advanced Technologies Ltd

# New interfaces: High level overview

Custom Data  
Interface

Published! Online!

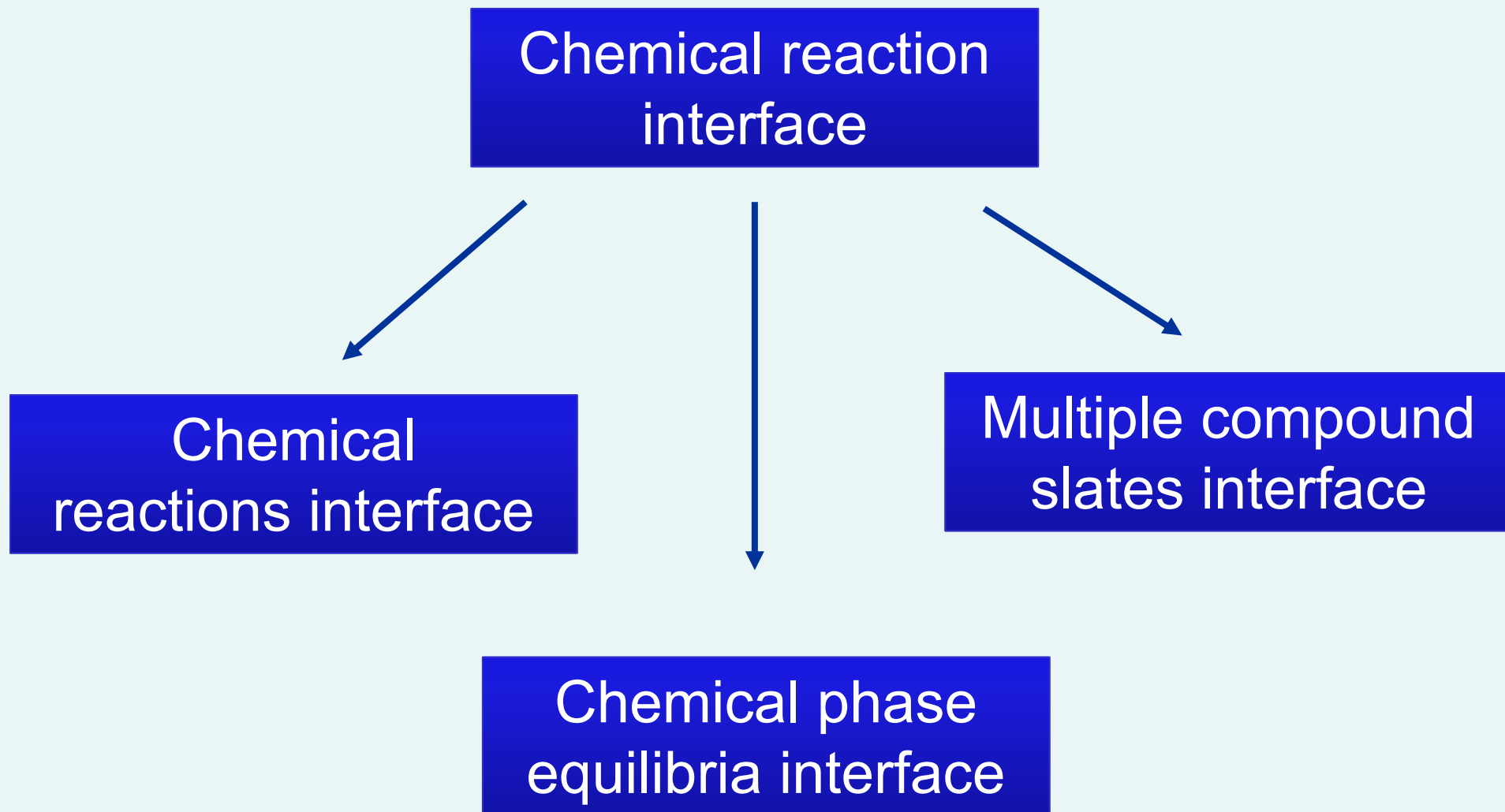
Manager  
Interface

Coming soon!  
2020-2021

Chemical reaction  
interface

Out for RFC!  
Please provide feedback

# Chemical reaction interface? Interfaces!



# Summary of activities 2019-2020

- **Errata Thermo 1.1**
  - **No additions**
  - **RFC about new properties:**
    - **Dielectric constant; depends on frequency**
    - **Refractive index; depends on wavelength**
    - **Need to establish business cases for these. Your input is welcome.**

# Summary of activities 2019-2020

- **Custom Data interface specification**
  - **Published!** (web site pending, complete in repo)
  - **IDL part of latest type library installer** (pending)
  - **Ready for implementation by software vendors**
  - **Obligatory for PME's that support chemical phase equilibria and multiple compounds slates**
- **Chemical Reactions interface specification v1.1**
  - **RFC Initiated!**
  - **Please provide your feedback!**

# Goals set for 2020: comparison with expected

- **Public Custom Data**  done
- **RFC initiated for Chemical Reactions**  done



# Errata Thermo & Physical Properties 1.1

- Investigated: dielectric constant, refractive index
- Issue: in addition to T, P, X, depends on frequency / wavelength
- Two possible solutions
  - Request calculation at specific frequency: requires new property (or interface)
  - Property package reports at which frequency the calculation is done
- Initial feedback
  - dielectric constant is available as internal property in some thermodynamic server
  - refractive index is available as measured property in some packages
  - no strong business cases exposed so far
- Thermo SIG is in process of establishing what current software implementations can offer: is there a business case?
- Your feedback is welcome. *If no further feedback: abandon.*

# Thermo SIG plan 2020-2021

- **Manager interface:**
  - Desired as generalization for Property Package Manager, Reaction Package Manager, (Unit Operation Manager?), ...
  - Deals with shortcomings in ICapePropertyPackageManager
  - Really a Common Interface
  - Needs to be published in order for Chemical Reactions interface to be completed.
- **Material Manager:**
  - Replacement for material template system
- **Resume SIG responsibilities:**
  - COBIA: document CAPE-OPEN 1.2 adaptations
  - Errata & Clarifications

# Requests to audience:

- **RFC for Chemical Reaction Interface is coming up**
  - This is a big document
  - Please take your time to read it
  - Your feedback is essential
  - Ideas for Manager Interface are outlined, also here feedback is welcome
  
- **Custom Data Interface is released.**
  - Please implement support in your MO

# Questions?



# Go CAPE-OPEN!

Thank you for your attention!