

# Thermo SIG Progress Report 2010 and Future Outlook

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# Thermodynamics Special Interest Group (Thermo SIG)

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 Members, September 2011

- ◆ Sergej Blagov, BASF (SIG co-leader)
- ◆ Jasper van Baten, AmsterCHEM (SIG co-leader)
- ◆ Richard Szczepanski, Infochem Computer Services
- ◆ Suphat Watanisiri, AspenTech
- ◆ Ensheng Zhao, Honeywell
- ◆ Murugesh Palanisamy, Honeywell
- ◆ Mallikarjun Lavate, Honeywell
- ◆ Rafael Lugo, IFP
- ◆ Jean-Charles de Hemptinne, IFP
- ◆ Alan Scott, contractor for TÜV-SÜD-NEL
- ◆ Michel Pons, CO-LaN

Join? Contact Sergej

# Thermo SIG Accomplishments 2010

## ◆ Interface specification documents

- Revision completed (authorized for publication in May 2011)  
**Thermodynamic and Physical Properties** interface specification v1.0 & v1.1
- Revision on-going  
**Chemical Reactions** interface specification  
(add to **Thermodynamic and Physical Properties** interface specification v1.1)
- New proposal under discussion  
**Compound Server** interface specification

## ◆ Help to developers

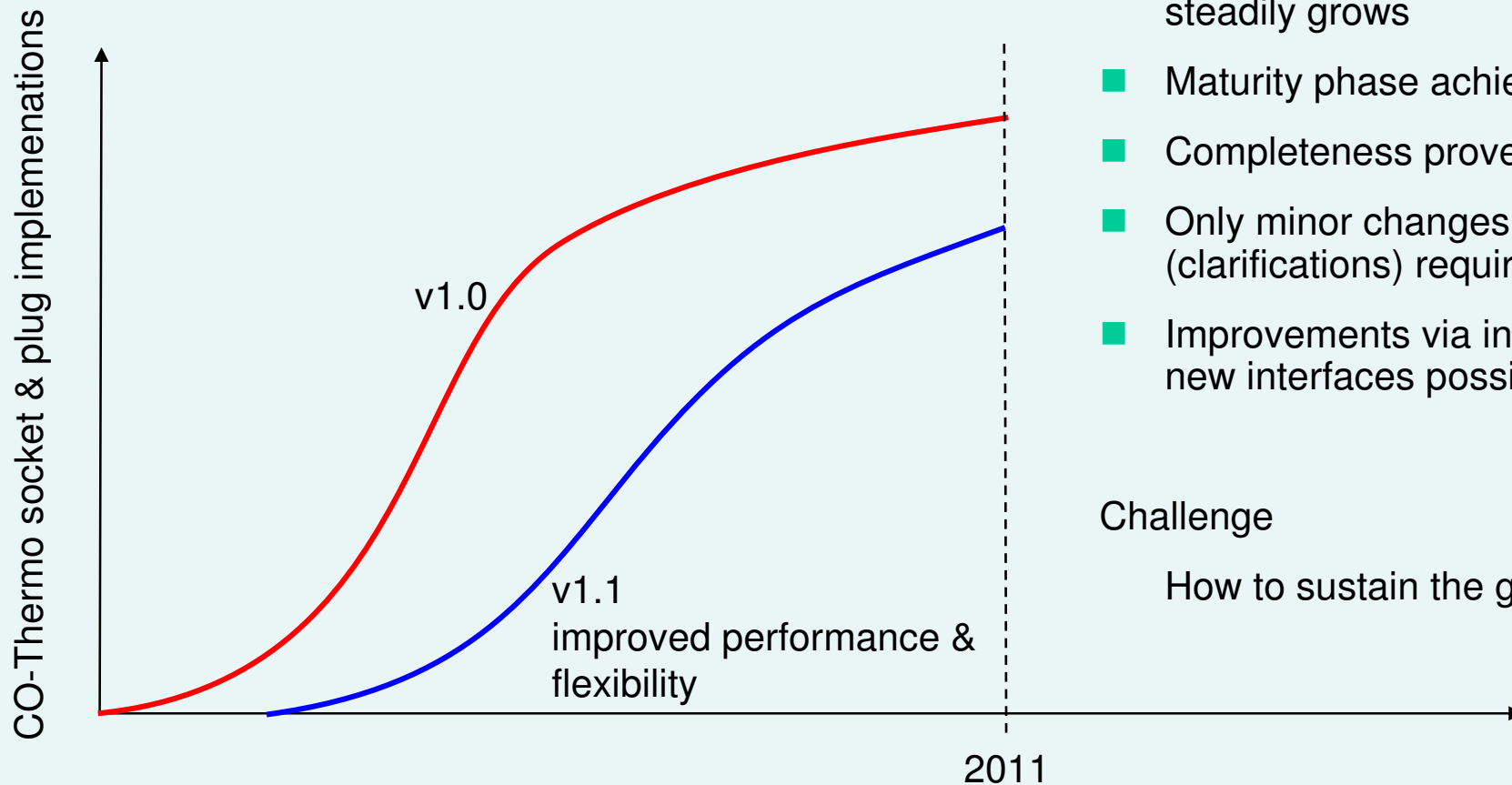
- Proposal for Open Source Examples of **Property Package & Property Package Manager** (v1.1) and **ThermoSystem** (v1.0)

## ◆ Regular bi-monthly phone meetings

# Revision of Interface Specification Documents

- ◆ Included “Errata & Clarifications” for both v1.0 & v1.1
  - ◆ Updated descriptions of phases and phase lists
  - ◆ Clarified values for CalcType
  - ◆ Clarified requirements for CalcEquilibrium
  - ◆ Updated Use Cases
  - ◆ ... (lots more)
- New specification documents available from <http://www.colan.org>
  - No impact on formal interface definitions

# v1.0 & v1.1 Life Cycle Curves till now



- Number of implementations steadily grows
- Maturity phase achieved
- Completeness proven
- Only minor changes (clarifications) required
- Improvements via inclusion of new interfaces possible

Challenge

How to sustain the growth?

# Main Deliverables for 2011

## ◆ Interface specification documents

- Revised **Chemical Reactions** interface specification as part of v1.1
- **Thermodynamic and Physical Properties** interface specification
- New **Compound Server** interface specification (Honeywell proposal)

## ◆ Help to developers

- **Open Source C++/VB6 examples of implementation**
  - **Property Package** and **Property Package Manager** (v1.1)
  - **ThermoSystem** (v1.0)
  - **CO-LaN** contracted **AmsterCHEM**

# Chemical Reactions Interface

- ◆ **Several issues exist with current v1.0 Reactions specification**
  - Reaction basis is not clearly defined
  - Units of measure require revision (non-SI)
  - Several concepts not well defined
- ◆ **Large overlap with v1.1 Thermodynamic and Physical Properties**
  - Compound definitions
  - Material contexts
- ◆ **Conclusions:**
  - Need of a new **Reactions** interface specification
  - Need for integration with v1.1 **Thermodynamic and Physical Properties** interface specification
- ◆ **Status:**
  - Draft under revision, not yet published

# Compound Server Interface Proposal

- ◆ **Existing CAPE-OPEN PPDB interface is complex**
  - Very wide scope
  - Not targeted at delivering single recommended values
- ◆ **Need for pure compound server delivering**
  - Compound constants
  - Compound correlation descriptor
  - Compound correlation coefficients
- ◆ **Current proposal: no support for mixture model data**
  - Too complex
  - Models not always uniquely defined
  - Model coefficients may depend on other models
- ◆ **Status**
  - New, simplified interfaces applicable for both v1.0 and v1.1 thermodynamic component specifications
  - Proposal made by Honeywell. Under discussion; IDL proposal expected

# Thermodynamic Data Workflow

## CAPE-OPEN Property Package

1. Collection of compounds

← **Compound Server**

2. Selection of models

← User experience,  
operating conditions

3. Binary interactions

← Binary data

4. Integrate in simulations

← Equipment data, etc

# Examples of Thermodynamic Components

- ◆ CO-LaN contracted AmsterCHEM
- ◆ Ideal Mixture Thermodynamics Library as an example
- ◆ Full Implementation
  - Property Package & Property Package Manager (v1.1)
  - ThermoServer (v1.0)
- ◆ C++ and VB6 versions
- ◆ ‘How to’ implementation
- ◆ Clarity is focus; no optimization for performance
- ◆ Open source published:

**[www.colan.org/News/Y11/news-1125.htm](http://www.colan.org/News/Y11/news-1125.htm)**

# Initial Feedback on Examples

## ◆ BASF adaptation experience

- C++ version
- No skills in **ATL/COM** programming
- 2 weeks demand for ~ 1/3 of all v1.1 interfaces
- Most time – adjustment of the native thermo-library
- Still complex for inexperienced program developer
- Requires ‘step-by-step’ guidelines
  
- **More feedback needed!**

# Perceptions of CAPE OPEN Are Not Always Right

## ◆ Conflicting statements:

- Too slow
- Too complex

## ◆ Complexity of Thermodynamic Standard results from the requirements for

- high flexibility
- high performance

## ◆ Ways to reduce the perceived complexity

- Detailed step-by-step guidelines
- Further investigations needed
  - Simplified 'Thermo'-Wizard/Template with built-in COM-support ?
  - New CAPE-OPEN **Object Model** without COM ?  
(proposal of **Methods and Tools SIG**)

# Performance Issue

## ◆ Problem of implementation and not of specification

**BASF** performance tests for several thermodynamic packages

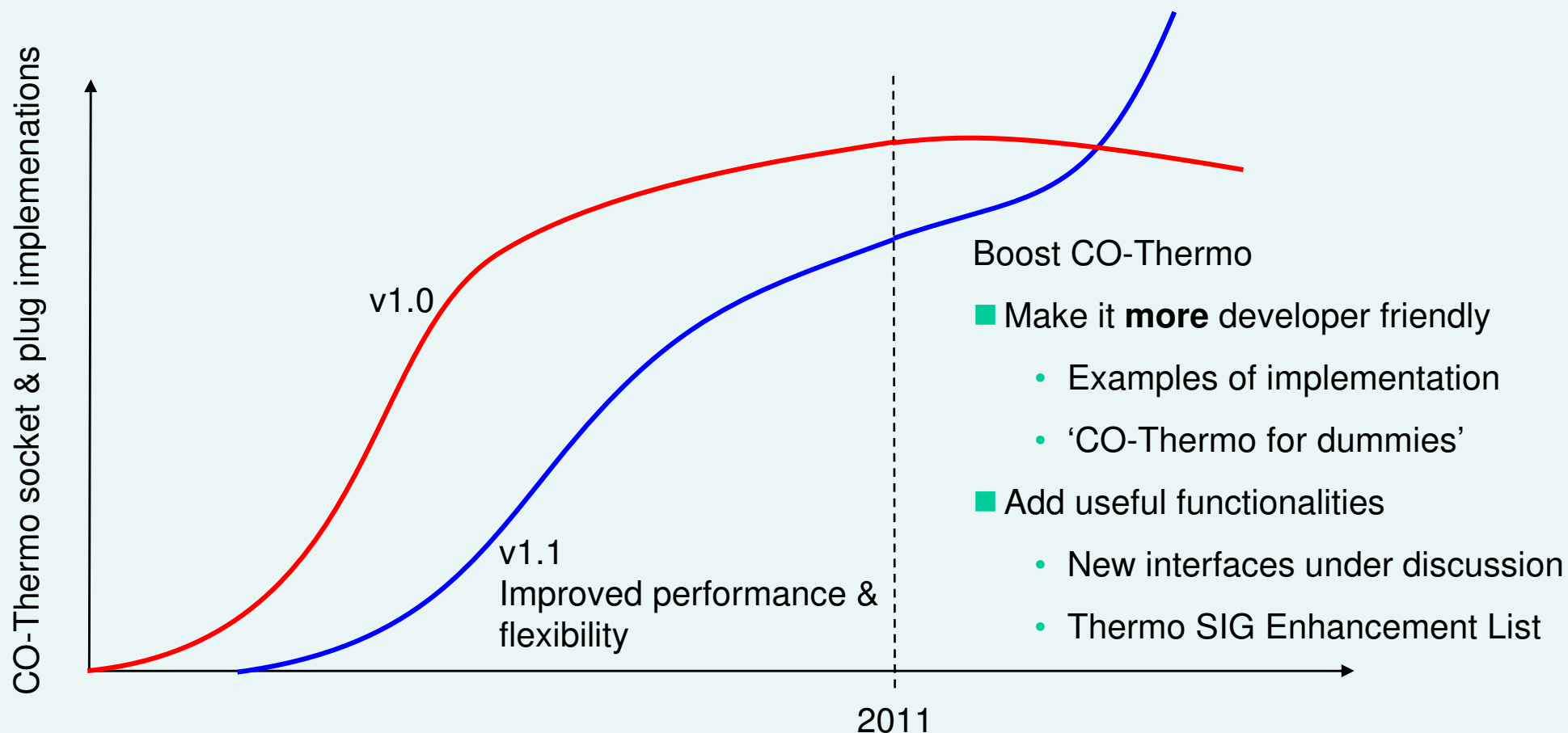
Simulator:	Thermodynamic Package			
<i>Chemasim</i>	Native BASF Thermo-Library	BASF EOS-Library via ForeignObject interface by gProms	CO compliant Multiflash via	
12 comp. mixture PSRK-NRTL ~ 100 eq. stages			general: FORTRAN- Thermo-Wrapper ( <i>ProSim</i> )	tailor-made: BASF- AmsterCHEM Material Object
Performance: CPU-time, sec	1.01	12.94	8.55	1.86

### Tailor-made Material Object

- High performance compared to EOS-Library or Thermo-Wrapper
- Good acceptance by end users; growing number of users
- High potential for further performance improvements (e.g., batch calculation of properties in a single call)

# Thermo SIG Challenges

- ◆ Increase acceptance by academics and small companies
- ◆ Accelerate migration from v1.0 to more powerful and better structured v1.1



# Enhancement List

- Addressing Compounds, Properties, etc., via integer IDs, not strings
  - GetCompoundIdList in addition to GetCompoundList
  - SetPhaseConditions to set (T,p,x) in one call
  - Support for array-wise property calculations
  - Access to information on validity domain for correlations/models
  - ...
- 
- ◆ **Currently: no need to start with v1.2**
  - ◆ **Extensions might be incorporated as additional interfaces**
  - ◆ **Future v1.2 must be binary compatible with v1.1**

# Summary

- ◆ Thermo v1.0 & v1.1: applicability proven
- ◆ Thermo specifications maintenance
  - Relies successfully on Thermo SIG
- ◆ Looking forward to more and further usage
  - New extension interfaces under discussion
    - Compound server interface
    - Reactions interfaces
    - Round-table Thermo SIG session here
- ◆ CO Thermo interfaces are working well
  - Spread the word!

# Questions?

Thank you for your attention!



# Go CAPE-OPEN!