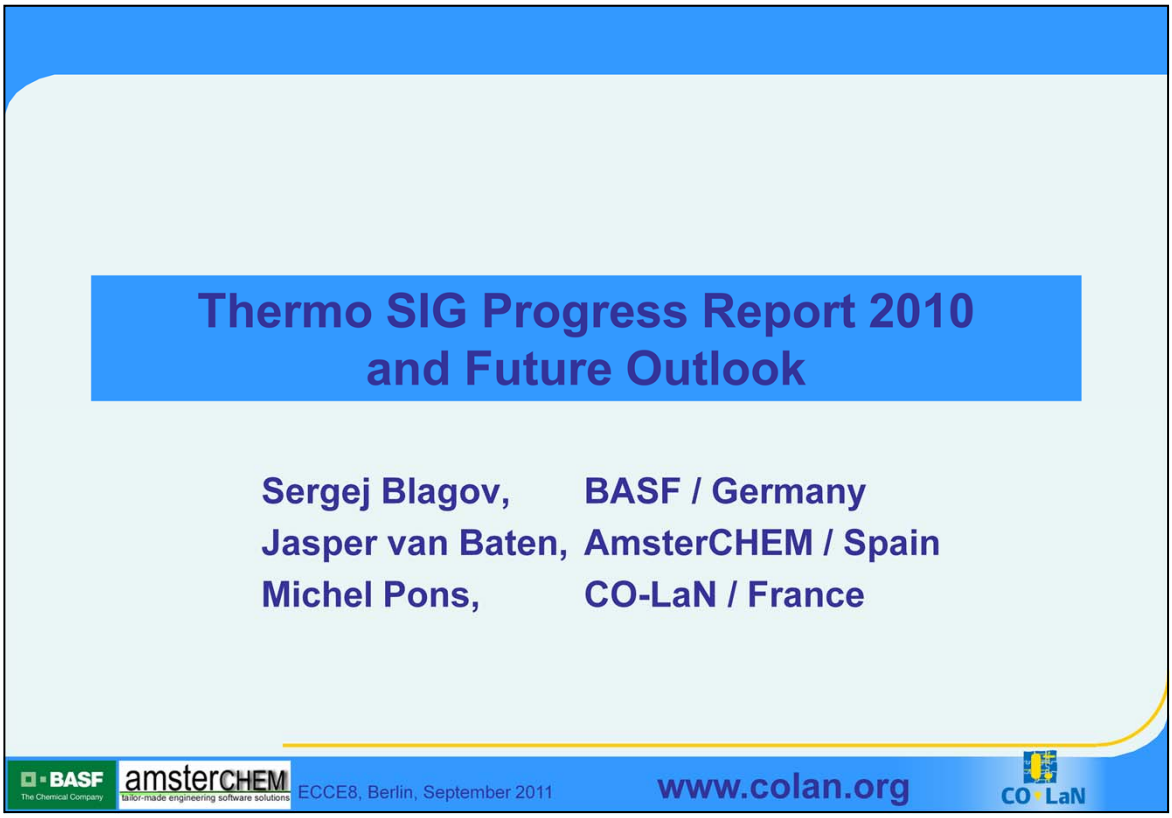


Good afternoon,

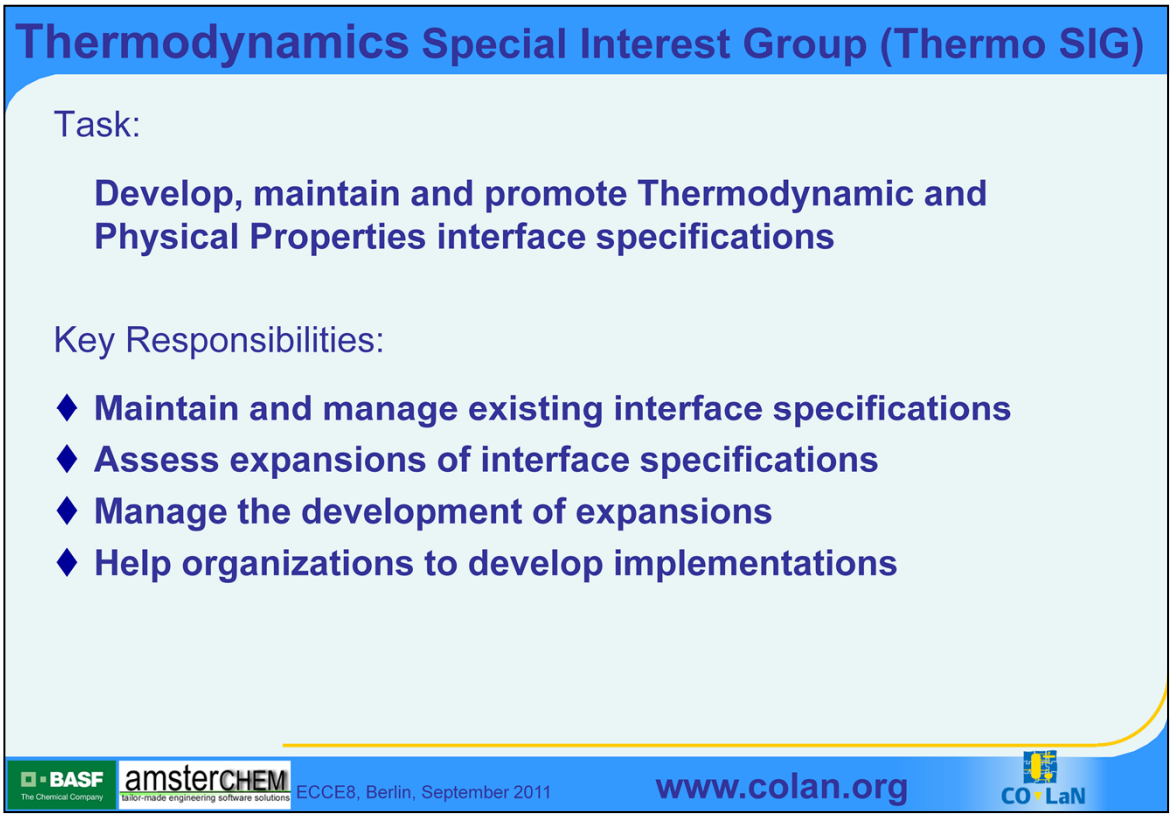
my name is Sergej Blagov and two years ago I undertook the leadership of Thermodynamics Special Interest Group from my precursor – Werner Drewitz after he retired from the BASF.

As I was new in CAPE-OPEN, and I feel me still new even now, Jasper van Baten – one of the most experienced persons in CAPE OPEN has agreed to assist me as a co-leader of Thermo SIG and he is also my co-author today.

Michel Pons – the chief technology officer of the CAPE OPEN Laboratory Network who coordinates activities of different special interest groups is the third author.

Our presentation today is aimed to provide a brief overview of the Thermo SIG activities in the last two years as well as to present some issues that will be addressed in the nearest future.

On that way we will also discuss some controversial statements on CAPE OPEN standard specifications like low performance and exorbitant complexity issues.



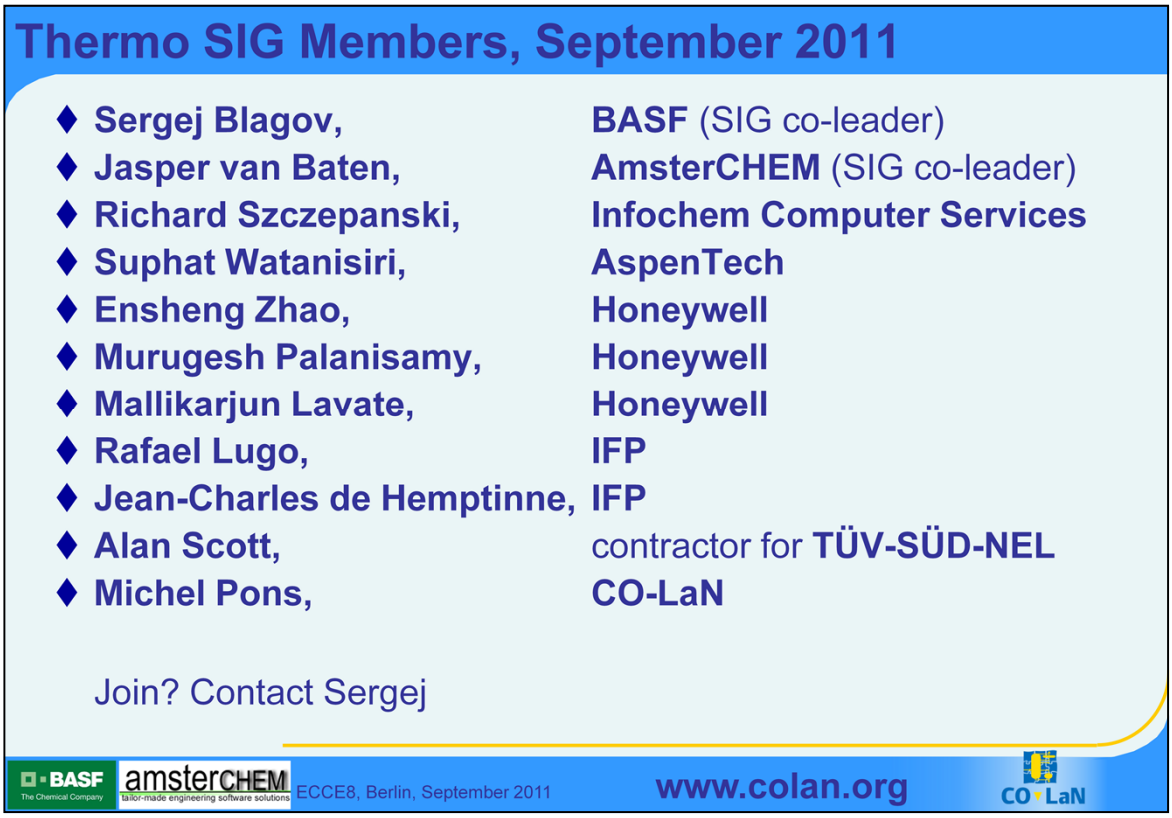
Well, let us begin!

As already mentioned, the abbreviation ‘Thermo SIG’ stands for Thermodynamucs Special Interest Group – an organizational unit within the CAPE OPEN Laboratory Network with the task to ‘develop, maintain and promote Thermodynamic and Physical Properties interface specifications’.

The Thermo SIG is one among several other groups like Unit Operation SIG, Methods and Tools SIG, etc., but still the Thermo SIG is of extreme importance for CAPE OPEN as thermodynamic calculations are in most cases at the heart of all process simulations.

The key responsibilities of our group are listed on the slide and they include:

1) Maintain and manage existing interface specifications
2) Assess expansions of interface specifications
3) Manage the development of theses expansions
4) Provide help support to developers of CAPE OPEN compliant software



To accomplish all these tasks, the Thermo SIG is comprised of representatives of chemical companies, process licensors and vendors of process simulation tools and currently includes 11 members from 8 companies.

At this point, on behalf of our group, I would like to express our gratitude to Andy Johns from TÜV-SÜD-NEL for his efforts and activities in CAPE OPEN in the past. He is not listed here as he left our group at the end of last year after his retirement.

Although Thermo SIG consists currently of full or associate CO-LaN members, it is not a some kind of a closed association and there is no restrictions on participating on Thermo SIG.

So, everyone, who has interest on developing and maintaining of internationally accepted CAPE OPEN interface standards, is welcome to join and you may contact me or Jasper or Michel to clarify the details.

The next slide gives a very brief overview of what has been accomplished in the last year. More details on separate items will be given a bit later and summarizing we may state the following:

1) First, the revision of the existing Thermodynamic and Physical Properties interface specifications of both version 1.0 and 1.1 was in focus in the past. The internally approved revisions have been authorized for publication by the CO-LaN Management Board and are now available on the web.

2) Second, the necessity of extending of the existing interfaces has been realized.

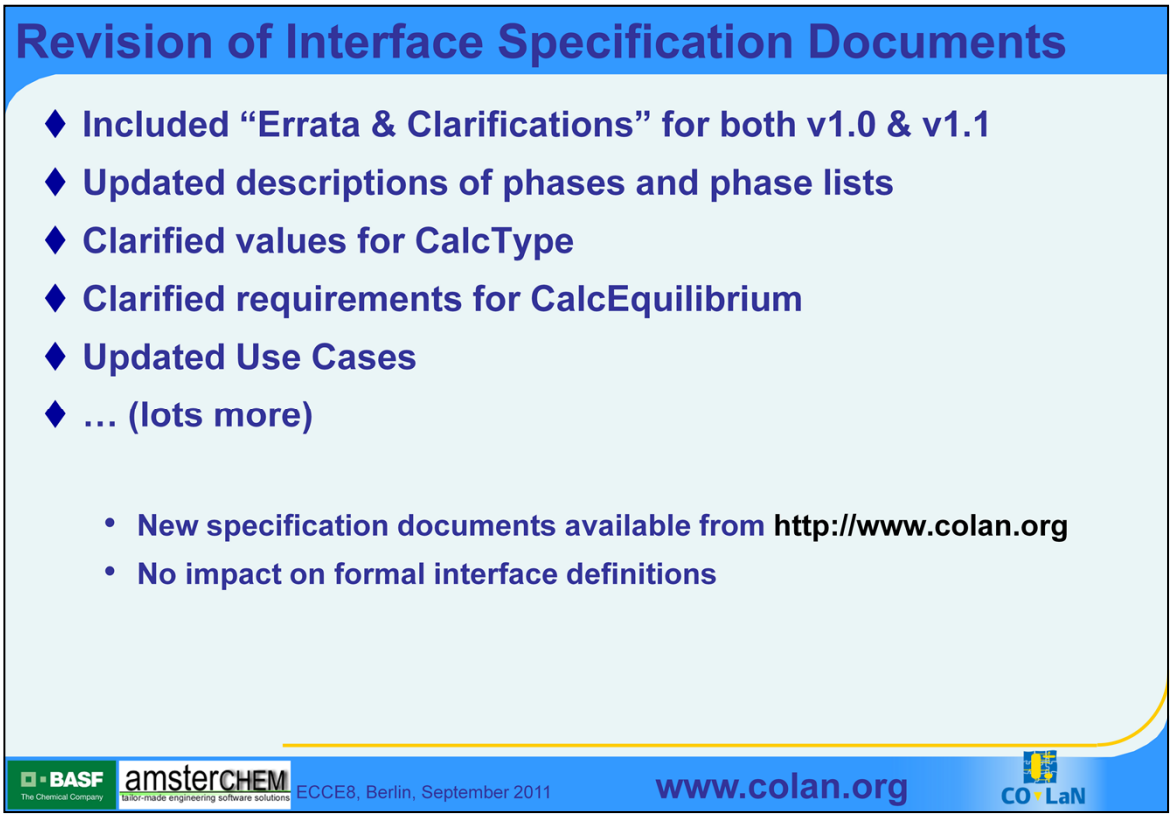
   This concerns particularly the Chemical Reactions interface specification.

   The existing version of this interface does not properly fit into the Thermodynamic version 1.1 standard and it was decided to add the revised version of the Chemical Reactions specification document to the Thermodynamic version 1.1 standard. This work is under way.

   Furthermore, Honeywell proposed to develop a target-oriented Compound Server interface in order to simplify querying databanks for pure compound data from within Thermodynamic software components. This proposal has been accepted and the new extension interface specification is to be developed this year.

3) One of the important tasks of Thermo SIG is to provide software develops with help materials how the things are to be properly handled with CAPE OPEN. Realizing that the CAPE-OPEN compliant implementation of Thermodynamic servers, i.e. software components yielding the results of thermodynamic calculations to the clients, might be complicated for inexperienced programmers, Thermo SIG proposed for a development of open source examples of such implementations for the both specification versions 1.0 and 1.1

The communication within the Thermo SIG is carried out per emails and on the bi-monthly phone meetings.



Now some more words on the revised specification documents

These revisions for both versions fully include the ‘Errata and Clarification’ documents that were collected and recorded in the past based on the feedback from the developers both within Thermo SIG and from outside.

As listed on the slide, these clarifications include:

- Updated descriptions of phases and phase lists,

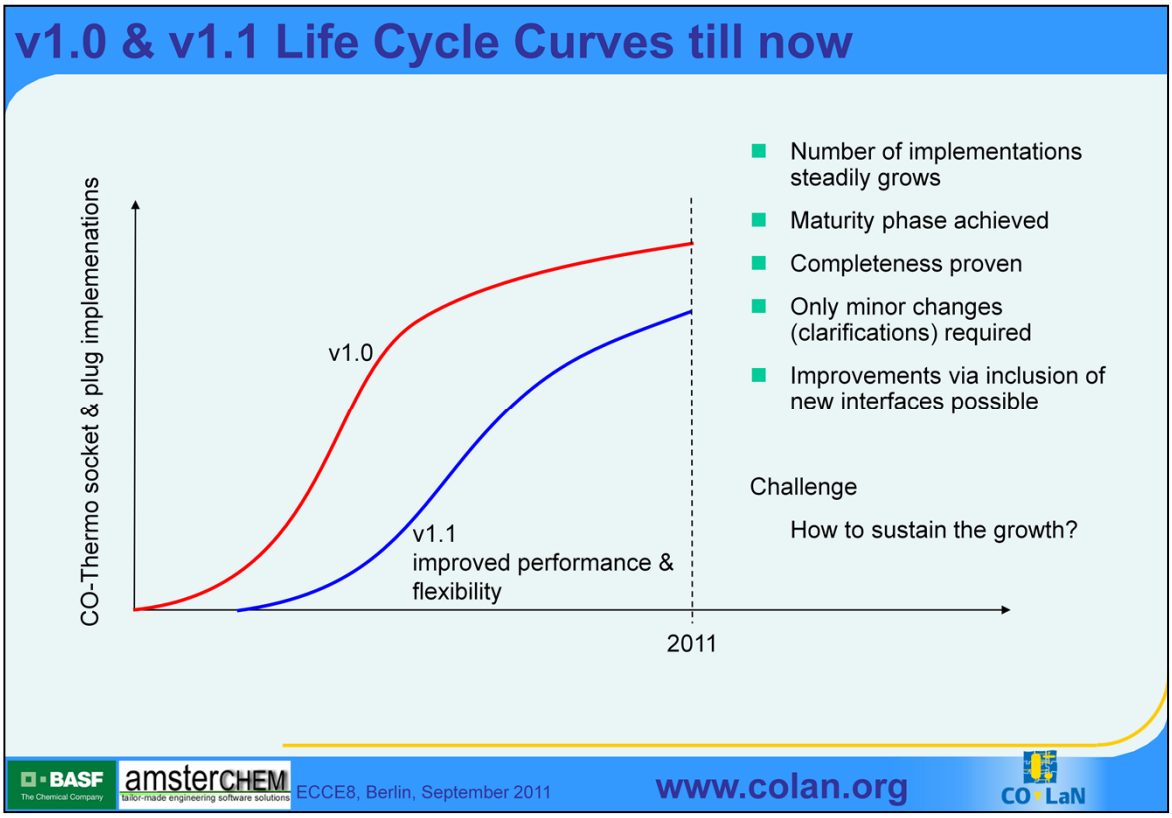
- Clarified values for the CalcType variable,

- and much more other issues …

Furthermore, the documents have been extended and now contain additional chapters, e.g., the one describing some details on Persistence interface implementation and emphasizing its importance.

So, the revised documents contain various clarifications and corrections; they are now published and it is worth for everybody involved in the CAPE-OPEN compliant thermodynamic software development to download the new official thermodynamic standards.

And last not least is to emphasize here that while the changes clarify some former ambiguities, they do not have impact on the formal interface definitions, so that downward compatibility is assured.



Before we begin with the discussion of on-going projects and future plans, let us try to realize where we are and where we want to go to. Here you see a very qualitative representation of life cycle curves for both thermodynamic standard version v1.0 and v1.1 reflecting the number of socket and plug implementations over the years till now.

The CAPE-OPEN thermodynamic standards at this point in time have two versions: version v1.0 and version v1.1; the former is still more widely supported, but the version 1.1 has a better design and solves a number of issues that were not dealt with the version 1.0 specification.

The reason for that is that implementation of the CAPE-OPEN standard by commercial software vendors is generally not driven by ideology, but rather by customer demand.

In particular this seems to hold for moving from the version 1.0 thermodynamic standard to the version 1.1 thermodynamic standard. For the software vendors to move forward with their implementation, it is important that the end-users, in particular the large chemical companies and full CO-LaN members, request their software vendors to provide support for CAPE-OPEN.

Currently, this is surely a certain drawback as, in fact, up to date any of full-functional thermodynamic servers has to support the both concurrent versions of the interface.

One may see in the Figure that the number of implementations continues to steadily grow. As to be expected the steepness of the growth is not so large as at the beginning, thus reflecting probably the fact that many of commercially available thermodynamic software is already CAPE-OPEN compliant and non-commercial developers could be addressed in the future.

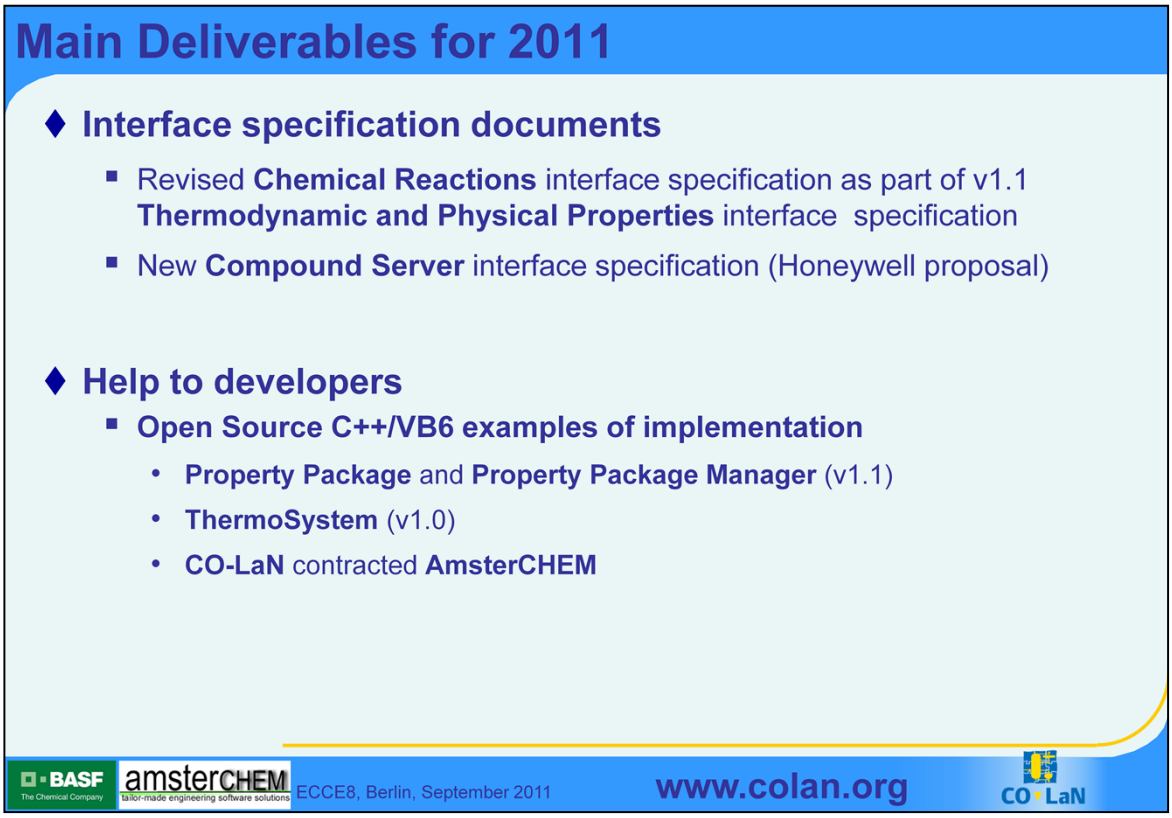
Analyzing our work on the revision, we can state that both versions have proven their applicability and completeness as generally only minor changes in form of clarifications have been required.

The main question to answer here is how to sustain or even to boost the growth.

One of the evident answers is to enlarge its applicability by providing new functionalities.

This challenge does not contradict with the idea to hold the formal interface specification fixed as improvements via inclusion of new useful interfaces still remains possible.

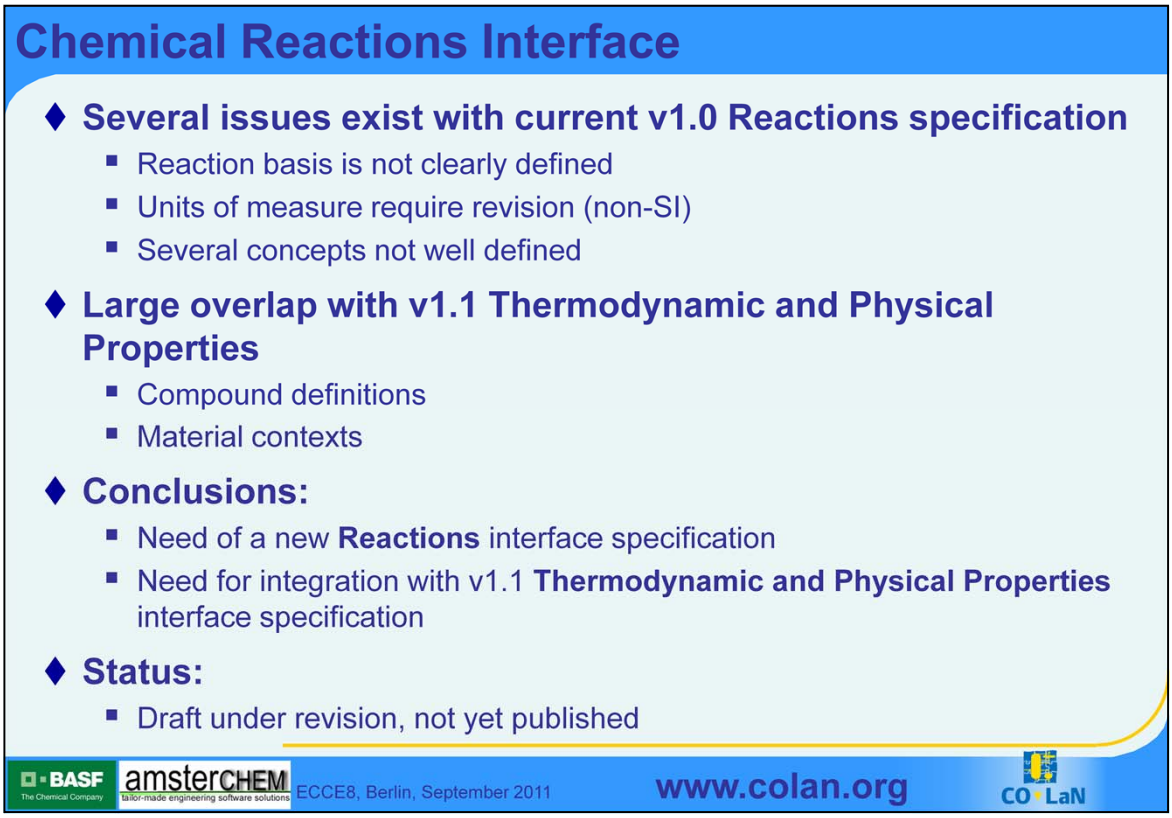
Another, and probably even more important issue here is to provide more help support to allow inexperienced software developers to start with their implementations.



The plan of Thermo SIG for 2011 addresses exactly these issues:

1) First, we work on extension interfaces for Chemical Reactions and Compound Server
2) Second, open source examples of implementation of thermodynamic servers for both interface versions v1.0 and v1.1 are to be developed. For that purpose, CO-LaN contracted AmsterCHEM and the Thermo SIG is coordinating that work.

Let us consider these works in more details



Chemical Reactions Interface

What is unsatisfactory with the current specification v1.0 which is a part of the entire CAPE-OPEN standard package?

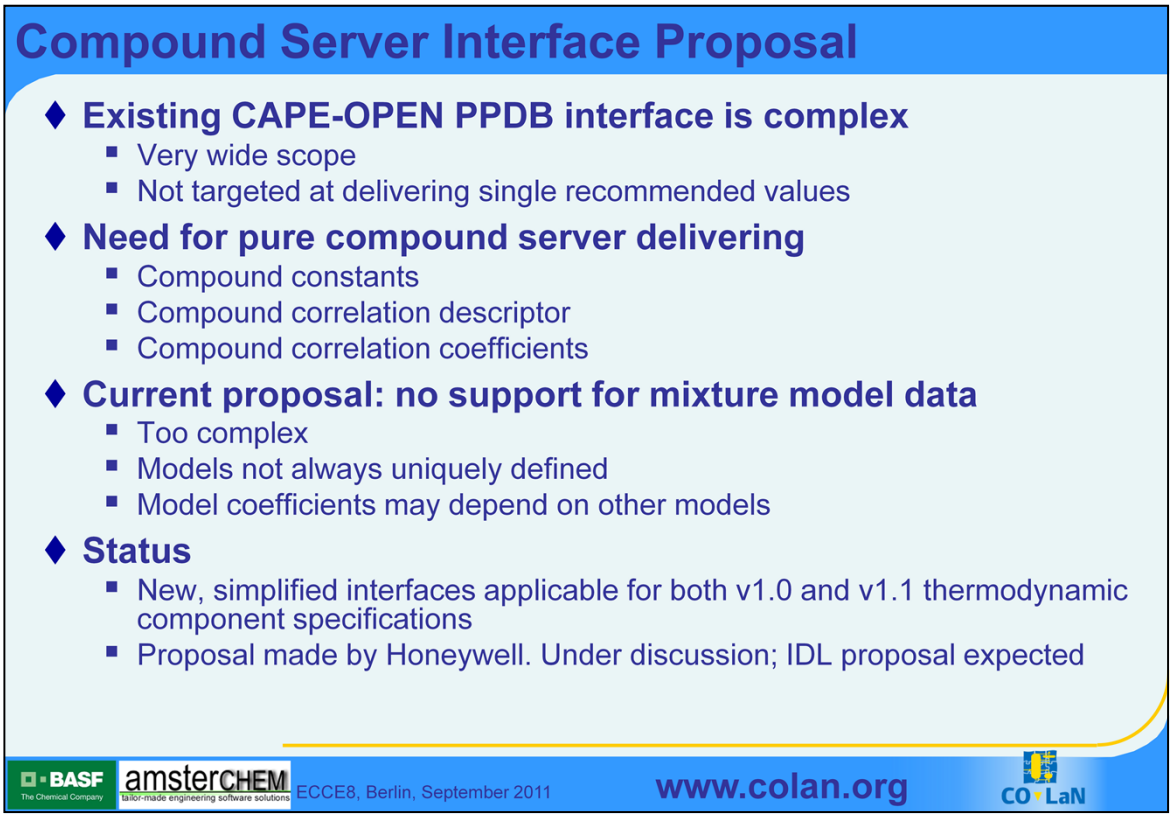
There exist several issues with that version, like that:

1) Reaction basis is not clearly defined;
2) Units of measure used are non-SI and then require revision.
3) …

Still the most important problem was seen to be the large overlap with the version v1.1 Thermodynamic and Physical Properties Interface that lead to duplication of such concepts like compound definition or material contexts.

Therefore, it was concluded to start with the revision of the existing Chemical Reaction interface with the aim to integrate it as a constituent part of the thermodynamic standard v1.1 and thus to avoid redundant coding.

The draft of the revised document is under discussion now and not yet published.



Compound Server Interface

The CAPE-OPEN standard package provides a comprehensive Physical Properties Data Base interface for communicating with databanks.

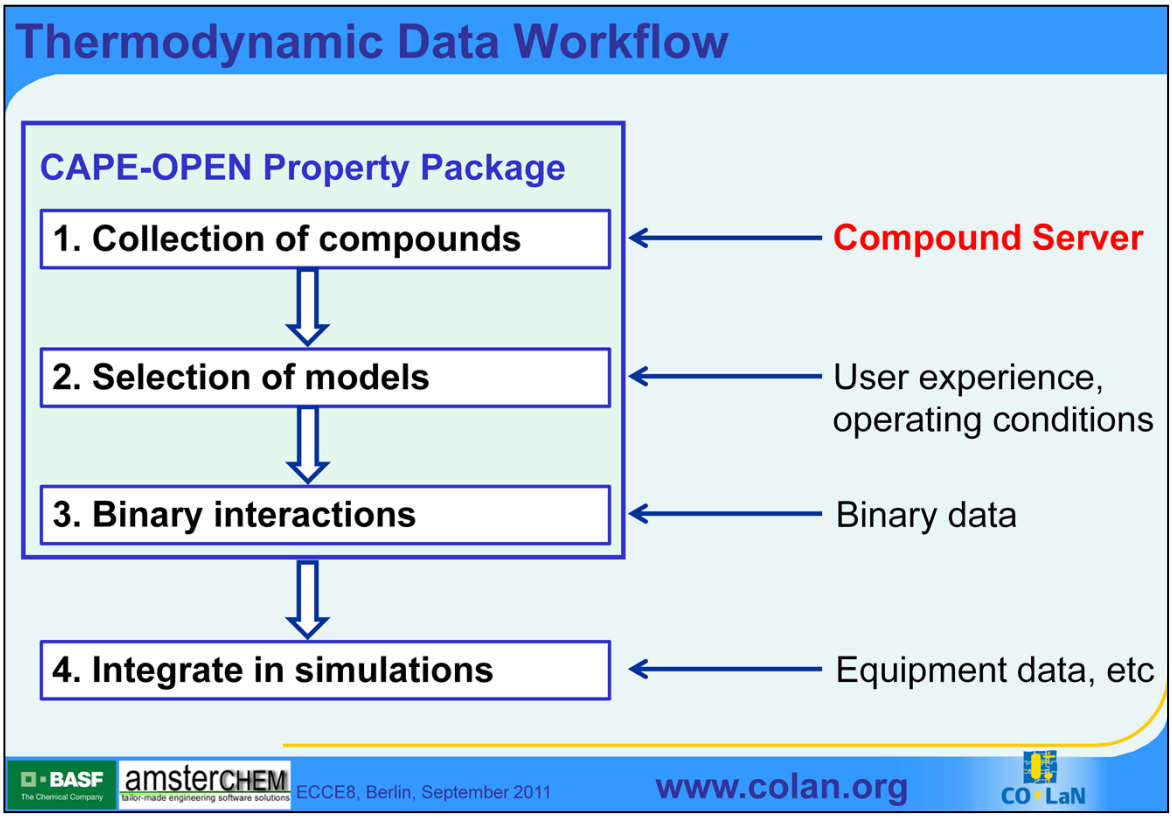
However, the usage of the existing PPDB interface coupled on thermodynamic server needs has some drawbacks. In this case, the PPDB interface seems to be overcomplicated and not really fit in, as it has a very wide scope and is not targeted at delivering single sets of recommended values.

The necessity for a simplified and target-oriented compound server interface has been realized. And this interface should provide simple and quick access to information on compound constants, compound correlation description and correlation coefficients.

All this concerns, in principle, not only the pure compound data but the real mixture model data too. However, Thermo SIG decided to start first the with pure compound data only, as handling of mixture data might generally be extreme complicated especially as the mixture model coefficients might be interrelated and thus not uniquely defined.

This new Compound Server interface seems to be useful for both specification versions v1.0 and v1.1 and so it is considered as an extension for them both.

The proposal of this interface has been made by Honeywell and it is currently under discussion.



Let us take a look on how the compound server would fit in.

Typically, designing a thermodynamic property package for a simulation consists out of the following steps:

1) create the collection of compounds, with the pure compound data,
2) select the thermodynamic and physical property models, e.g. an equation of state, and transport models,
3) adapt the model to predict the mixtures properly by adjusting binary interaction coefficients,

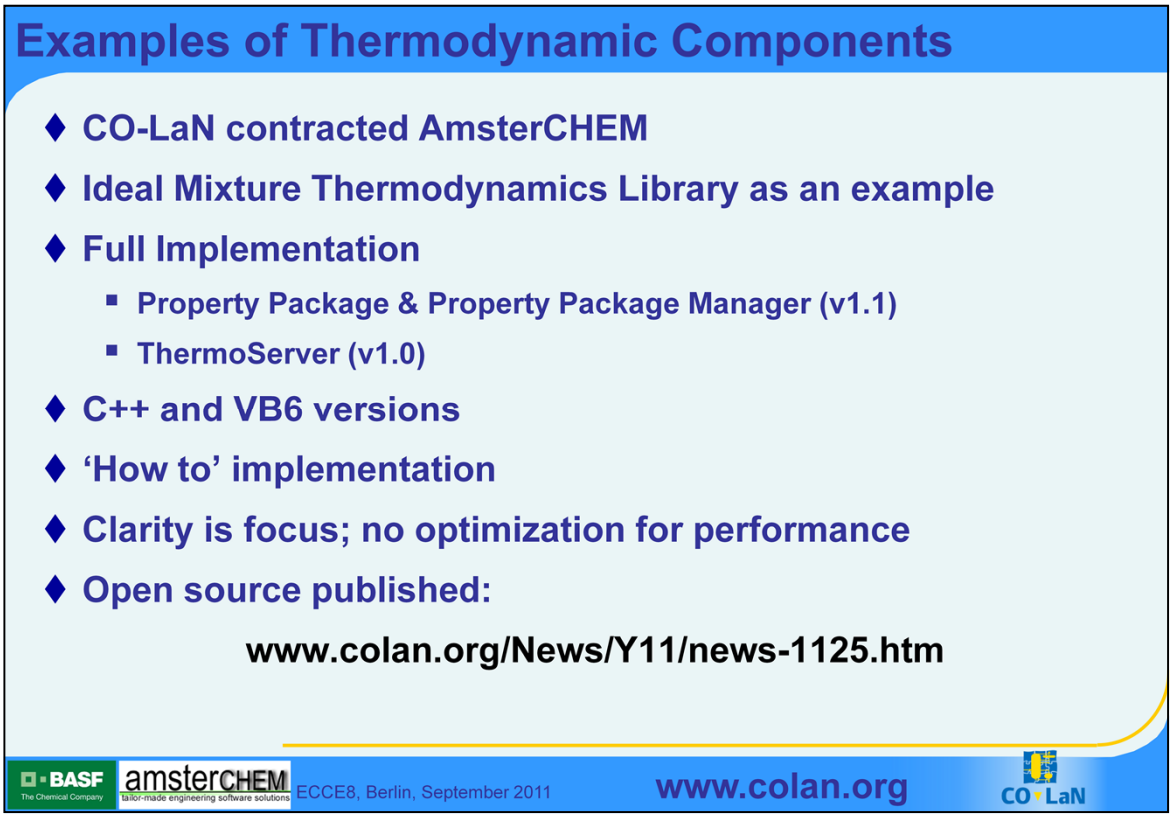
and, after the CAPE-OPEN property package has been created, we can

4) use it in the simulation.

In the first step we envision the new compound server concept to be useful.

The selection of models in the 2nd step depends on operating ranges such as pressures, temperatures and concentrations and relies on experience of the engineer.

The binary generally involve fitting coefficients to mixture data such as phase equilibria. As this step depends on the model selected in step 2, such information is hard to generalize …



Open Source Examples of Thermodynamic Servers Examples.

As mentioned above, for that purpose, CO-LaN contracted AmsterCHEM to develop the examples.

In order to keep the things as simple as possible and still to provide examples with full functionality it was decided to implement ideal mixture thermodynamics as native thermodynamic library.

As both thermodynamic specification version v1.0 and v1.1 are in use, the following objects had to be developed:

- Property Package and Property Package Manager in accordance with version 1.1 specification;

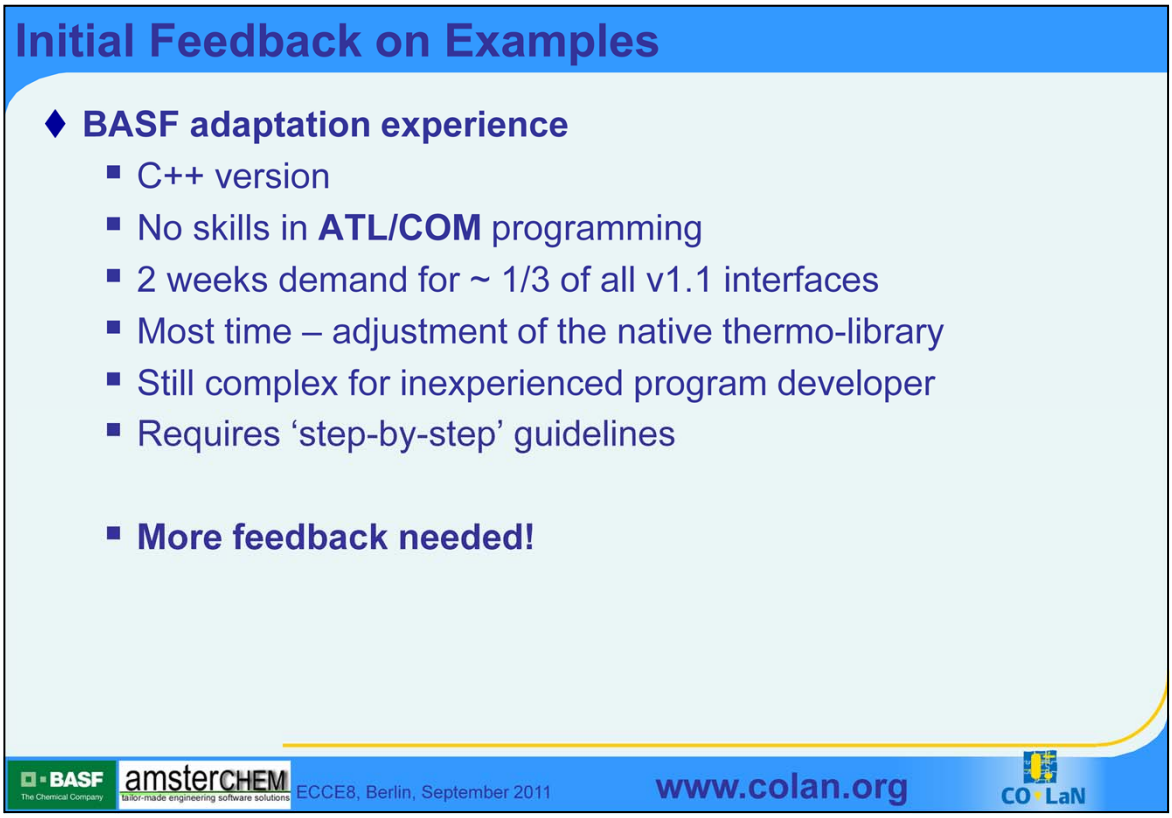
- and the ThermoServer from from the older version v1.0 specification.

The software written by AmsterCHEM for CO-LaN presents two implementation for the above objects either in C++ or in VB6, both coupled on the ideal mixture thermodynamics library written in C++.

It should be emphasized here that the examples are to be considered as 'how to' implementations with clarity in focus so that no optimization for performance has been done. For that reason, significant modifications of the example code are expected to be required for the production versions of Thermodynamic Servers.

But still we hope that the developed code might be a great help by getting started with CAPE OPEN thermodynamics.

AmsterCHEM has delivered the source code, it is now published on the web and available for testing.



At the BASF we also successfully tested the C++ version of example property package.

As the BASF-native thermodynamic library currently possesses a CAPE-OPEN socket to the third party thermodynamic server, and not the plug for using with external CAPE-OPEN compliant flowsheeting simulators, It was decided to make an adaptation of the example property package for initial tests and here you see our first feedback on this issue.

We have used the C++ version of the code for version v1.1 interface specification. The goal was to reuse the implementations of Property Package and Property Package Manager and to replace the ideal mixture thermodynamics library with the BASF native one.

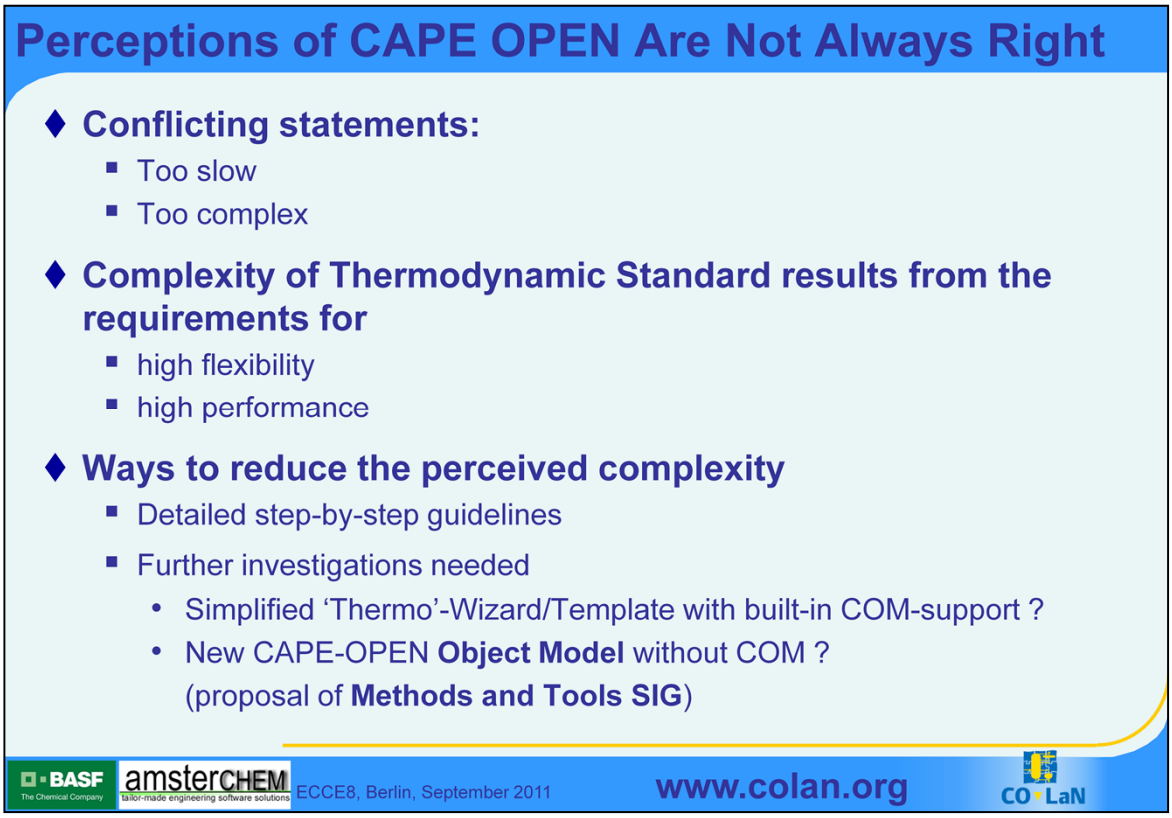
The adaptation has been carried out by me and please take into account that actually I have no experience with ATL/COM programming what may be considered as a prerequisite and this made the work more complicated.

Nevertheless, after 2 weeks I have succeeded to implement approximately one third of all version v1.1 interfaces and the most time was spent not for the replacement itself but for adjustment of the native library to CAPE-OPEN needs. So, from my personal point of view, this result should be considered as very positive.

On the other side, the initial goal of that test was different. A graduate student, who made his internship by us, was expected to carry out this work. This is a very good student with good programming skills, but still it was realized very soon, that he is not able to perform an adaptation without missing step-by-step guidelines.

So, summarizing, even having the examples at the hand, the developing of the thermodynamic server still remains complex for inexperienced program developers.

Well, this is a very subjective statement now, and actually we need more feedback on that issue to find out the ways how to improve situation if needed.



I have mentioned the complexity issue on the previous slide. And this issue coupled with the performance one are the two that are sometimes misunderstood.

Because these are, in fact, two conflicting statements: too slow and too complex.

After all, the existing CAPE-OPEN standards resulted from several years of discussions and tests within two European Collaboration projects and they aim to fulfill the two quite different requirements of high flexibility and high performance.

And here there is a possibility to stress either of these aspects: either generality at the expense of performance or high performance at the expense of flexibility.

However, either of these solutions needs a proper design! And the bad design will surely yield both bad flexibility and low performance.

The Thermo SIG is still aware of the perceptions related to CAPE-OPEN. As has been mentioned above, the necessity to provide detailed step-by-step guideline is realized. Further investigation are necessary to find out how to improve the situation.

Some of possible ways could be, e.g., providing some kinds of Wizards or Templates like it has been done for Unit Operations.

Probably, the introduction the new CAPE-OPEN Object Model as proposed by Methods and Tools SIG could also help to reduce the complexity as would not require COM programming.

Performance Issue

♦ **Problem of implementation and not of specification**

BASF performance tests for several thermodynamic packages

Simulator:	Thermodynamic Package			
Chemasim	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 (*ProSim*)	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)

BASF The Chemical Company | amsterCHEM tailor-made engineering software solutions | ECCE8, Berlin, September 2011 | www.colan.org | CO LaN

To justify my statements on performance, now I want to present the results of performance tests that were carried out at the BASF with several thermodynamic packages.

A test mixture of 12 compounds was modeled with PSRK-NRTL equation of state, the entire flow sheet comprised of several unit operations with entire complexity of approximately 100 equilibrium stages. Chemasim – the BASF in-house equation-oriented simulator – was used in all cases.

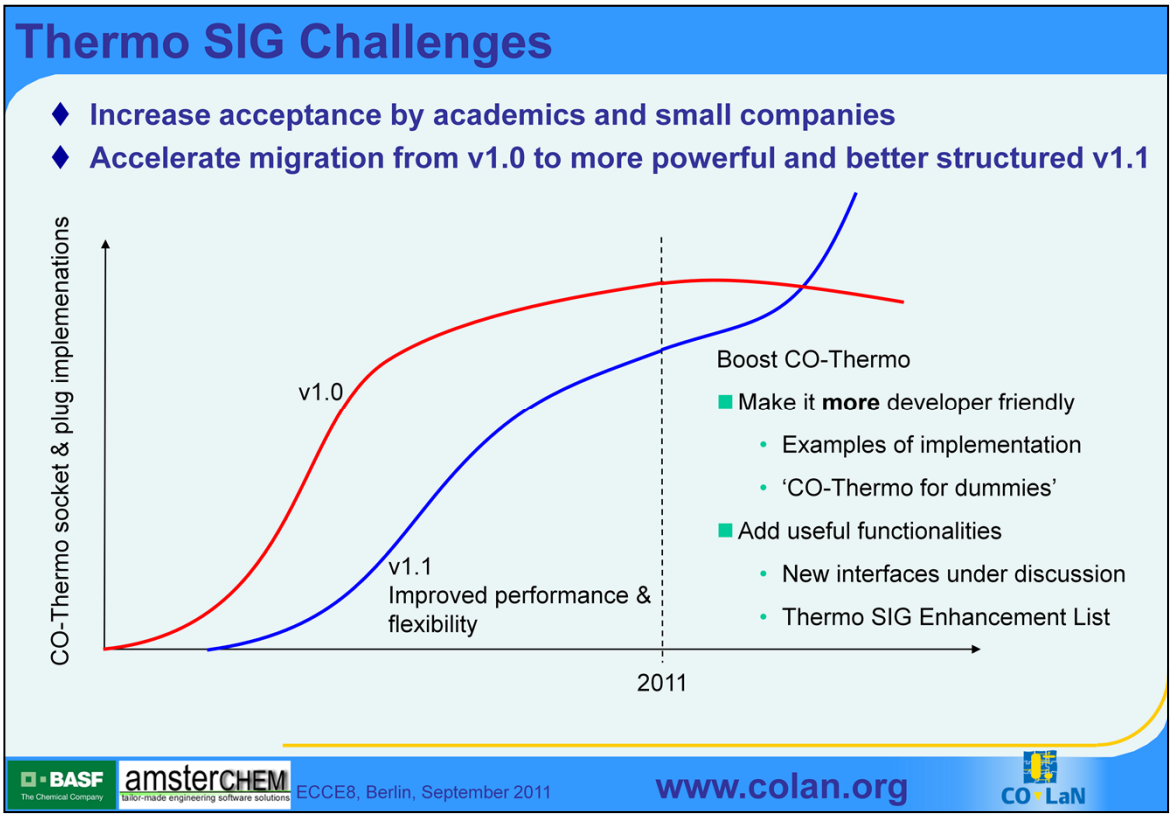
As expected, the performance benchmark corresponds to the native thermodynamic library that has been strongly optimized for usage with Chemasim. Another BASF in-house library, based on equation of states and driven via the so called ForeignObject interface by gProms, yielded the worst performance thus indicating problems either with the interface specification itself or with its implementation.

The two CAPE-OPEN compliant thermodynamic packages lie in the middle but one clearly see the significantly higher performance of the tailor-made implementation compared to a very general and flexible implementation via Thermo-Wrapper provided by Prosim.

The tailor-made implementation has now found a very good acceptance by the end users in the BASF and the number of CAPE-OPEN applications steadily grows.

As the internal architecture of the native BASF Thermo-Library is not really well suited for CAPE-OPEN interface, there still remains high potential for further performance improvements after some refactoring. So we expect the number 1.86 to go down after further optimization; in particular, significant performance increase will be gained when batch calculations of properties in a single call will be available.

Thus, these performance tests justify the statement that the performance issue is actually the problem of implementation and not of specification itself.



Let us finally take a look on the further evolution of the life cycle curves as we could imagine and desire.

To boost the number of implementations in the future, Thermo SIG should probably find the ways to:

1) Increase acceptance of CAPE-OPEN by academics and small companies

2) Accelerate the migration from v1.0 to more powerful and better structured version v1.1

We expect future developments to focus more on version 1.1, while version 1.0 will slowly fade out as it is cumbersome to provide concurrent support for them both. It is important that the end-users, in particular the large chemical companies should request their software vendors to provide support for version v1.1 thermodynamic interface.

The first problem still seems to be more important and it is clear that one of the major goals here is to make CAPE-OPEN more developer friendly through examples of implementation and detailed guidelines as already discussed in the presentation.

Another way to increase acceptance is to provide new useful interfaces. Two such interfaces have been discussed in this talk.

Thermo SIG also records other suggestions how to enhance the specification.

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**

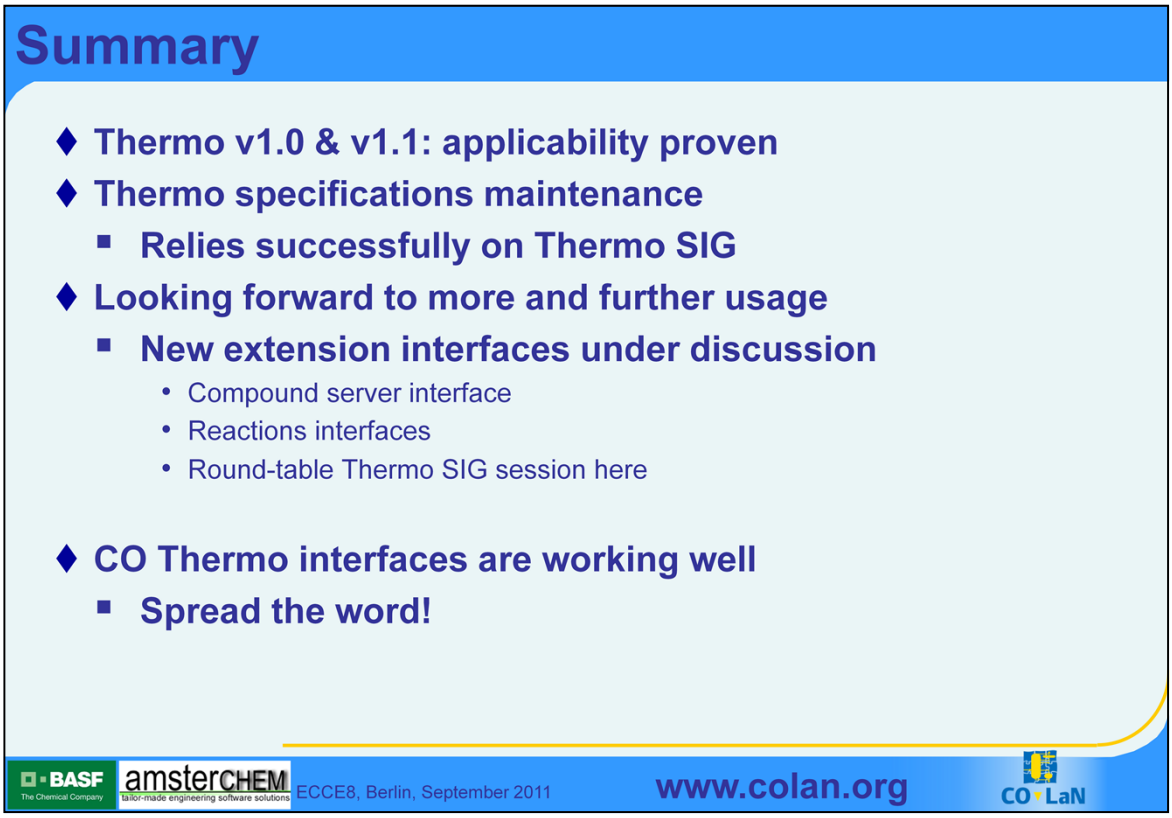
Some of these suggestions are listed here. It might be noted that many of them are aimed on the further performance increase, like

1) suggestion to avoid communications with strings or
2) setting calculation conditions in a single call or
3) providing support for array-wise property calculations.

Still, the analysis of all these suggestions revealed no necessity to start development of a new specification version v1.2 in the nearest future.

It might, however, be discussed whether some of these suggestions could be incorporated into existing interfaces.

And it has to be kept in mind when we start with version v1.2 that it must be binary compatible with the well proven version v1.1



To summarize the presentation I would like to point out that

1) The applicability of thermodynamic specification in both versions v1.0 and v1.1 has been proven over the years in real world applications
2) The maintenance of thermodynamic specifications successfully relies on Thermo SIG
3) We are looking forward to more and further usage and, hence, develop new extension interfaces like the two ones presented here
4) And after all, according to our experience now we can state that CAPE-OPEN thermodynamic interfaces are working well, so

Let it be better known !

Questions?

Thank you for your attention!

Go CAPE-OPEN!