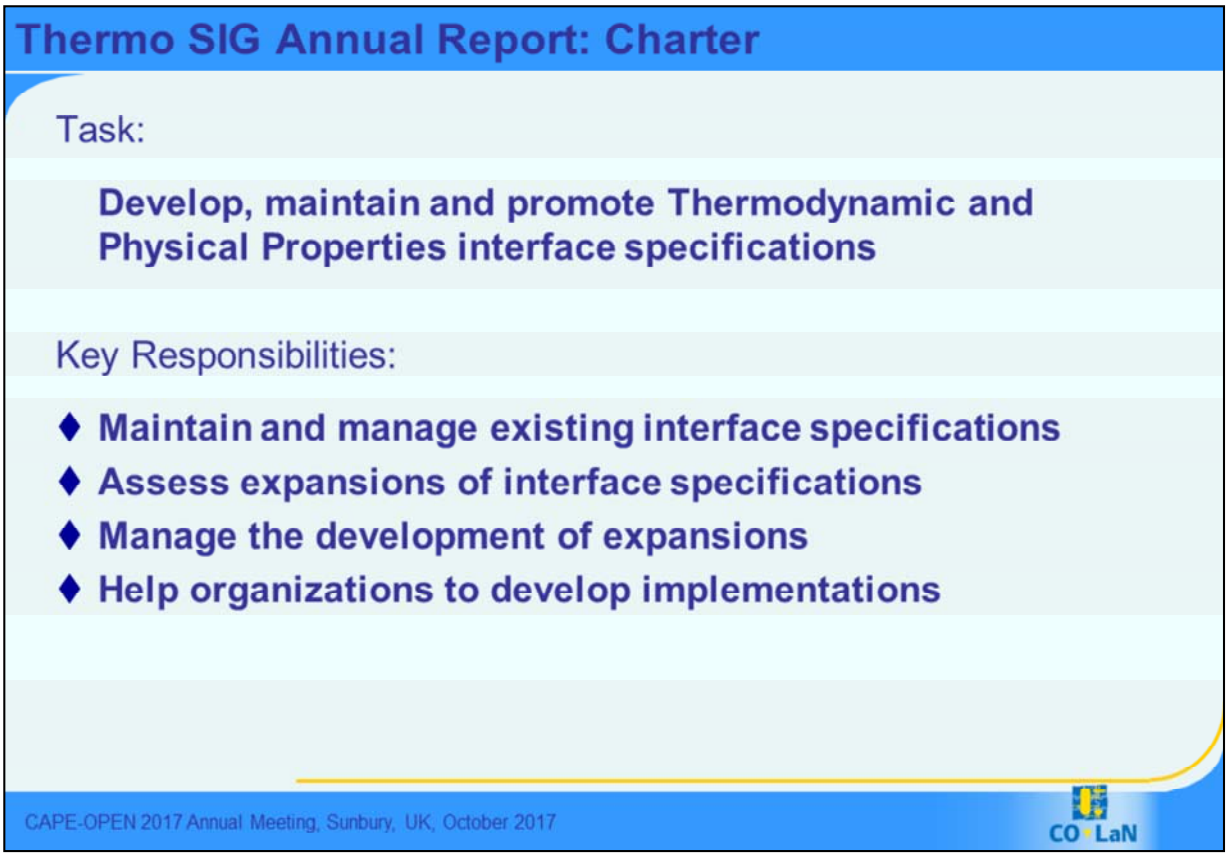
Good morning. This is the thermo SIG update for 2017. Normally Sergej would do this presentation, but he could not make it to this meeting alas. So you will have to do with me for today. I am Jasper. Mark Stijnman, Bjørn Maribo-Mogensen, Michel, Sergej and myself have been meeting 2 h / week this year, and we have been doing some work offline, so we made good progress.



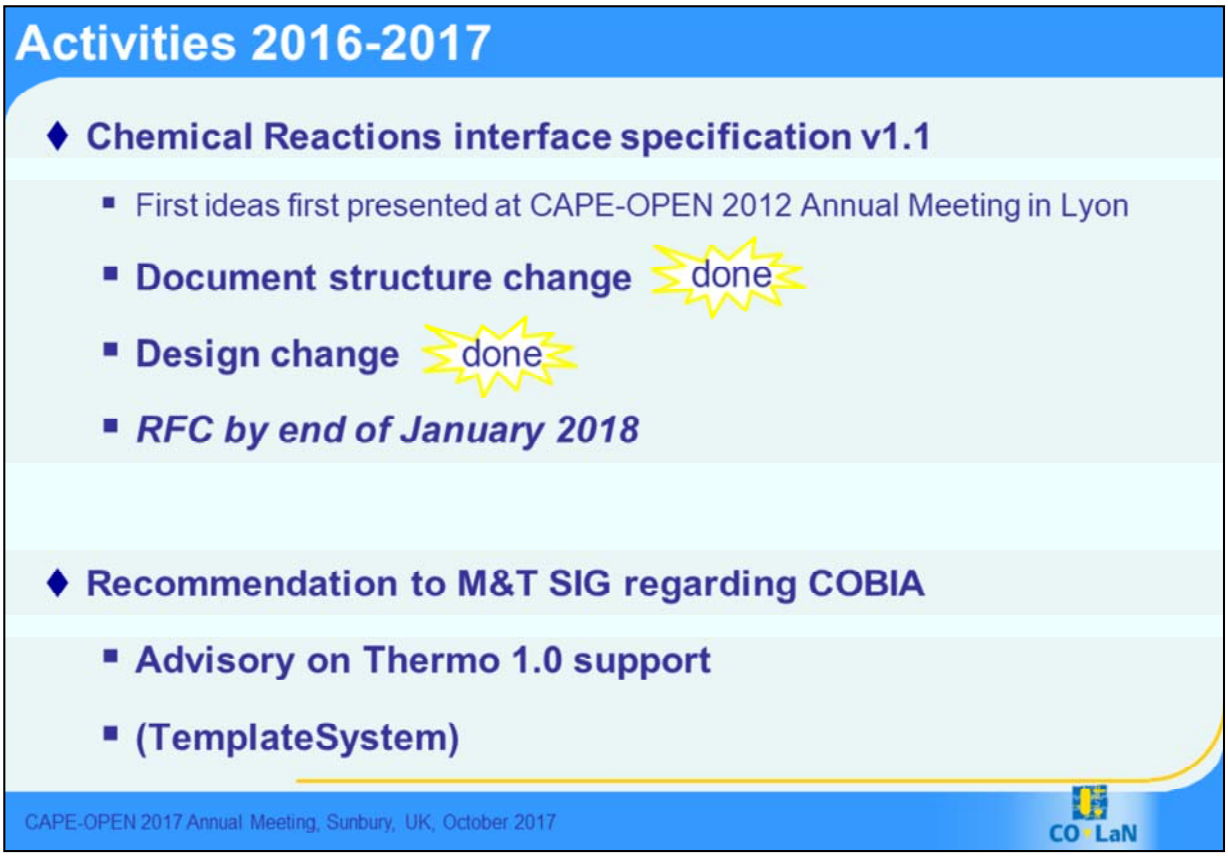
As always, the charter. The Thermodynamics Special Interest Group is an organizational unit within the CAPE OPEN Laboratories Network with the task to 'develop, maintain and promote Thermodynamic and Physical Properties interface specifications'.

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 these expansions
4) Provide help support to developers of CAPE OPEN compliant software

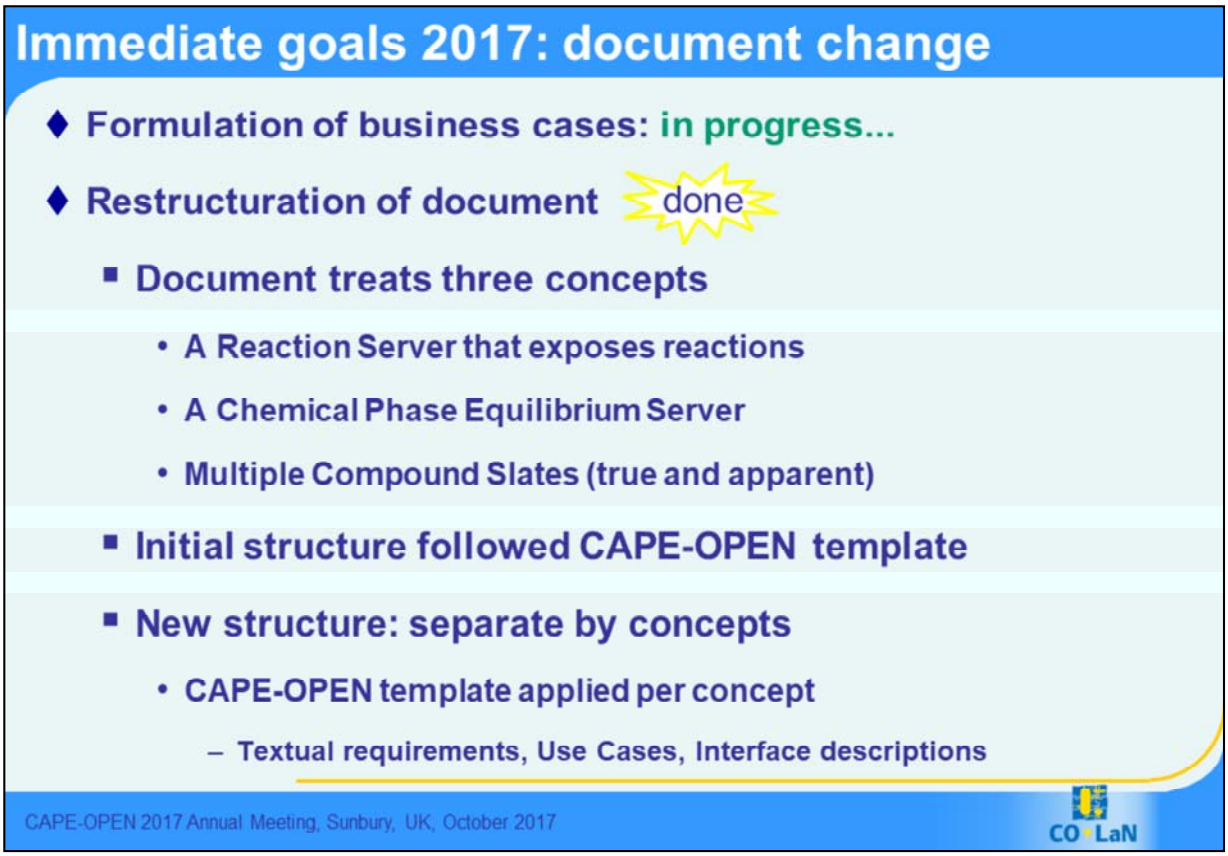
The people shown on this slide are currently member of the thermo SIG.

The highlighted people are the ones that visit nearly all phone meetings. You can join of course, if you are in



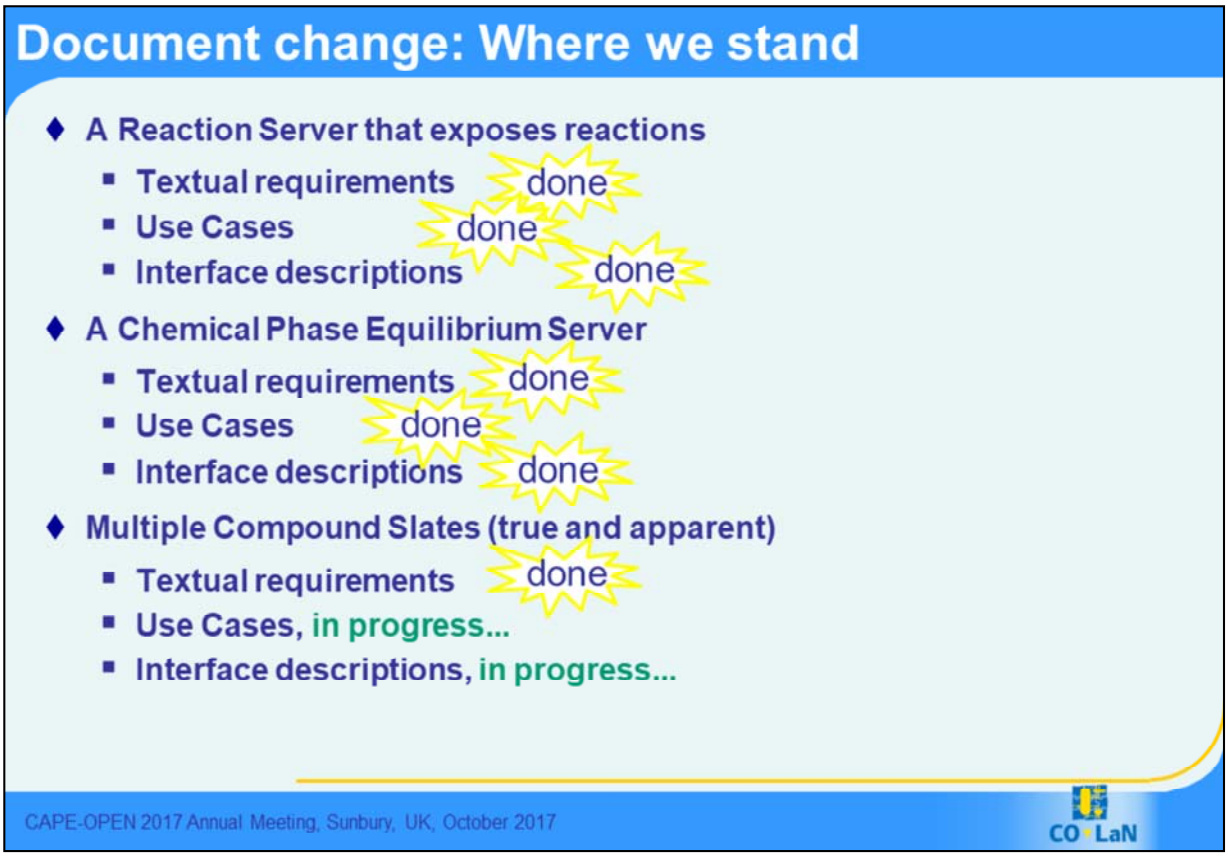
The first half of this slide presents what we were set out to do in 2017 for the Chemical Reaction specification. The document structure change that was proposed is done. The design changes that were proposed are done. In fact we made an additional design change. We aim to be ready to send this document out for RFC by the end of January.

In addition to the Chemical Reaction specification we performed some reviews and advisories to aid the M&T SIG with setting up COBIA.

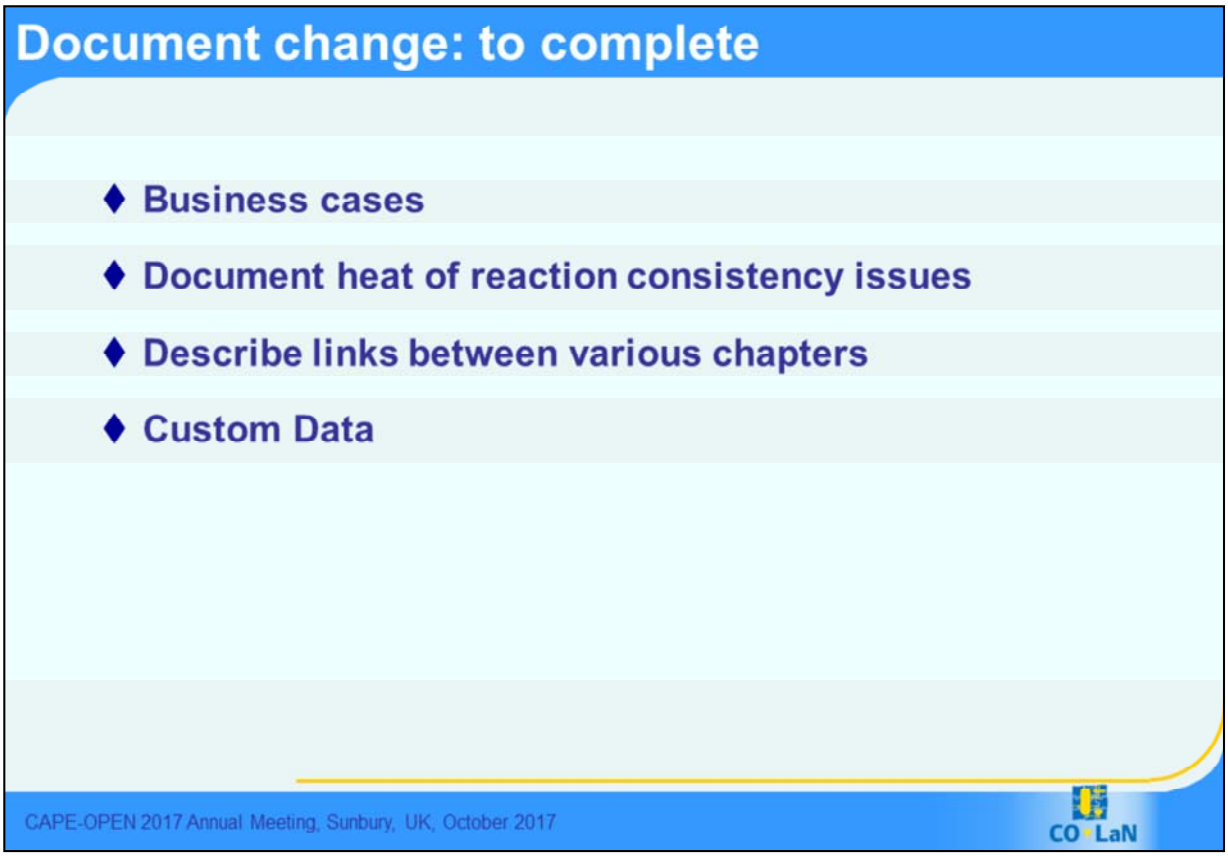


Firstly Mark reasoned that the business cases that demonstrate the relevance of the newly proposed interfaces were missing. The work on this aspect is not yet done.

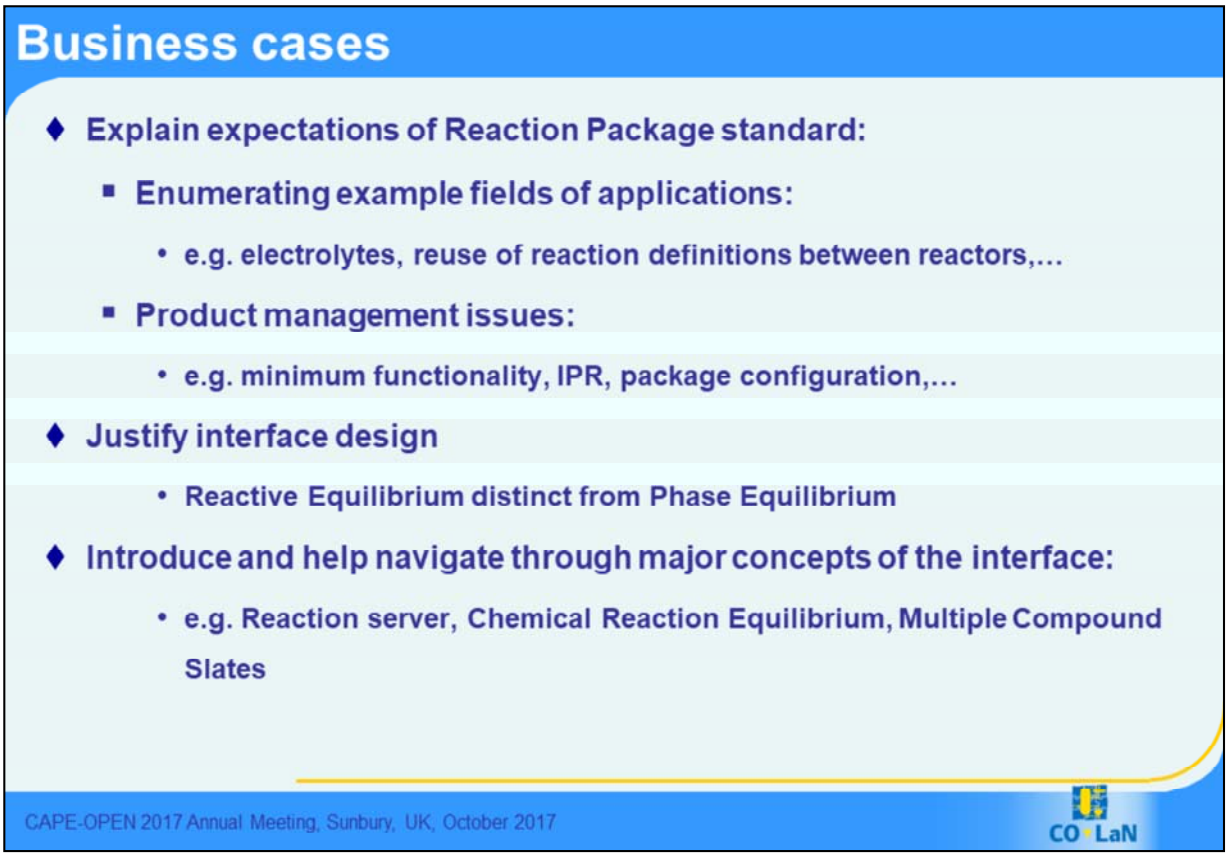
Mark also offered the suggestion to take the three separate topics that are treated, chemical reactions, chemical phase equilibria and compound slates, in a more readable fashion. At first the entire document was organized along the normal CAPE-OPEN structuring; introduction, textual requirements, use cases, analysis and design. Now each of the three subjects is structured as such and can be read as separate entities. But the coupling between these subjects is maintained through common introduction and theory chapters.



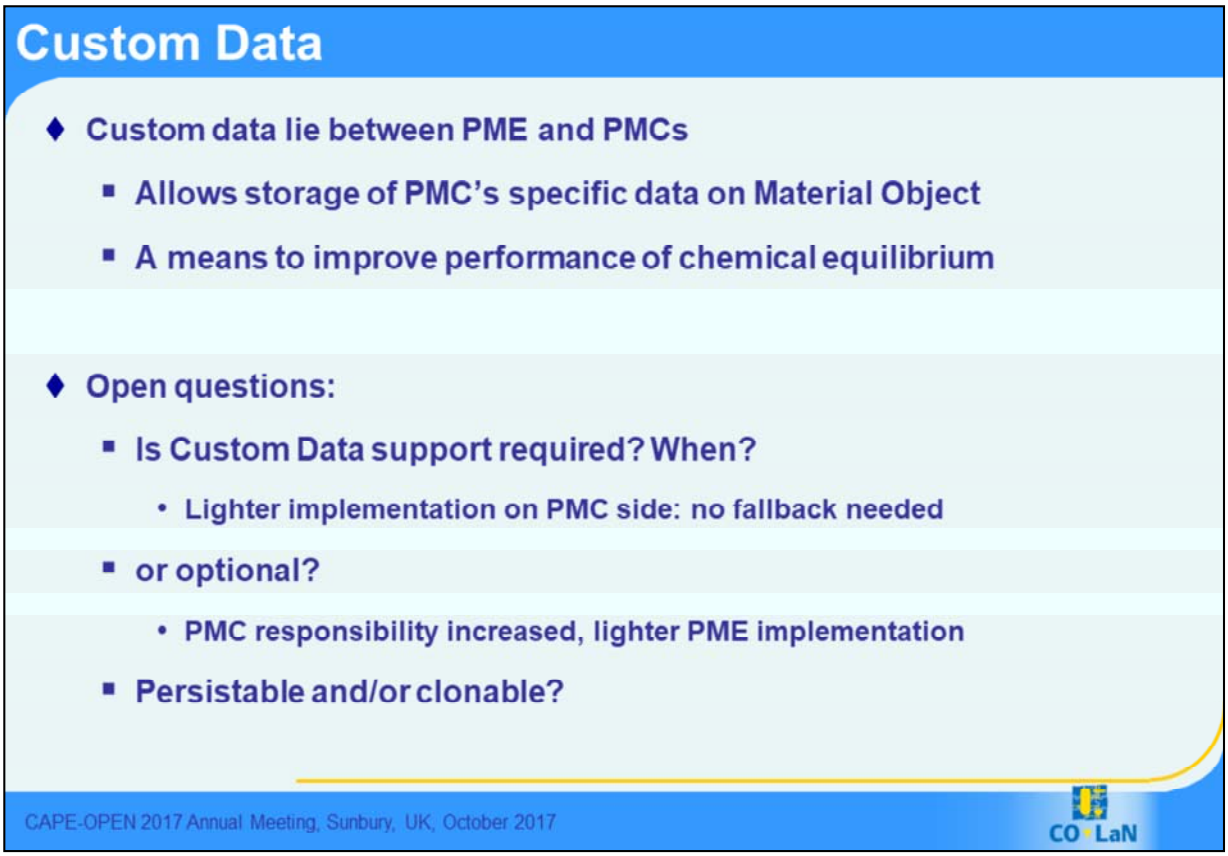
For each of the main topics we therefore now have textual requirements, use cases and analysis and design, where the interfaces desciptions live. For Reaction Servers and Chemical Phase Equilibria, each of these chapters is done. For the Compound Slates chapters, we completed the textual requirements, but some work is still to be done on the use cases and on the analysis and design chapter.



In addition to these main chapters, we have some work to complete in the remainder of the document. We need to describe business cases. We need to document heat of reaction – in particular we need to describe that heat of reactions is at operating conditions and how this relates to heat of reaction at reference conditions. We need to clean up the links between these chapters and how they may be used in conjunction. Finally we need to do some work on the Custom Data interface that was suggested and documented last year.



Business cases need to be described not only to illustrate the relevance of this standard specification, but also to clarify which part of the standard specification applies to which type of process model. Note that business cases are not the same as use cases that we find in each CAPE-OPEN document. Business cases are enumerations of possible applications, and illustrate what functionality is expected for each application. From this, a justification of the proposed interfaces will naturally follow. For example when you describe a process involving reactive phase equilibria, it becomes evident rapidly why the current non-reactive phase equilibria are not sufficient to fulfill the business case requirements. It also helps to identify which parts of the documents are to be read by which parties.



The Custom Data interface was proposed last year to help PMCs store any data on the Material Object. The reason we want to do that, is that data that pertains to describing a particular material should be coupled to the life time of the material. So attaching it to the material object make sense. When the material object no stops existing, so does the data that is associated with it. Even the data that is private to a PMC. Property packages are the PMCs we currently have in mind for his. Particularly property packages that provide the Material with a composition that is not the true composition known inside the property package, because the property package internally carries out reactions, will need the true composition each time a property calculation must be performed. No better place to store the true composition than on the material. But we cannot store it as composition as it does not match the exposed compound slate. So we store it as custom data. This will prevent the property package from having to reevaluate the chemical equilibrium in a particular phase over and over again.

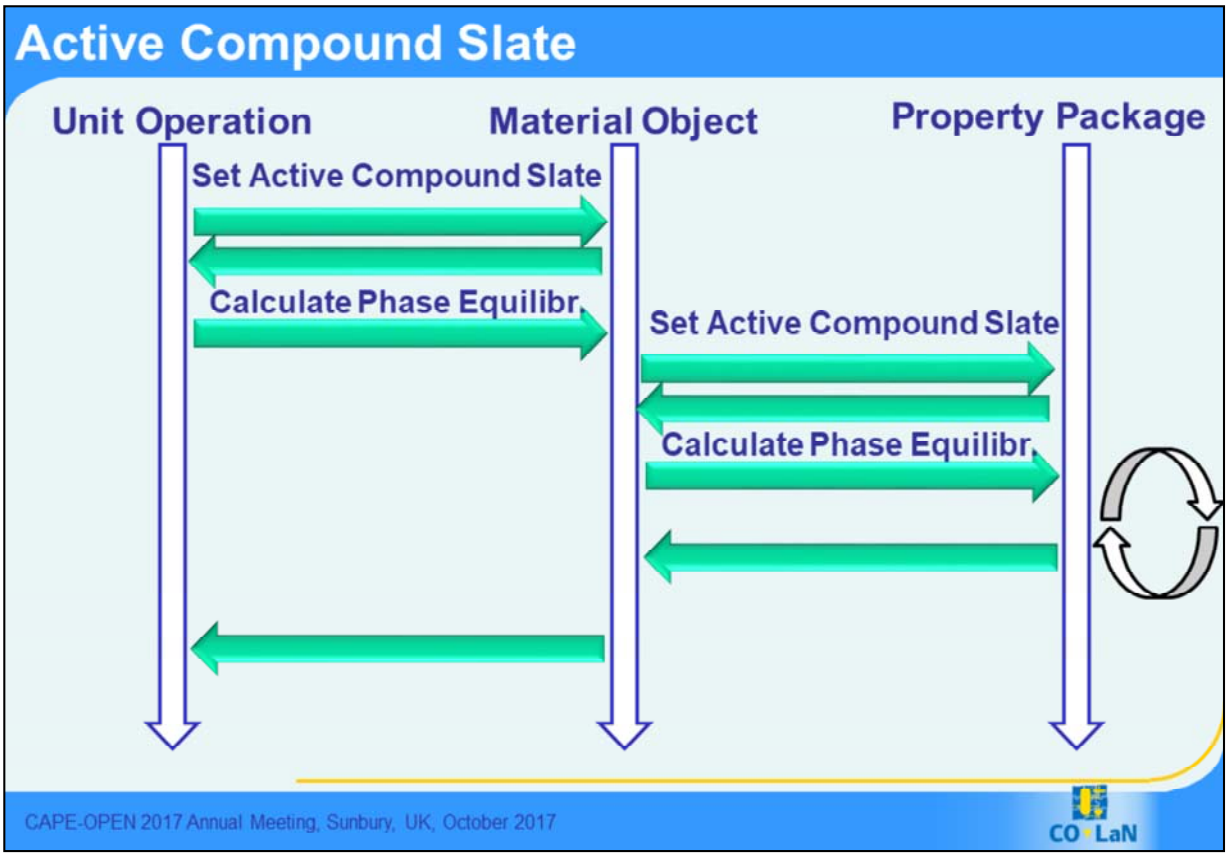
We would like this custom data interface to be implemented on each Material Object as a requirement. Of course this is not possible as there are currently many material object implementations around that do not do so. Nevertheless, there is a good business case to be made for custom data support to be required on a material object for dealing with property packages that internally perform reactions. If not, the property package internally needs to recalculate chemical equilibrium at each property call, which is prohibitly expensive, or need to set up some sort of caching mechanism for its private data, which is considerably more difficult than storing it on the Material Object as the Property Package has no way to know about the Material Object's life span and can at best guess at a cache size.

Finally as the Material Object specification allows for duplication of the material object, perhaps the custom data must be duplicatable as well. Or persistable. Or both. Something to be decided, still.

Structural changes made to the document in 2017 include: the hierarchy of reactions that was proposed earlier was deemed too complex and has been dropped. It is now clearer what is the difference between a reaction server that exposes reactions and a chemical phase equilibrium server that performs its reactions internally. Minor clarifications have been made for Chemical Equilibrium Servers. For multiple compounds slates we introduced last year the concept of delegates. A delegate was essentially another copy of a material object on which one operates in a different compound slate. The state between a material object and its delegates was shared, which is temperature, pressure, composition, phase fraction. But the thermophysical properties are specific to each delegate. Although effective, it was observed that the concept of a delegate was slightly overwhelming, and this has been changed to a simpler notion of an active compound slate on a material object. Functionality-wise it is more or less the same; change the active compound slate and you share the same state, but different thermophysical properties. Some additional bookkeeping is required on the Material Object implementation to ensure that if one PMC sets the active compound slate, it does not affect another PMC. So some new work flows have been defined for this.

New slide: explain active Compound Slate

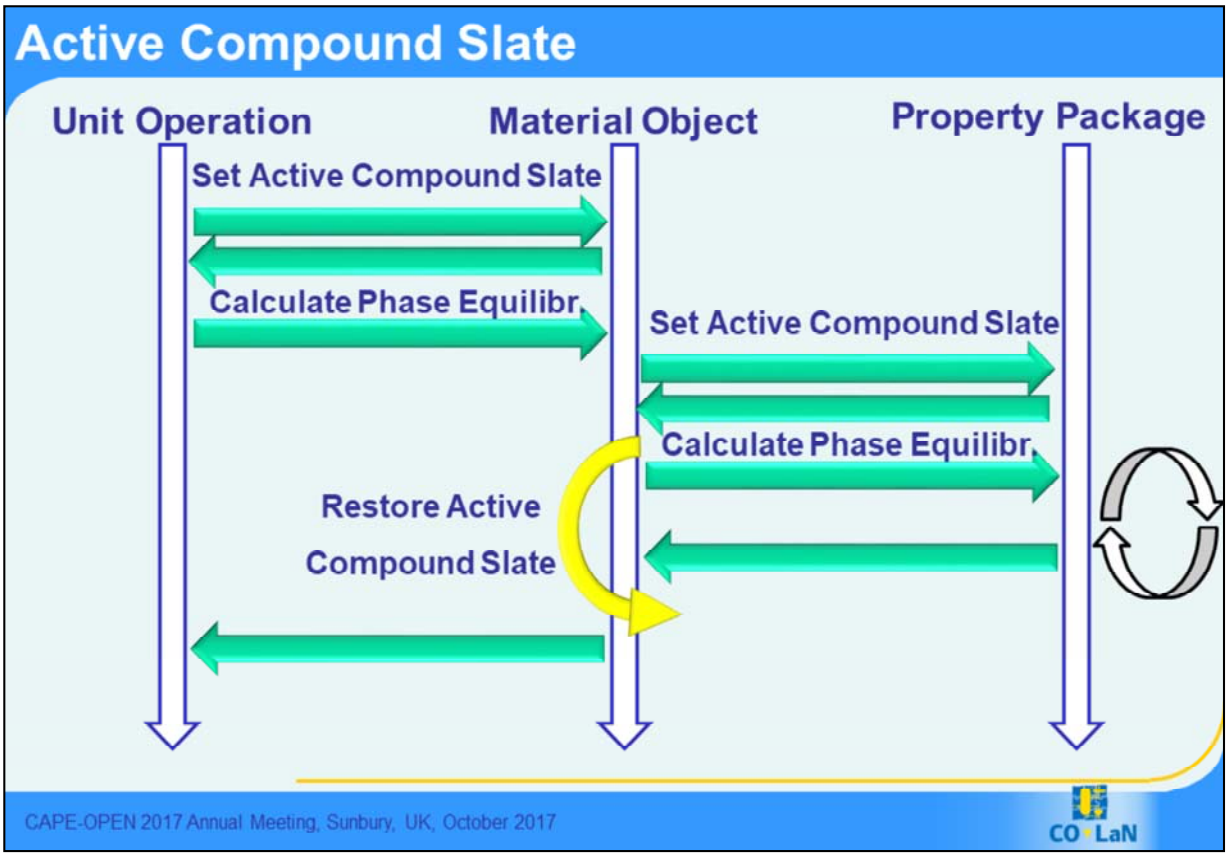
- Reasons
- Why drop Delegate?



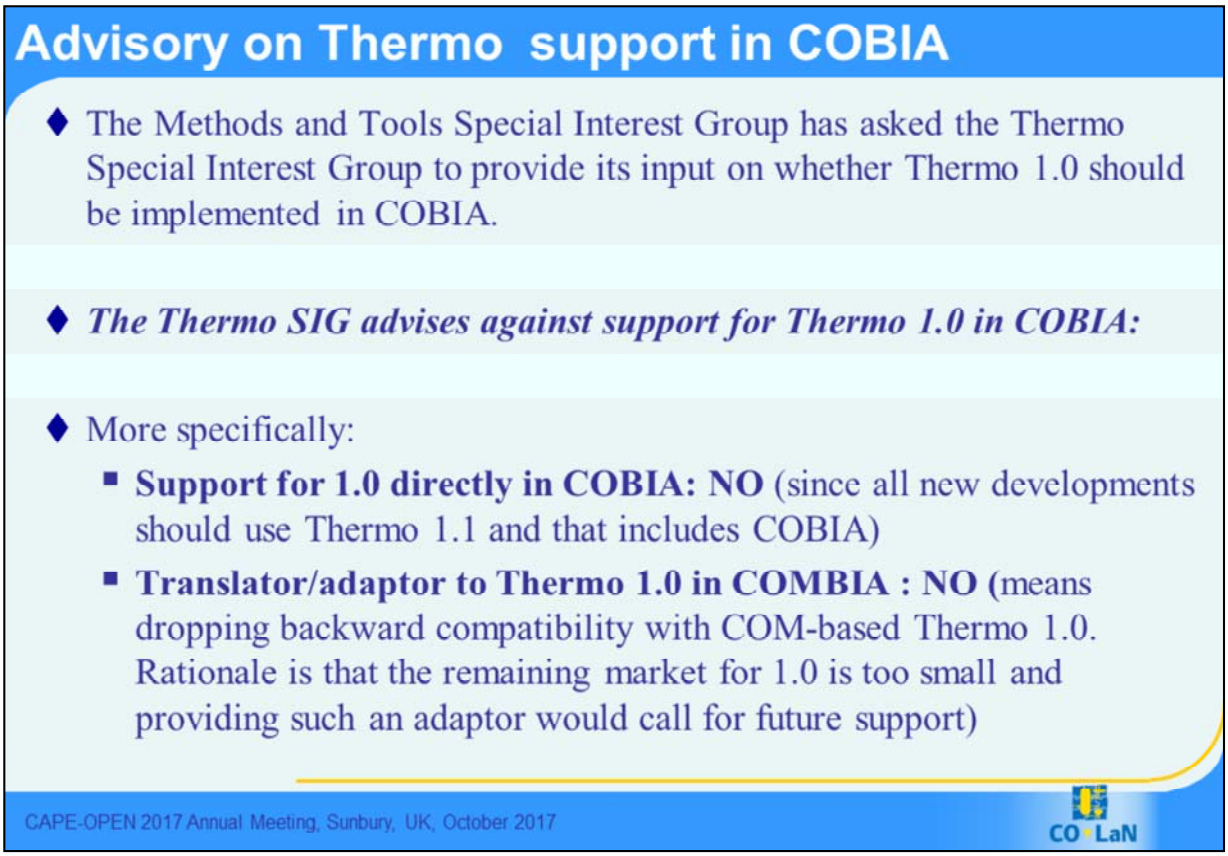
As an illustration, the interaction between a Unit Operation, a Material Object and Property Package might look like this, when the Unit Operation want to perform a phase equilibrium calculation in a particular compound slate. First, it sets the compound slate as active on the Material Object. Then it requests the property calculation. The Material Object in turn needs to ask the Property Package for the property calculation. To do so it first makes sure the active compound slate on the Property Package is selected to reflect the active compound slate on the Material Object.

As a side effect of the phase equilibrium calculation, the Property Package may or may not decide to change the active compound slate on the Material Object. After, as state is shared between all compound slates, the Property Package may set the composition of the resulting equilibrium phases in a compound slate of its choice. Should the Unit Operation later on query phase composition in the target compound slate, machinery is in place for just-in-time composition conversion. Much like the Material Object's just-in-time basis conversion.

As a side effect, when coming out of the Property Package's CalcEquilibrium, the active compound slate on the Material Object may have changed. This would lead to an unpredictable situation in the Unit Operation, as the active Compound Slate on the Material Object no longer is that what was specified by the Unit Operation. Hence, the additional book-keeping the Material Object must to do ensure PMCs are not affected by change of active compound slate by other PMCs.

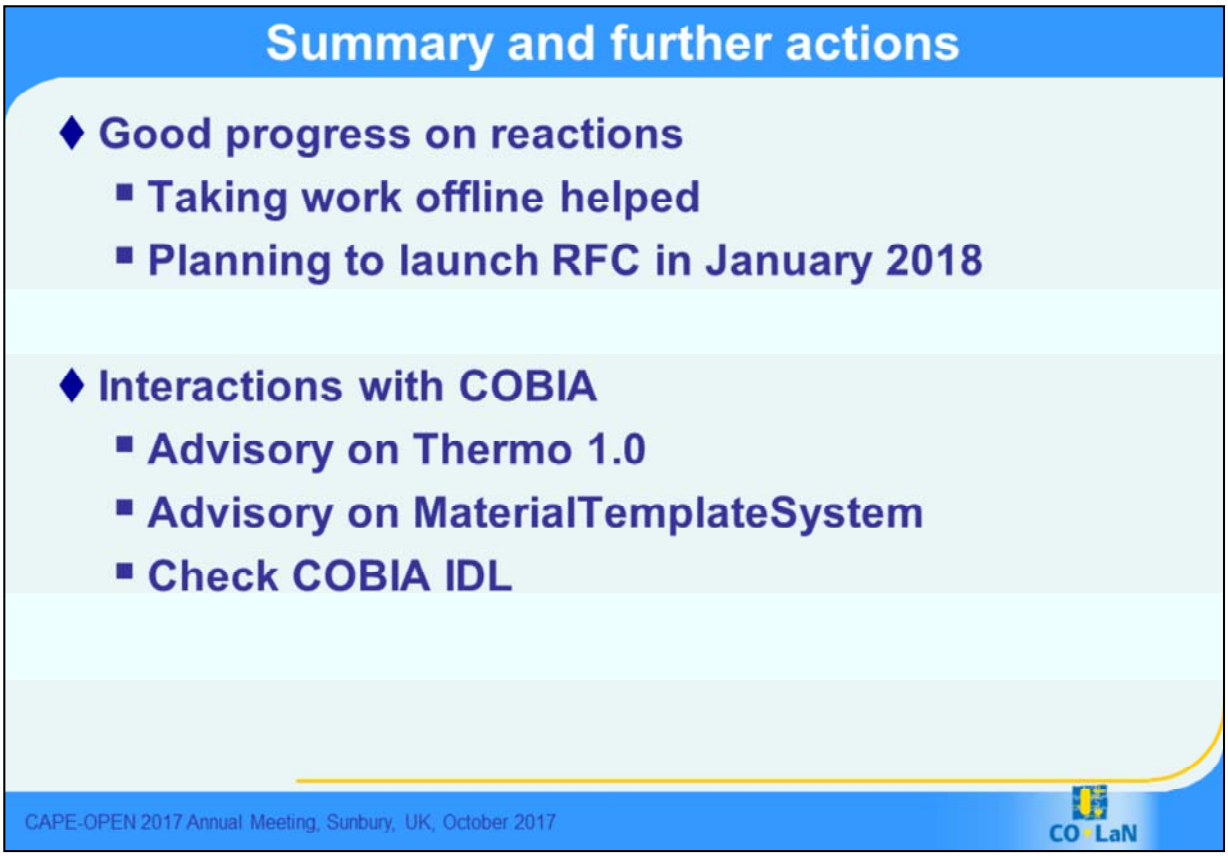


As a general rule, it is the PME's responsibility to restore the active Compound Slate on Material Object after each external call. In this slide the call to the Property Package's CalcEquilibrium.



The M&T SIG asked for whether we should or should not implement support for CAPE-OPEN 1.0 in COBIA. The Thermo SIG's outcome was unanimous. The answer is no. The issue is not so much that the use for 1.0 gets less and less, but rather that if we implement new software to cover 1.0 support, people will continue to develop in 1.0. And we have advised already long ago that all new developments should use 1.1.

So do we support the interfaces themselves? No. Do we put a layer in between that automatically converts between 1.0 on the COM side and 1.1 on the COBIA side? No – this option is even worse, as the conversion between 1.0 and 1.1 is not one-to-one, so is subject to interpretation of the standard. This will surely be subject of debate and of future support. And we have better things to do.



To summarize:....

Thank you very much for your attention, and I will be happy to answer any questions.