

Thermo SIG Progress Report 2010 and future outlook

Sergej Blagov, BASF, Ludwigshafen / GERMANY

Jasper van Baten, Amsterchem, Cuevas del Almanzora / SPAIN

Michel Pons, CO-LaN, Lyon / FRANCE

The CAPE-OPEN Special Interest Group on the thermodynamic standards (Thermo SIG) is responsible for maintaining, revising and managing the CAPE-OPEN thermodynamic standard specifications. Its members consist of representatives from simulation software vendors and industrial companies. This presentation will report on the accomplishments of the Thermo SIG in 2010 and deliverables for 2011.

In 2010, revisions of CAPE-OPEN thermodynamic standard specifications versions 1.0 and 1.1 have been formulated and internally approved; revised documents are published and contain various clarifications and corrections.

While the changes clarify some former ambiguities, they do not have impact on the formal interface definitions, so that downward compatibility is assured. The developed standards have proven their completeness in the past and have successfully been used in various applications for solving real world simulation problems. As examples, some experiences at BASF regarding the use of CAPE-OPEN will also be presented.

Amongst the deliverables for 2011 is the incorporation of the Chemical Reaction Interface specification into the thermodynamic standards specification version 1.1. Although chemical reactions are an important part of process simulation interoperability, its standard specifications have not been yet developed properly to fit into the CAPE-OPEN thermodynamic version 1.1 standard framework. The current presentation will highlight the application of the chemical reactions standard, and discuss some of the improvements over the older version 1.0 chemical reactions interface definition. An example application will demonstrate the intended use of the new interface specification.