Using COSMOtherm in Process Modelling Environments

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**COSMOthermCO: The COSMOtherm – CAPE OPEN Interface**

- **CAPE-OPEN (Computer-Aided Process Engineering Open Simulation Environment)** is a collaborative project between a group of operating companies, technology vendors and academic groups, sponsored by the EC:

  - Different simulators have different strengths, so that to obtain the best results for a particular problem, access to more than one vendor simulator and to in-house software containing company specific methods or data is usually required.

  - The main objective of **CAPE-OPEN** is to enable native components of a simulator to be replaced by those from another independent source, or that are part of another simulator, with minimal effort in as seamless a manner as possible. So that it will be possible to assemble a process model from a set of software components encapsulating **physical property methods**, **unit operation models** and **numerical algorithms** that are communicating through the open standard interfaces.

  - **CAPE-OPEN** delivered interface standard specifications for the main components of a process simulation.
**Rationale:** Make available COSMOtherm calculated properties in Process Modeling & Engineering software applications via CAPE-OPEN standard interface definitions.
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- A CAPE-OPEN compliant *ICapeThermoPropertyRoutine* was developed in collaboration with Amsterchem (J. van Baten, R. Baur): COSMOthermCO

- **COSMOthermCO** provides:
  - Activity Coefficient $\gamma$
  - Unconstrained derivatives of $\gamma$ with respect to temperature
  - Unconstrained derivatives of $\gamma$ with respect to concentration
  - Properties related to $\gamma$ and its derivatives: $G^E$, $H^E$, activity, ...
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The interoperability and CAPE-OPEN compliant of COSMOtherm CO has been verified with all major Process Modeling & Engineering (PME) programs:

- Aspen+ (Version 2004.1 and later) by AspenTech
- Hysys (2007 Release and later) by AspenTech
- PRO/II (Version 8.0 and later) by SimSci/Invensys
- ProSim and ProSimPlus (2007 Release and later) by Simulis
- COCO-TEA (Version 1.05 and later) by AmsterChem
- ChemSep LITE (Version 5.5 and later) by ChemSep
- gPROMS (2007 Release and later) by PSE
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- Demonstration Version:
  - A *free* version of COSMOthermCO (COSMOthermCO-LITE) is available within the *free* PME COCO-TEA by AmsterChem
  - The latest version of COCO can be downloaded from:

  http://www.cocosimulator.org/index_download.html

- For more information see:

  http://www.amsterchem.com/coco.html