

Engineering &
Maintenance

Experiences with **THERMO Wrapper in BASF**

Competitive
Engineering

 **BASF**
The Chemical Company

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CHEMASIM - Inhouse Simulator in BASF

- > 25 years experience
- Calculation in FORTRAN, user interface in VB
- Equation oriented
- Very fast (typical calculation time in secs not minutes)
- ~ 250 users
- < 400 000 calculations in 2008
- Mainly low-pressure region
 - => Thermodynamics
 - strong in activity coefficient models
 - weak in EOS
- More demand for complex EOS models like PSRK, PCSAFT...
 - special solution (restricted)

=> Decision to use CO THERMO interface

CO-THERMO Interface in CHEMASIM

Need of:

- Property Package
 - Multiflash from Infochem - or others

- Material Object
 - Implementation in VB 6
 - Seemed simpler
 - some knowledge in VB 6 and COM existed

CO-THERMO (Version 1.0) Interface in CHEMASIM

Experiences:

- Implementation more difficult than expected
 - Use of ‘magic art’ in VB 6 (lack of knowledge?)
 - Calling COM from Fortran through “Variants&SafeArrays” is complicated
 - more “trial and error” than reading help docs

- Result
 - Bad performance (factor of 2 to 10, depending on example)
 - Not flexible enough
 - Mixing of different Properties Packages

=> Question: improve MO?

CO-THERMO (version 1.1) Wrapper Fortran 90 Library

- Developed by ProSim SA for TOTAL SA
 - Visual Studio 2005 / Intel Fortran, latest version 2009
 - Given to CO community by TOTAL SA
 - Available on CO-LaN website
- Well documented
 - Reference guide
 - Comprehensive test example
 - Source code is open
- With Material Object
 - As dll

⇒ Decision to use this Wrapper

instead of improving the MO with old THERMO V. 1.0

Implementation of THERMO Wrapper in CHEMASIM

It seemed simple but needed more time than expected!

- VS 2005 / Intel Fortran \Leftrightarrow VS 6.0 / Compaq Fortran
 - Experiences with VS 2005 needed

- VS 2005 instable: many crashes, even blue screens

- Complex interacting of 4 parts – 2 black boxes
 - CHEMASIM
 - THERMO Wrapper
 - Material Object (non debuggable)
 - Property Package (non debuggable)

THERMO Wrapper in CHEMASIM /2

- Project settings different in CHEMASIM and Wrapper
 - Not really a problem thanks to interface routines in Wrapper

- Use of many dlls
 - For MO, Wrapper, Multiflash, CO connection.
 - To register or not?
 - Where to locate?

- not always really helpful: THERMO error codes
 - hr = -2147220213
= 0x80040501 meaning “ECapeUnknown“, see error.idl
 - “ECapeThrmPropertyNotAvailable“
 - But why?

THERMO Wrapper in CHEMASIM /3

- You implement what is in your head not what is in the docs
 - But the docs are large...
 - `MO_Get_SinglePhaseProp(..., sBasis,...)`, `sBasis` = „mole“ / „mass“ / undefined
 - For `molecularWeight`: `sBasis` = undefined
 - Otherwise:
`hr = -2147220218`
`= 0x80040506` = „`ECapeInvalidArgument`“, but which one?
 - Undefined means „ “ and not „undefined“!

- Very helpful:
 - logging of debug&diagnosis information in MF PP (esp. in MF 3.8)
 - ...”P=0. is not allowed”
 - Wrapper test example
 - If PP call is ok comparison with test example finds often wrong parameter list

State of THERMO Wrapper Implementation in CHEMASIM

- test version
 - only small examples tested
 - ready for tests by other users

- production version in June

- First performance impressions
 - Ok for single PPs
 - Bad when change of PPs needed between iterations (“Create_PP“)