# Experiences with CAPE OPEN Thermo Interface v.1.0 in BASF in-House Simulator CHEMASIM

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# ProcessNet: The Users Environment at BASF and Users Requirements



- ~ 30,000 PCs at BASF Europe
- ~ 250 heavy users of ProcessNet in Chemical Engineering and Process Design Departments (~ 800 users in total incl. cost eval.)
- ProcessNet integrates commercial and in-house software, e.g.:
  - AspenTech
  - Chemasim (in-house)
  - gProms
  - HTRI
  - HyproTech
  - Kolfluid (in-house)
  - Konver (in-house)
  - Multiflash
  - PinchExpress
  - SuperTarget
  - Umberto
  - Vali
  - Zyqad

# ProcessNet: The Users Environment at BASF and Users Requirements (contd.)



- > 500,000 runs of CHEMASIM per year

- > 50 other utilities (programs) available, e.g.
  - Column Design
  - Heat Exchanger Design
  - Visualization of Physical Data Properties
  - Reconciliation / Fitting of phase equilibrium data

- OPEN CHEMASIM available (http://chemasim.itt.uni-stuttgart.de/); next Update with CAPE OPEN Thermo Interface ?

# General remarks to Interface definitions and Implementations

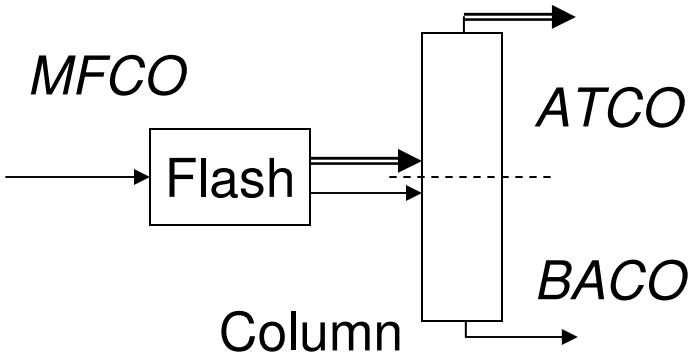


- Many Interfaces (Common, Error, Unit, ThermoSystem, …)
- Documentation typically for Professional Computer Scientist, not for Technical Programmers
  **More & simple Examples needed!**
- Communication between Objects nice, but too complicated! ⇒ „KISS“
- Implementation supplier depended: AT ≠ MF (v.1.0)
  - E.g. using PP.GetNumComponents() is supplier dependend
  - Raw COM functions like IUnknown::QueryInterface() should not be necessary
  - Too much help from supplier needed
  - Hidden "standards" of providers implementation (ρ or/and $v_{mol}$?)
  - Some properties not always available

# Administration of Thermo Systems (TS) and Property Packages (PP)



- How to manage different Thermo Systems?
  - Interfaces v.1.0 ≠ v.1.1
- For users input files stable expressions are necessary
  Example Input for simulator:
  - <keyword> <ID> <ProgID> <PathPropertyPackage>
  - E.g. COPP 3 MFCOProperties.MFCOPPack C:\data\MF\hg.mfl
    (recommended naming convention exists)



# Constructing the Material Object (MO)

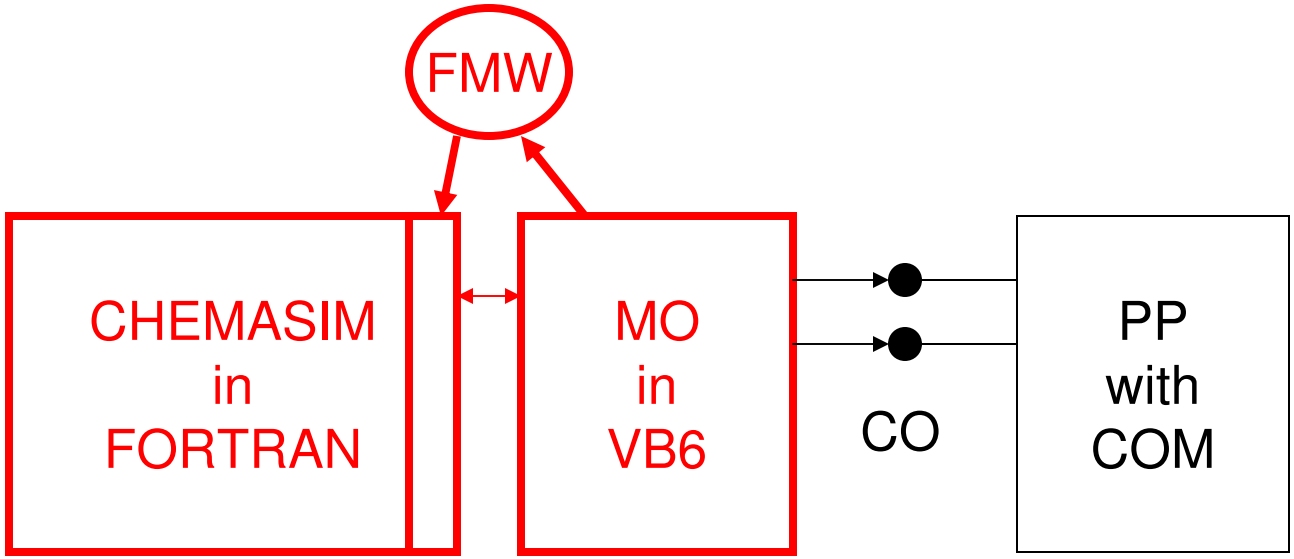


- MO couples Simulator and PP
  - MO is part of the simulator!!!
- Features of the Simulator
  - Component Reduction!
  - Phases! (e.g. 3 liquid phases, polymeres etc.)
- Features of the PP
  - Does the PP support all phases of the simulator and vice versa?
- Problems
  - Efficient administration of component lists
  - Efficient calculation of physical properties
- Our Implementation: in Visual Basic, usage from FORTRAN

# Interactions between the MO and the Simulator CHEMASIM



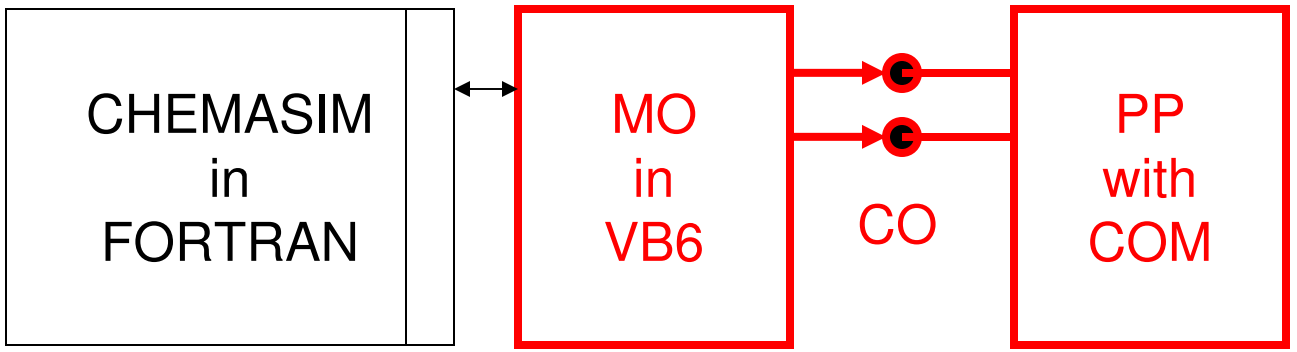
- Used Software Development Environment: MS Visual Studio v.6
- MO in Visual Basic v.6
- Simulator essantially in Compaq FORTRAN v.6
- COM Interfaces used with the Compaq "Fortran Module Wizard"



# Interactions between the MO and PP



- Communication between MO and PP is very intensive
- V.1.0: Different MOs with different Component Lists needed
- Raw COM functions like IUnknown::QueryInterface() should not be necessary
  - E.g. using PP.GetNumComponents() is supplier dependend
- **Debugging mode of PP during developing MO important**



# ⇒ Future Requirements



- For Providers of Physical Properties Packages
  - More robustness / "Plug & Play" Usage (managing different ThermoSystems)
  - Bug fixing (e.g. VaporPressure AT)
  - Better performance (for low level usage)
  - Take care of three liquid phases

- For the CAPE OPEN Standard itself (Thermo Interface)
  - More precise documentation with simple examples, especially communication between MO and PP (as simple as possible!)
  - Possibility to calculate Physical Properties like Residue Curves and Azeotropic Points instantaneously