

AixCAPE



Experiences in interfacing the IK-CAPE thermodynamics package to CAPE-OPEN

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Situation

- IK-CAPE as a calling convention for thermodynamic routines
- Developed in late eighties by „Industriekonsortium CAPE“
 - Dow, Bayer, Degussa, Hoechst, ...
- Idea: Unify efforts for use and development of thermodynamic models
- Used in many in-house tools, academic developments
- Large amount of input files exists
- Implementation distributed by DECHEMA e.V.
- Bayer interested to permit **use of existing parameter sets** in state-of-the-art process modeling tools

IK-CAPE details

- Written in FORTRAN 77
- Detailed documentation available
- Available subroutines
 - Configuration, setup
 - Computation
 - Including analytic derivatives
- Use textual input files
- Subroutine headers (examples)
 - **SUBROUTINE** T_G_COMP_NUMBER (TASK, NUMBER, MIST)
 - **SUBROUTINE** T_ENTH (WHAT, PHASE, T, P, MOLES, ENTHALPY, MIST)
 - **SUBROUTINE** T_ENTH_DERIVATIVE (WHAT, PHASE, DERIVATIVE, MIST)



IK-CAPE input file format

```
THER      3    75    8    12
SYST DATA      1    3
SHOR      1 MCH
NAME      1 METHYLCYCLOHEXAN
CASN      1 108-87-2
MOLW      1 BASE    9.81896000D+01
CL        1 DIPP POLY      3  3.83234290D+02  4.575000D+02
          2.39926D+05 -8. 3042D+01  7. 98345550D-01
HVAP      1 DIPP WATS      4  4.1499453490D+02  2.49990D+02
          5.365878D+04  2.234563D-01  6.190000D+02  0.00000000D+00
VP        1 DIPP ANTO      3  2.93149990D+02  1.454567768D+03
          4.432348D+01  5.36567578D+03 -2.4534657D+02
INKR      1 UFGR      3
          1    1    1    3.01099980D-01    5.47999990D-01
          2    5    1    4.74399972D-01    3.40000021D-01
          3    1    1    6.46900010D-01    3.28000000D-01
..
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```



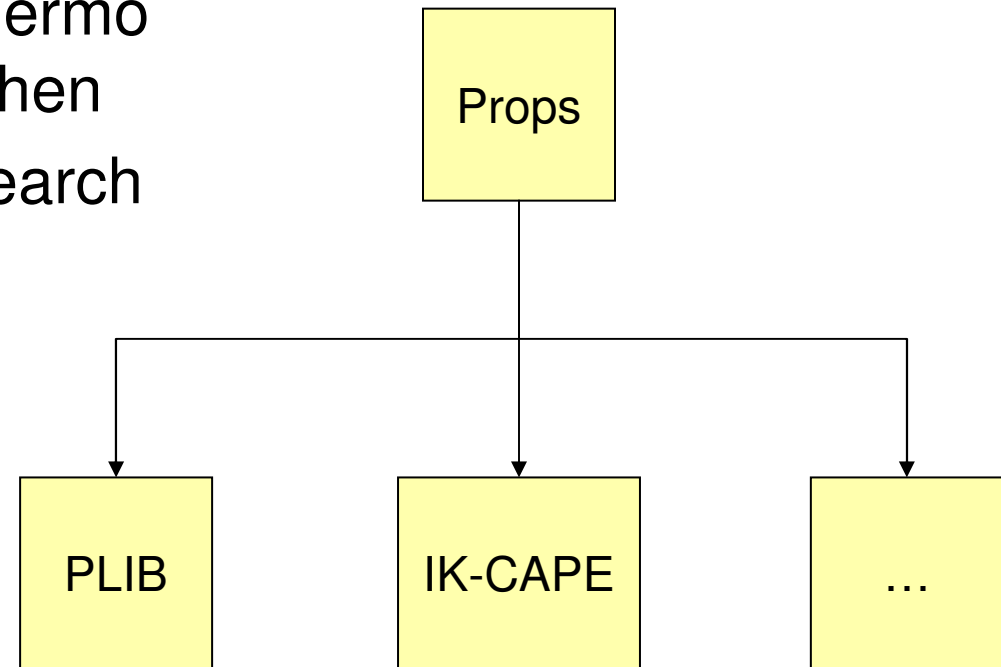
Conceptual mapping



IK-CAPE <-> CAPE-OPEN

- Configuration file <-> Property package
- Constant properties identifiers
 - Critical point (T, p, density)
 - Melting point, heat
 - Specific volume at standard temperature
 - Formation enthalpies
 - ...
- Non-constant properties
 - Enthalpy
 - Volume
 - Viscosity, vapor pressure, thermal conductivity
 - (Activity coefficient, Fugacity coefficient)
- K-values
 - vs. Fugacity coefficients in 1.0
- No entropy
- No flashes

- Interface layer for thermo at LPT / RWTH Aachen
- Used in several research codes in Aachen
- Implements flashes
- Interfaces IK-CAPE
- Interfaces PLIB
 - „In-House“ implementation of common thermo models
- Written in C
- Makes interfacing FORTRAN a bit easier



Migration strategy

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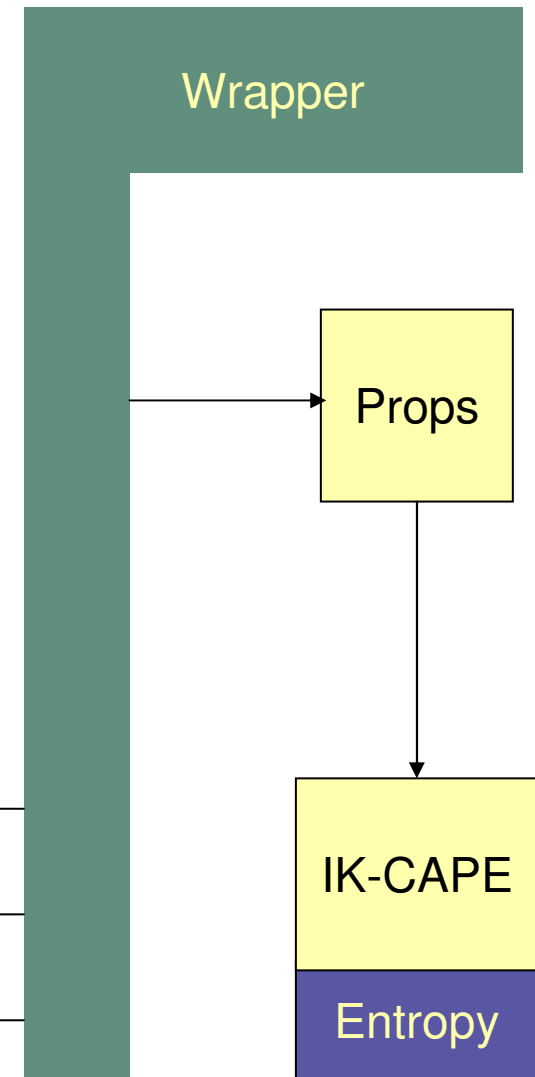


- Wrapper
 - Implements property system
 - Implements property package
 - Makes use of Props
 - Looks at certain directories to find available property packages
 - Written using C# / .NET
- Entropy to be added to IK-CAPE

ICapeThermoPropertySystem ●

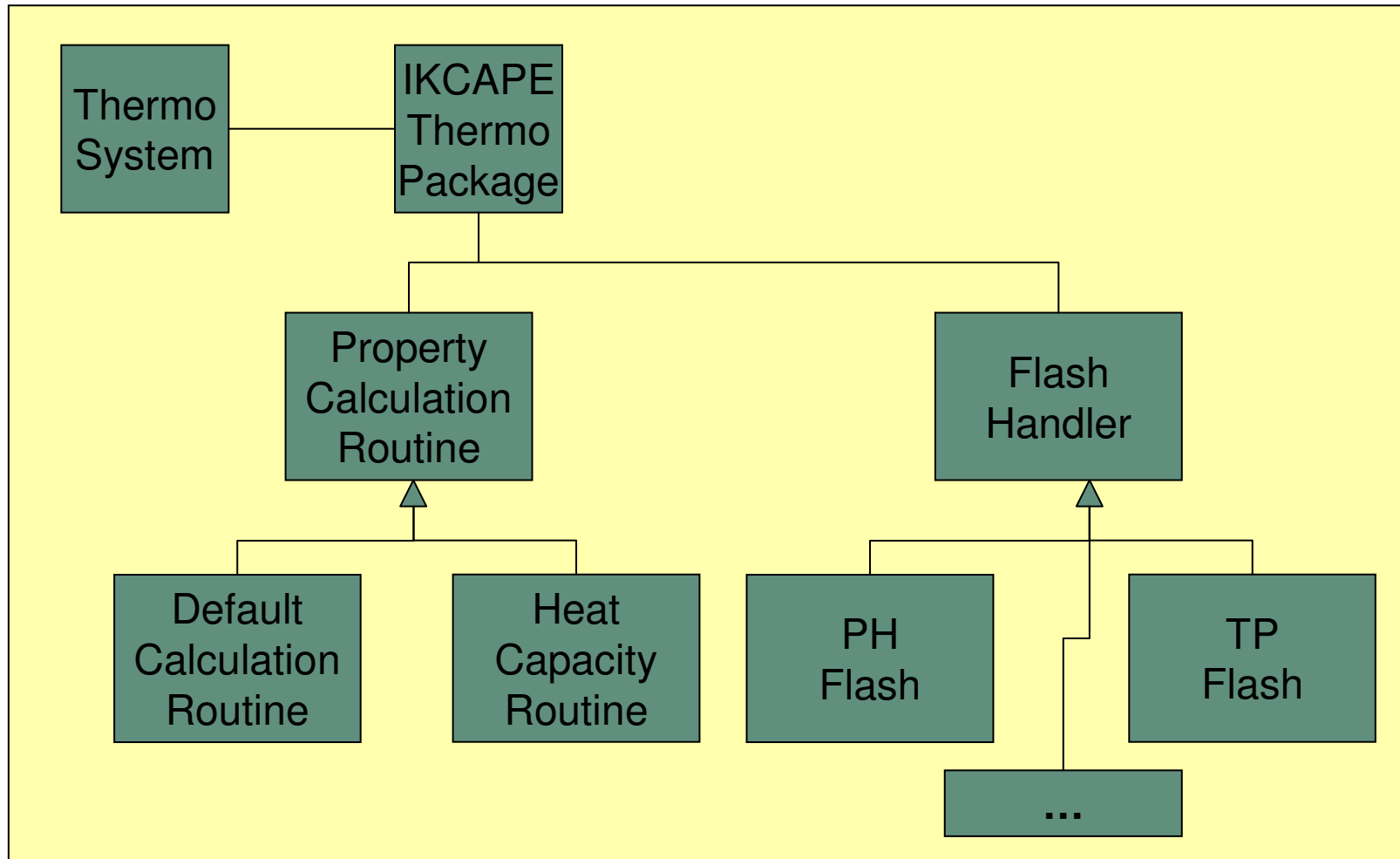
ICapeThermoPropertyPackage ●

ICapeIdentification ●



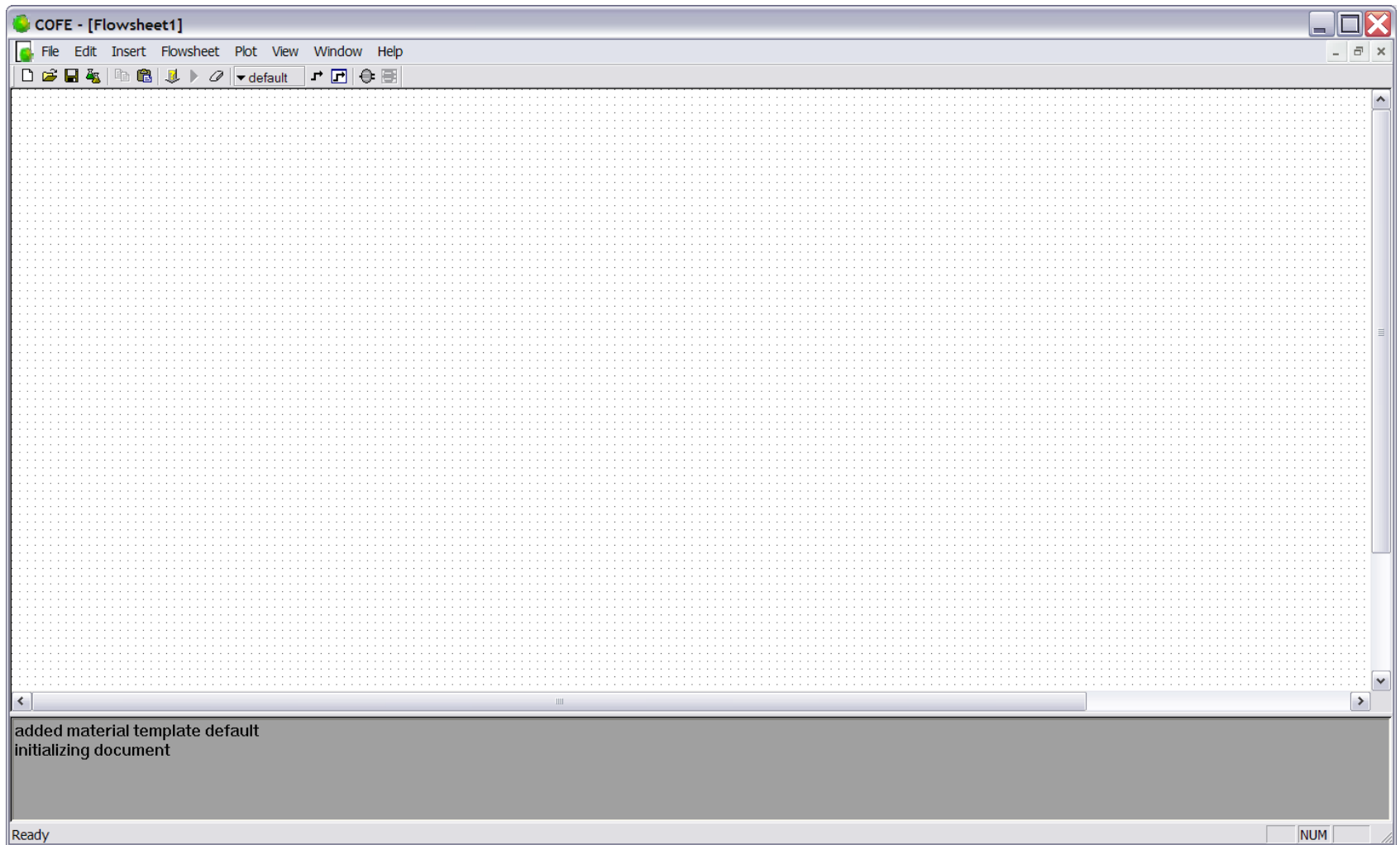
Wrapper architecture

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Little Demo

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Demo results

Just flashed a
single stream:

name	1	unit
▶ Stream		
▶ Connections		
▼ Overall		
pressure	100000	Pa
temperature	385	K
mole fraction [METHYLCYCLOHEXAN]	0.3	
mole fraction [TOLUOL]	0.4	
mole fraction [PHENOL]	0.3	
flow	2	mol / s
MW	94.54783	g / mol
▶ Phase Fractions		
▼ Vapor composition		
mole fraction [METHYLCYCLOHEXAN]	0.48536965	
mole fraction [TOLUOL]	0.46037413	
mole fraction [PHENOL]	0.05425622	
▼ Liquid composition		
mole fraction [METHYLCYCLOHEXAN]	0.20257803	
mole fraction [TOLUOL]	0.36827007	
mole fraction [PHENOL]	0.4291519	
▶ Overall properties		
▶ Vapor properties		
▼ Liquid properties		
activityCoefficient[METHYLCYCLOHEXAN]	1.7542269	-
activityCoefficient[TOLUOL]	1.1911848	-
activityCoefficient[PHENOL]	1.3631367	-
fugacityCoefficient[METHYLCYCLOHEXAN]	2.3959639	-
fugacityCoefficient[TOLUOL]	1.2500992	-
fugacityCoefficient[PHENOL]	0.12642661	-
enthalpy	21255844	J / mol
heatCapacityCp	210165.79	J / mol K
entropy	21255844	J / mol K
volume	N/A	m ³ / mol

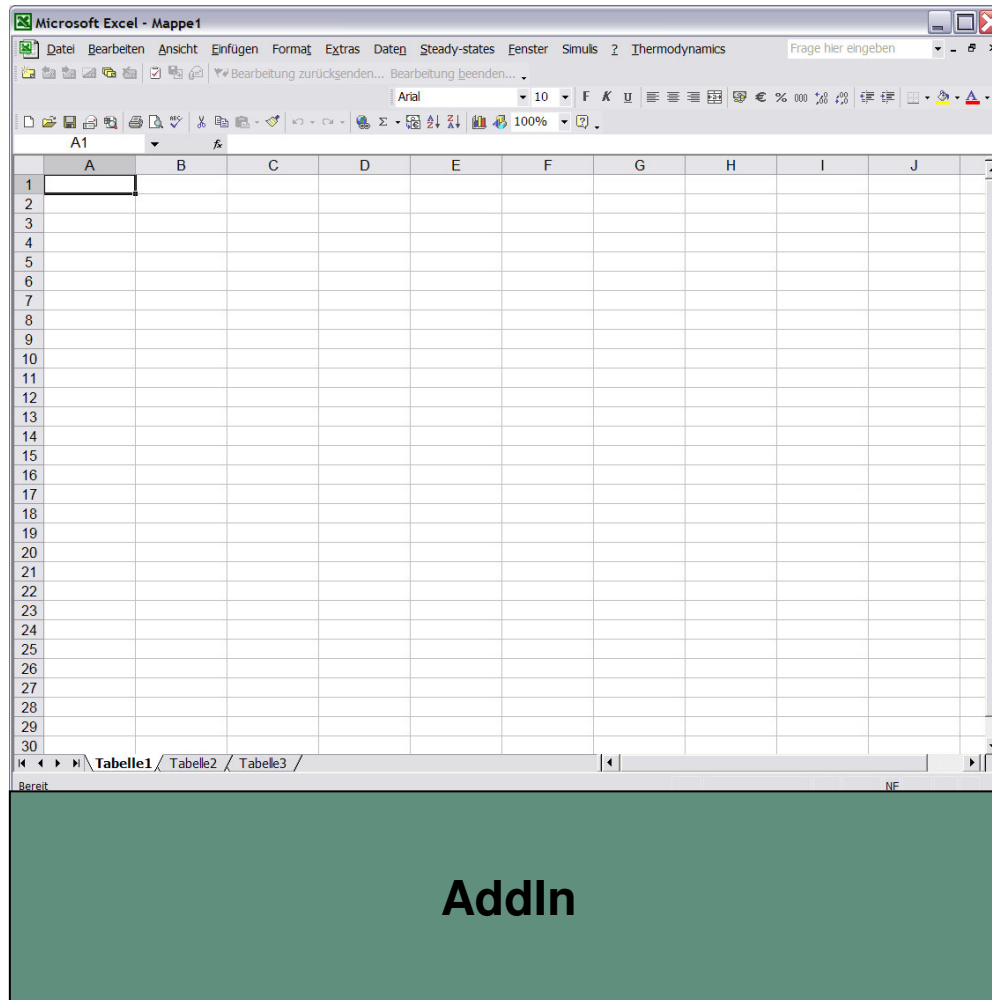
Mole fractions

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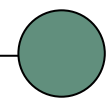
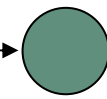
Excel Interface

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PropertyPackage

ICapeThermoPropertyPackage



ICapeThermoMaterialObject



- Thermodynamics package IK-CAPE provided as CAPE-OPEN component
 - CAPE-OPEN v1.0
 - Wrapper in C# / .NET
- C-based wrapper from research used
 - adds flash calculations
- Excel interface
- Successful interoperability tests
 - COCO (yes)
 - AspenPlus (yes, but entropy is missing)
 - Uses „backup model“ to compute missing properties
 - Pro/II (basic T,P-diagrams, yes)
 - Simulis Thermodynamics (and thereby ProSimPlus)
 - gPROMS



- Flashes from VT-PLAN
 - Standard 2-phase flash
 - More robust 3-phase flash including reactions
 - (not as separate component)
- Reactions
 - Supported by IK-CAPE
- More interoperability testing with other tools
 - gPROMS
 - AspenPlus (once entropy is added)
 - ...
- Thermo 1.1