



nel

technology for life





PPDS Cape-Open Development

Present Status and Future Plans

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TUV NEL - Background



- **Originally a UK Government primary laboratory for engineering R&D (1947 - 95)**
- **Privatised Nov 1995 - our parent company is TÜV Süddeutschland Holding AG**
- **120+ staff of whom 80% are qualified scientists and engineers**
- **Four core market groups, including**
 - Oil, Gas & Chemicals (PPDS,...)



PPDS Cape-Open Development



- **Trials and tribulations**
- **The never-ending story**
- **The long and winding road**
- **but, interesting and rewarding**



PPDS Functionality : Databases



- **Quality-assured data for pure compounds (~1600) and mixtures (~7000 BIPs)**
- **Support packages to create user databanks for pure compounds and binary parameters**
- **Pseudo-components (petfrac) database**
- **Special databanks of high-quality data, e.g. IAPS95**

- **Complete restructure of databases in v4 release**

- **Cape-Open opportunity for**
 - Physical Property Data Base Interface
 - Petroleum Fraction Interface



PPDS Functionality : Calculations

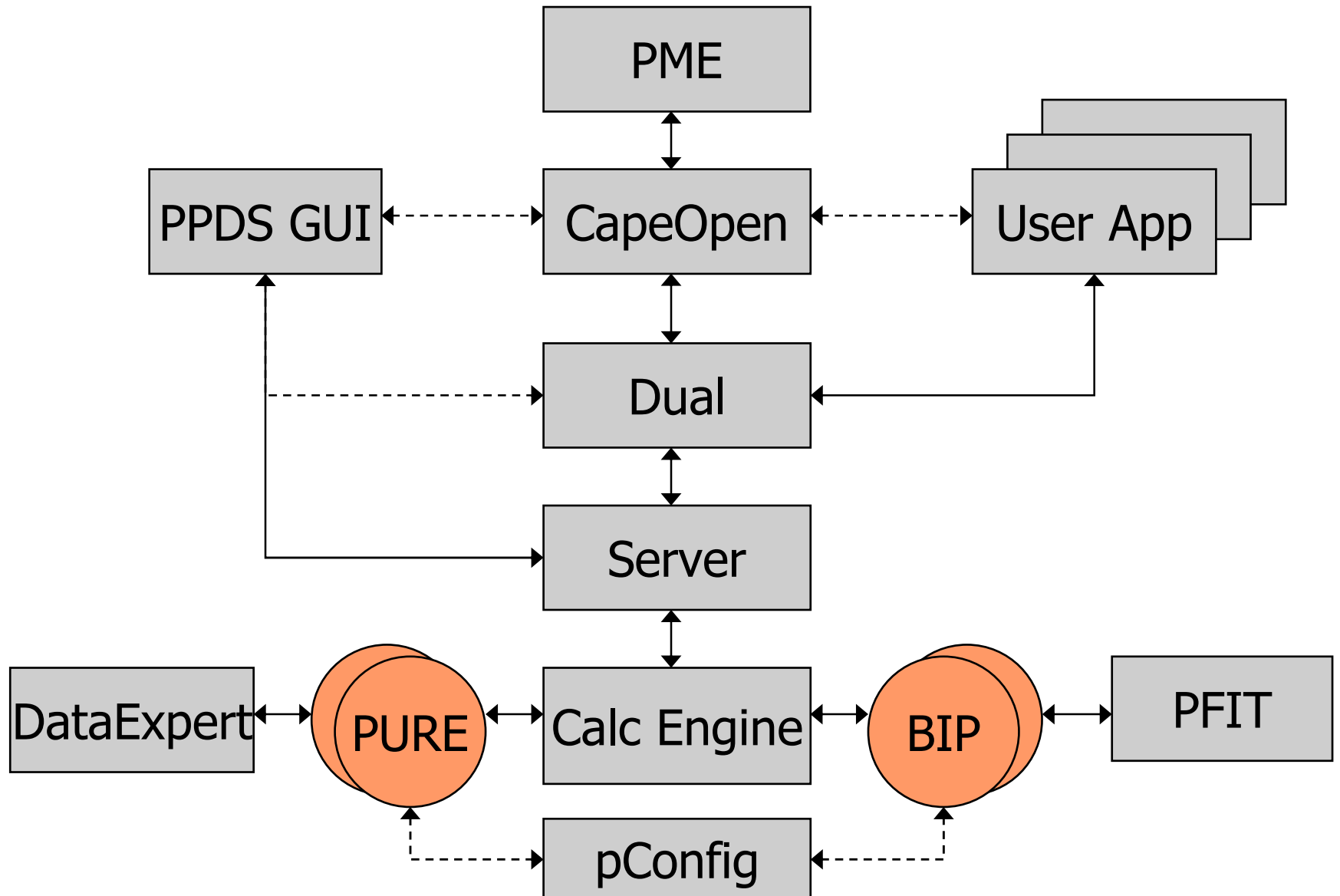


- **General purpose physical property and phase equilibrium calculation package**
- **All standard thermodynamic models**
- **Recommended mixing rules**
- **Flexible (COM) interface for access by client applications, including web-based apps.**

- **Cape-Open opportunity for:**
 - ThermoSystem Interface
 - Property Package Interface
 - Property Calculator Interface
 - Equilibrium Calculator Interface



PPDS Structure





PPDS Cape-Open Development



- **Original development mid-2001**
- **ppdsCapeOpen dll for testing with PPDS v3 during period Jan 2003 to Dec 2006**
- **PPDS v4 release Feb 2007**
 - Better management of packages within ThermoSystem
 - Upgrade path for Thermo v1.1
 - Capability for 'bankless' operation
 - Release has ThermoSystem with 3 test packages
 - Hydrocarbon (20 compounds, PR model)
 - Chemical (12 compounds, NRTL model)
 - INDISS (5 compounds, PR model)
 - and one standalone package
 - IAPS84 Steam Tables (plus flash calculations)



Tests with COSEs



- **Originally**
 - CO Tester v0.9, v0.9.3
 - AspenPlus, HYSYS, Simulis
- **Currently (v1.0 Thermo)**
 - General testing by M Pons
 - At NEL
 - COCO-COFE
 - AspenPlus
 - At Chemstations
 - CHEMCAD
 - COLTT tester very useful
- **General thanks to suppliers of test software**



Demo 1 : COFE - PPDS



- **Run PPDS GUI**
 - Create a new problem
 - Water, Ethanol, Methanol
 - Set VLE models – Ideal Gas / Wilson-A
 - Run typical calculation (e.g. TP flash)
 - Save as CO package in PPDS ThermoSystem
 - Open CO package view and check list
 - Exit program

- **Run COFE**
 - Create simple stream
 - Add new CO package from PPDS ThermoSystem
 - Set stream data
 - Check results



Demo 2 : AspenPlus – PEL



- **Run PhysPack GUI**
 - Open saved problem
 - R115, R134A, R114, HF with VPA / Wilson-O
 - Run standard calculation
 - Save as PPDS CO Package
 - Exit program

- **Run AspenPlus**
 - Create simple sheet with flash drum
 - Import CO package
 - Set calculation data
 - Run simulation



Thermo v1.0 Issues



- **General issues with Complds, Name, CAS**
- **One PropertyList to cover both “mixture” and “pure” attributes**
- **Use of “overall” in CalcProp call**
- **Dew / bubble points as Properties**
- **Setting MO T and/or P after CalcEquilibrium for all valid phases**
- **How much of the MO data should the PP set as a result of the CalcEquilibrium call**
- **Amount of info required in Windows Registry**
- **Many of these are better with Thermo v1.1**



Thermo v1.1 Plan



- **PPDS will be configured as ThermoSystem & PropertyPackages as per v1.0**
- **No plans at present for separate Property Calculator or Equilibrium Calculator**
- **Development starts March 2007**
- **Target date for test package June 2007**
- **Update PPDS release Oct 2007**

- **Preliminary design**
 - Rebuild PPDS v4 with Thermo v1.1 tlb – OK
 - Can use same list of property packages
 - Most of calculation code is reusable
 - v1.0 and v1.1 within same dll



End of presentation

Thank you for listening

Any questions?