Using ChemApp and ChemSage data files with Aspen Plus

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Aspentech

Overview

- Who is Aspentech, what do we do?
- Why use use ChemApp inside Aspen Plus
- Interface in version 2004.1 and previous
- Changes in 2006
- Q&A

AspenTech Today

- Is the leading provider of software and services to process industries, with $320M+ annual revenues
  - Engineering & Innovation (PLM)
  - Plant Operations (MES)
  - Supply Chain Management (SCM)
- Offers 20+ years of experience in serving the process industries
  - Founded in 1981; public company since 1994 (NASD:AZPN)
  - 1,500+ employees operating in 20 offices worldwide
  - World-class industry partners and global support
- Provides proven solutions that reduce costs, improve margins, increase capital efficiency and improve customer loyalty
- Is the only provider with a unified offering for Enterprise Operations Management (EOM)

Market Segments & Products

	Engineering & Construction	Exploration & Production	Refining & Marketing	Chemicals	Polymers	Spec Chem	Pharma	Growth Markets
Process Engineering Process Development	●	●	●	●	●	●	●	●
Planning & Scheduling	●		●	●	●	●	●	●
Advanced Process Control		●	●	●	●	●		●
Production Management & Execution		●	●	●	●	●	●	●
Supply & Distribution			●					

● *Identifies relevant point products available*

aspenONE for Chemical Process Engineering

	Chemicals
Aspen Plus	
Aspen Simulation Workbook	
Aspen Dynamics	
Aspen Tasc+	
Aspen Acol+	
Aspen Icarus Process Evaluator	
Aspen Polymers Plus	
Aspen Custom Modeler	
Aspen Batch Plus	
Aspen Properties	
Aspen BatchSep	

V2006 for Chemicals notes:

- New feature to update dynamic models from steady-state models – first step towards tight integration of AD and Aspen Plus
- Support for AD/ACM dynamic simulation in Aspen Simulation Workbook
- New Plate+ plate & frame exchanger module integrated into Aspen Plus
- New Database infrastructure for Aspen Properties

aspenONE Users in Minerals Applications

- Aspen Plus used to model cement process
  - UBE
  - Finnsementti
  - Cementa
- HuntsmanTioxide
  - Use ACM for solid phase reactions in a rotary kiln
- ALCAN Aluminium: Simulation of Arvida facilities.
- Umicore: Zinc and precious metal production. Pilot plant scale up.
- CODELCO: Portrellios smelting operations and solvent extraction at Chuquicamata.
- Corus: Exergy analysis of blast furnaces and coke oven gas treatment.
- A Steel Company (Japan): Coke oven gas treatment.
- Buss AG: Model the production of HF from fluorospar

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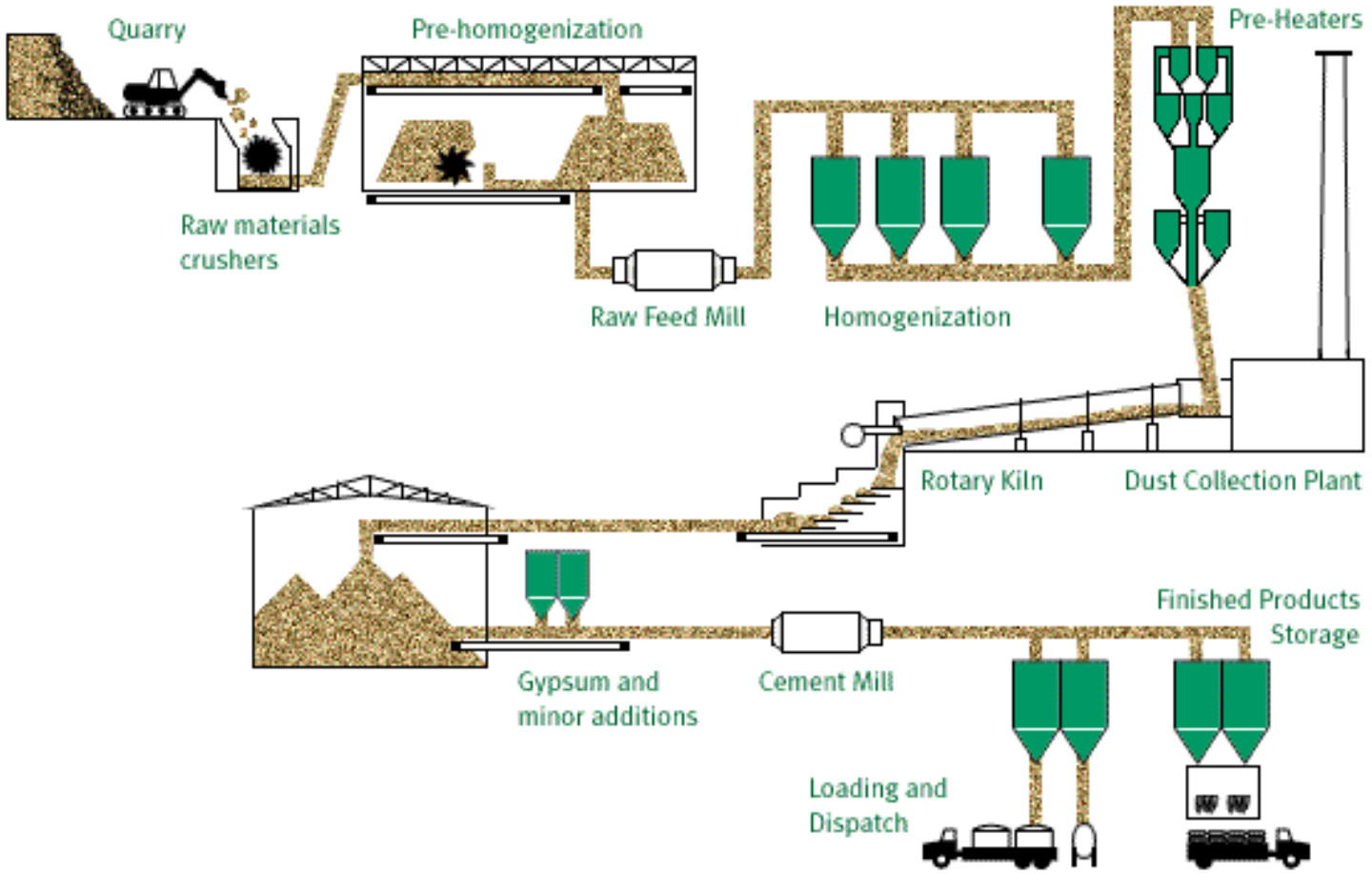
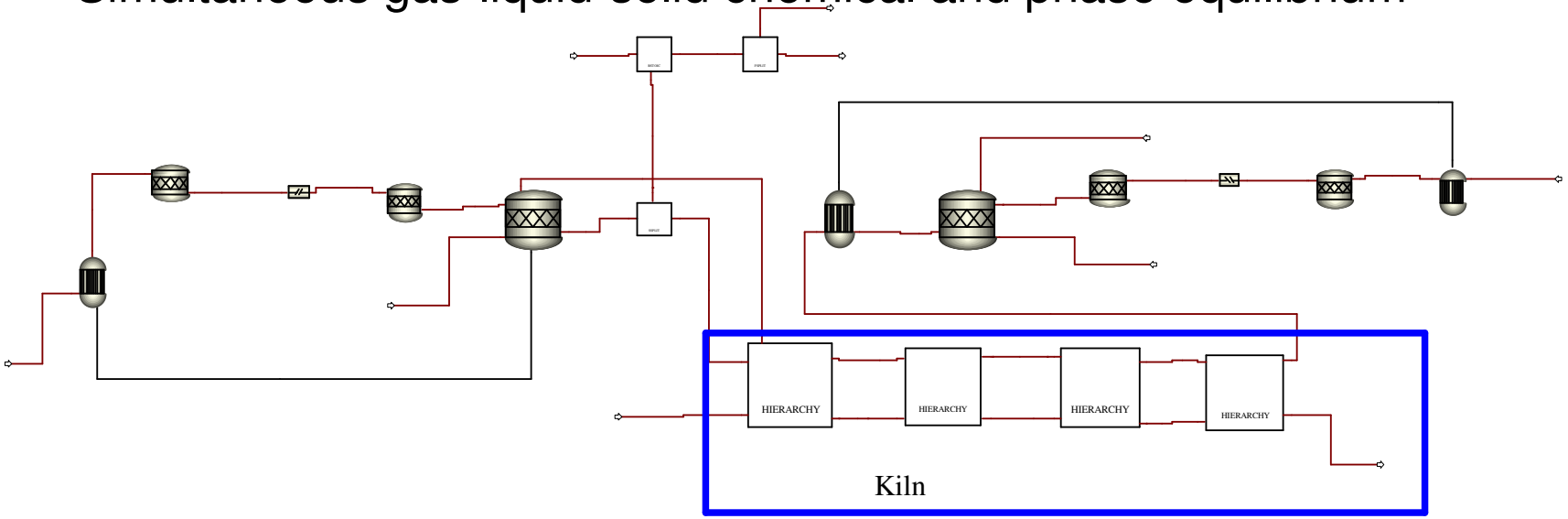
A process has many connected operations, example, a Cement Process

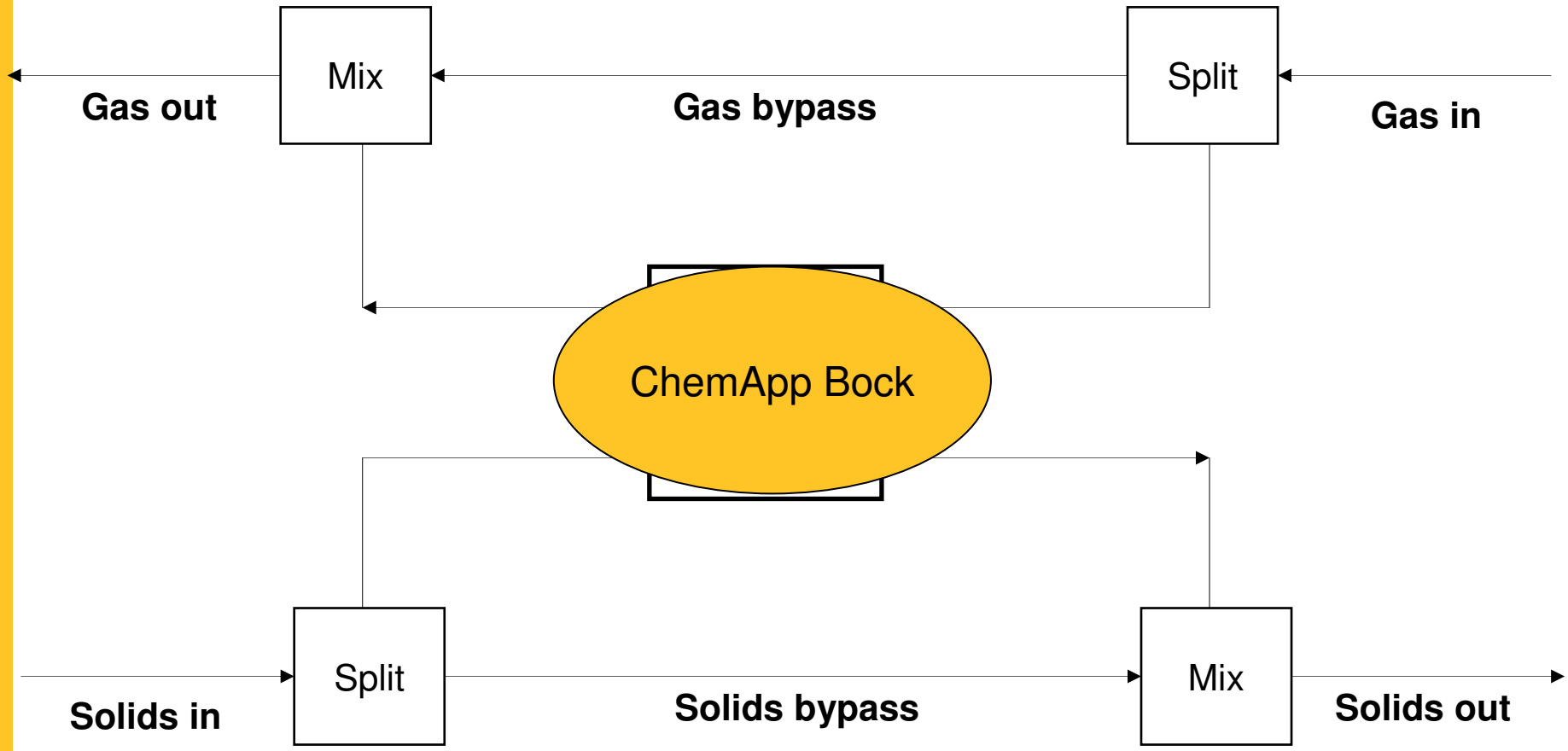


Cement model in Aspen Plus

- Standard Unit Op models used to model pre-heating, cyclones, fuel combustion for example
- The kiln is modelled as a series of linked Gibbs Equilibrium reactor blocks with counter-current gas and solids flow
  - Simultaneous gas-liquid-solid chemical and phase equilibrium



Model scheme of a reaction cell without thermal equilibrium



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When does it get difficult

- Aspen plus comes with old FACTPCD
- You want to use a newer version
- You want to add you own components

In Short

- Mapping Aspen Plus components
- Making the Aspen Plus Databanks
  - Making the main calculation engine databank file
  - Making the Aspen Plus User Interface Databank
- Using the databank in Aspen Plus
  - Selecting Aspen Plus component databanks
  - Change the phase name mapping file in Aspen Plus
  - Setting the name of the ChemSage data file

Mapping Aspen Plus components

- Components in Aspen Plus are identified by the component ID
  - This is an 8 letter name.
- The Aspen+ component name is used to map to ChemSage components
- Aspen+ has a standard databank that maps the FACT 5.0 database
- For other components a “user-added” Aspen+ databank is needed
  - The component name cannot be changed for a user-added component entered directly in Aspen+
- The user-added Aspen+ databank needs:
  - Component names
  - Formulae
  - Molecular weights
  - The main physical property data come from the ChemSage data file

Mapping Rules

- ChemApp component names in Aspen+ Plus have two parts
  - NAME:PHASE, Example: C:G1 = Carbon in the gas phase (G1)
  - Phases may be pure component phases or solution phases
- Pure solid components in the ChemSage data files naming syntax:
  - ChemicalFormula_Description(solid phase number)
    - e.g. C_Graphite(S), or Fe3C_Cementite(S2)
  - Aspen Plus name should use “ChemicalFormula” & “solid phase nbr”
    - C_Graphite(S) maps to C:S1
    - Fe3C_Cementite(S2) maps to FE3C:S2
- ChemSage datafiles can contain data for mixture or solution phases
  - The PHASE in the Aspen+ component name is limited to 4 letters
  - File factsoln.txt maps the Aspen+ PHASE to the Chemsage name
- For example, a component C_(carbon) in phase LIQUOR
  - Could be called C:LQOR in Aspen+
  - factsoln.txt needs to be updated with LQOR / LIQUOR mapping

Mapping Examples

ChemSage name	Phase	Description	Aspen+ name
C	Gas	C in gas phase	C:G1
C2	Gas	C2 in gas phase	C2:G1
O	Gas	O in gas phase	O:G1
O2	Gas	O2 in gas phase	O2:G1
O3	Gas	O3 in gas phase	O3:G1
Si	Gas	Si in gas phase	SI:G1
Si2	Gas	Si2 in gas phase	S12:G1
Si2C	Gas	Si2C in gas phase	SI2C:G1
C(s)	pure solid	solid C	C:S1
Si(s)	pure solid	solid Si	SI:S1
SiC(s)	pure solid	solid SiC	SIC:S1
SiO2_quartz(s)	pure solid	solid quartz	SIO2:S1

- In Aspen+ the component type should reflect the state
  - Liquids and gases designated as Conventional (the default)
  - Solids and solid solutions designated as Solids
- This is useful when assigning products to substreams

Making Aspen+ user databanks

- These instructions are for v12.1, 2004 and 2004.1 of Aspen+
- Aspen+ user databanks have two separate parts:
  - One databank for use by the User Interface
    - this contains component name, formula and mol weight.
  - A second databank for use by the Aspen+ Calculation Engine
    - Normally this databank contains the full data for those components
    - BUT here this databank only contains component names and mol weights
- Aspen Plus User databanks come in different formats
  - e.g. In-House, USRPP1
  - Instructions to create can be found in the Aspen+ documentation
  - This document explains how to make a USRPP1 type of databank

Making the calculation engine databank

- Make a text input file called xxxx.INP
- Use Notepad or similar text editor
- Format should be similar to the example (next slide)

Example DFMS input file

```
; FILE NAME: FE-C_DATA_INPUTFILE.INP
;
FILE USRPP1A USR1 NEW
WRFILE USR1
;
NEW-COMP
   'C:G1'        'C'           /
   'C2:G1'       'C2'          /
   'C6:G1'       'C6'          /
   'C7:G1'       'C7'          /
   'FE:G1'       'FE'          /
   'C:LIQU'        'C(LIQ)'    /
   'FE:LIQU'       'FE(LIQ)'   /
   'FEC3:BCC_'     'FEC3(BCC)' /
   'FEV:BCC_'    'FEV(BCC)'    /
   'FEC:FCC_'    'FEC(FCC)'    /
   'FE:FCC_'     'FE(FCC)'     /
   'C:S1'        'C(S)'        /
   'FE3C:S2'     'FE3C(S)'

NEW-PROP    MW 1 / DHFORM 1 / DHSFRM 1
PROP-DATA
            PROP-LIST       MW 0      / DHFORM 0 / DHSFRM 0
        PVAL      'C:G1'   12.011 / -9999 / -9999
        PVAL      'C2:G1'  24.022 / -9999 / -9999
        PVAL      'C6:G1'  72.066 / -9999 / -9999
        PVAL      'C7:G1'  84.077 / -9999 / -9999
        PVAL      'FE:G1'  55.847 / -9999 / -9999
        PVAL      'C:LIQU'   12.011 / -9999 / -9999
        PVAL      'FE:LIQU'  55.847 / -9999 / -9999
        PVAL      'FEC3:BCC_'  91.880 / -9999 / -9999
        PVAL      'FEV:BCC_'  55.847 / -9999 / -9999
        PVAL      'FEC:FCC_'  67.858 / -9999 / -9999
        PVAL      'FE:FCC_'  55.847 / -9999 / -9999
        PVAL      'C:S1'     12.011 / -9999 / -9999
        PVAL      'FE3C:S2'  179.552 / -9999 / -9999
END-INPUT
```

Lines starting with ; are comments

These 2 lines should not be changed

NEW-COMP is the start of the component names and formulae in single quotes. Separated by spaces. Each component separated by a /

This part contains the MolWts along with dummy values for enthalpy and entropy of formation.

Making the calculation engine databank

- Start the Aspen Plus command window
- Change the working folder to where your input file is stored
- Run DFMS with this command: DFMS input-file runid
  - input-file is the name of the *.INP input file made above
  - runid is the name used for the output report from DFMS
- This will create the engine databank
- This file should be in the Aspen+ input file folder

Making the User Interface Databank

- The input file for the User Interface databank should be named *.DAT
- Format it as the example on the next slide

Making the User Interface Databank

```
/* all input starts at column 1                                    */
/* file name:     FE-C_GUI.DAT                                     */
DBANK ADD MYDATA1
USRPP1 USR1
USRPP1A.DAT
 C              C:G1                              0
      12.011 0.1E36  0.1E36
  *
 C2             C2:G1                              0
      24.022 0.1E36  0.1E36
  *
 C3             C3:G1                             0
      36.033 0.1E36  0.1E36
  *
 C4             C4:G1                             0
      48.044 0.1E36  0.1E36
  *
 C5             C5:G1                              0
      60.055 0.1E36  0.1E36
  *
 C6             C6:G1                             0
      36.033 0.1E36  0.1E36
  *
```

This is the name of the databank as it will appear in the Aspen Plus user interface e.g. MYDATA1

Component "formula"

Component name

Mol Wt followed by 2 dummy values

Making the User Interface Databank

- In Windows Explorer go to the folder: C:\Program Files\AspenTech\APrSystem 2004.1\GUI\Custom
- Locate file tbprop.dat (the MMTBS Driver File)
- Open tbprop.dat in a text editor
- Add an additional line referencing your xxxxx.DAT
  - INCLUDE c:\aspen\chemapp\FE-C_GUI.DAT
- Start the Aspen+ Simulation Engine command window
- Change location to folder with tbprop.dat
- Next type command: mmcustom mmtbs
- Now all local records have been updated

Making the User Interface Databank

- Verify that the User Interface databank is correct
  - Start Aspen Plus
  - Open file custom.bkp
    - Located in C:\Program Files\AspenTech\APrSystem 2004.1\GUI\Custom
  - This input file uses any local databanks.
  - Make sure you can find and use the new databank
- If the above steps work ok, the User Databank is correct
- Install the new user interface databank file
  - Open the Simulation Engine command window and type: custinst
- That finishes the database installation

Using the new databank in Aspen+

- Update phase mapping file if needed
  - Only if your ChemSage data file has named solution phases
  - This mapping file is called factsoln.txt and is found in the folder: C:\Program Files\AspenTech\APrSystem 2004.1\Engine\Xeq
  - Factsoln.txt is an ASCII text file
  - Update the second line to reflect total number of entries
  - Line format is:
    - A number: 2 for liquid and 3 for solid
    - The Aspen Plus phase name (4 letters or less)
    - The full phase name from the ChemSage data file.
- Selecting Aspen+ component databanks
  - Go to Components/Specifications and the Databanks Tab
  - Select MYDATA1 (or whatever name you gave it)
  - Deselect all others (except perhaps FACTPCD)

Setting the ChemSage data file in Aspen+

- Only use ASCII files (*.dat) or transparent ChemSage files (*.cst)
- The default ChemSage data file name is CHEMSAGE.CST
  - .CST files are called “Transparent” data files
  - An ASCII format data file can also be used with a file extension *.DAT.
- A Calculator block can be used to set another name for the data file.
  - This could be a *.CST file, or a *.DAT file
  - This requires the use of a Visual Fortran compiler!
- For Fortran syntax, see example Aspen+ file called ChemSage.bkp
  - C:\Program Files\AspenTech\Aspen Plus 2004.1\Gui\Xmp\Chemapp
- This file can be imported into any Aspen+ simulation
- The calculator block executes first and sets two variables:
  - Ppfact_FILEN: name of the ChemSage file, must be in local directory.
  - Ppfact_CADBG: controls if debugging info is sent to the Control Panel

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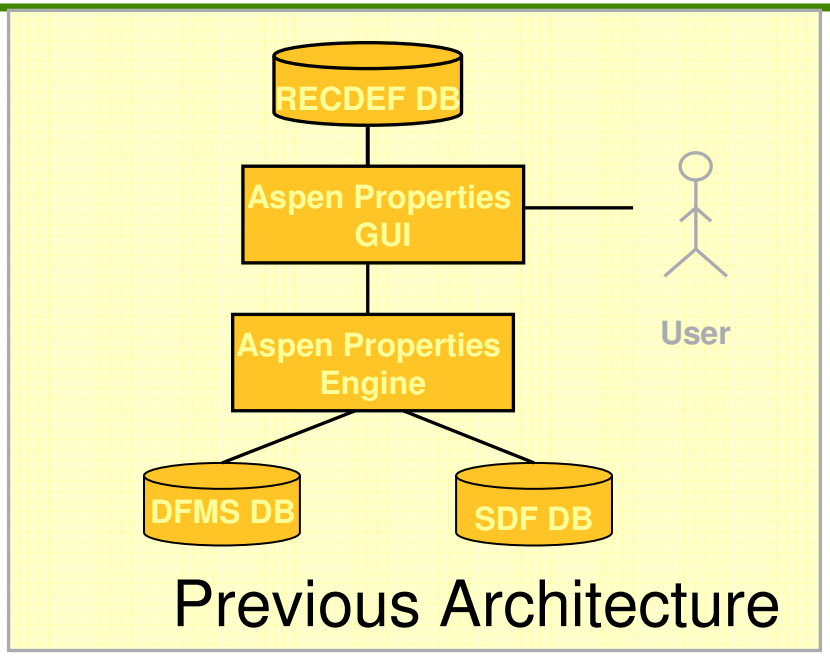
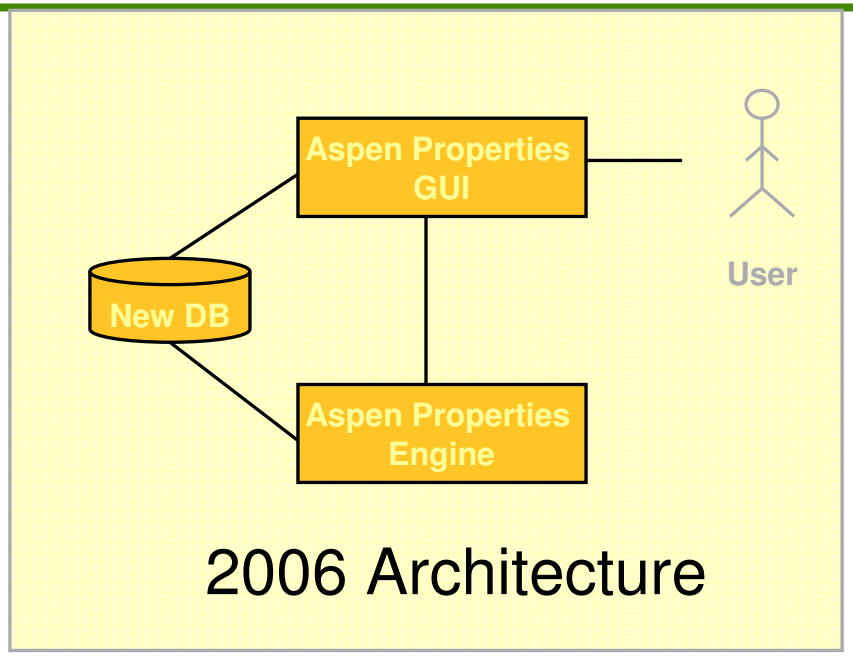
New Features – Aspen Properties Enterprise Database Architecture



Previous Architecture

- Many databases: Engine and GUI. Data dispersed and duplicated
- Maintenance, customization difficult
  - No user-friendly GUI
  - Very limited customization
- Cannot be deployed enterprise-wide



2006 Architecture

- Single modern database, (MSDE & SQL server)
- Ability to add properties, comments, and other data
- User-friendly GUI for database management
- Utility to convert legacy Aspen Properties data bank files

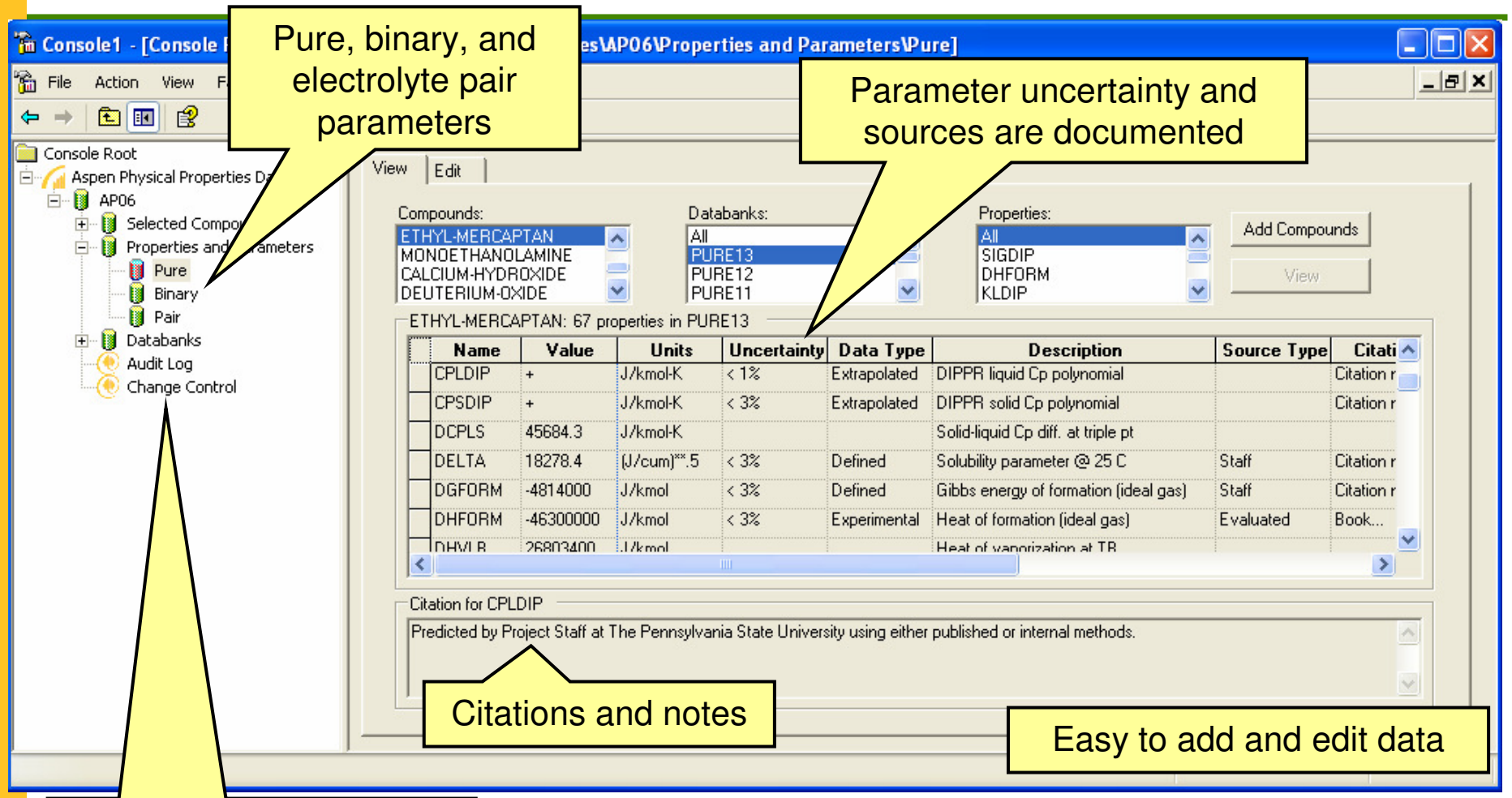
Adding Components to the Enterprise Database

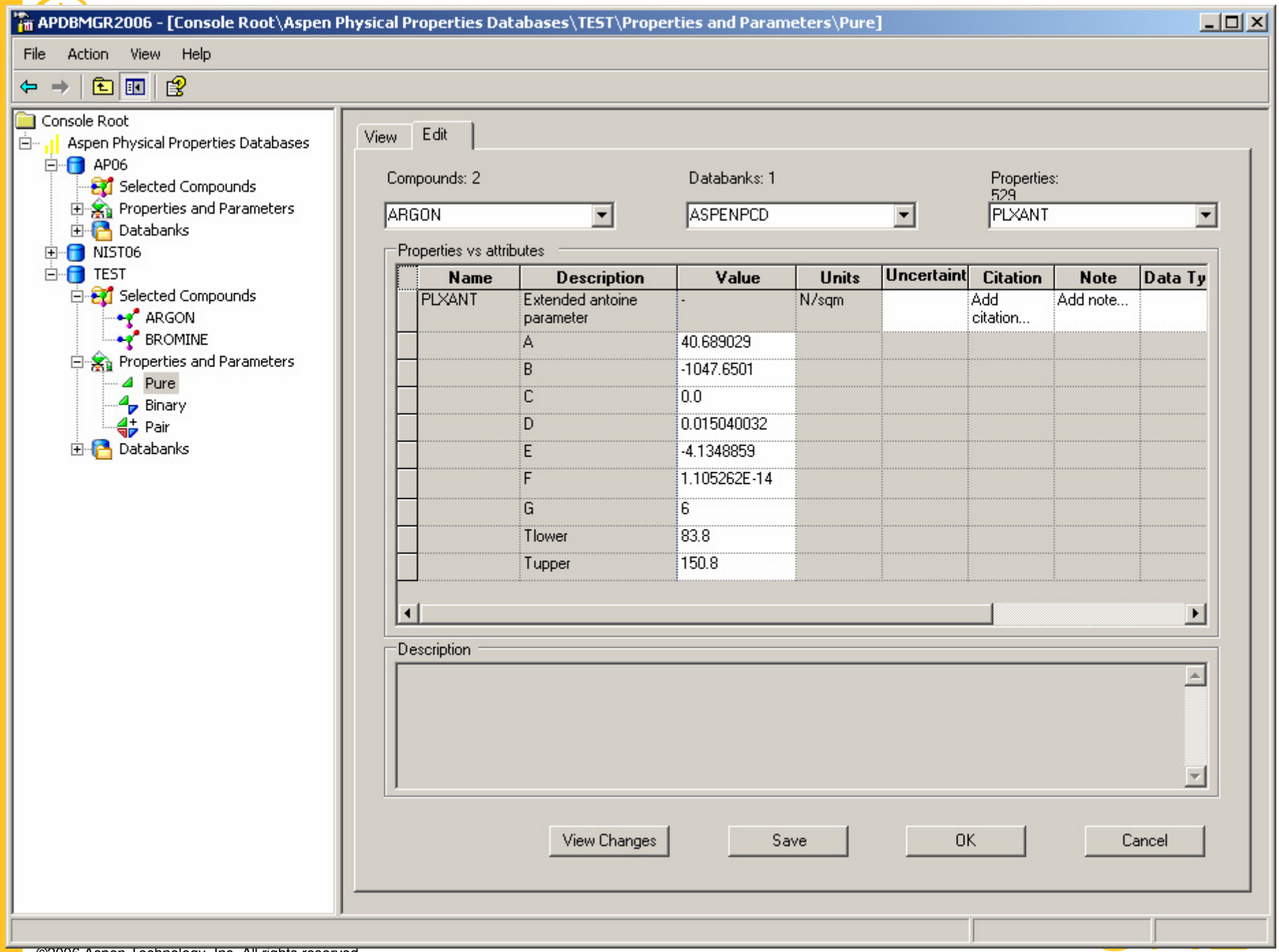
- When creating a user database, it is not necessary to customize the Aspen Plus and Aspen Properties simulation engine and GUI as was required in previous releases.
- Instead, you use the Database Manager…

Aspen Properties Database Manager

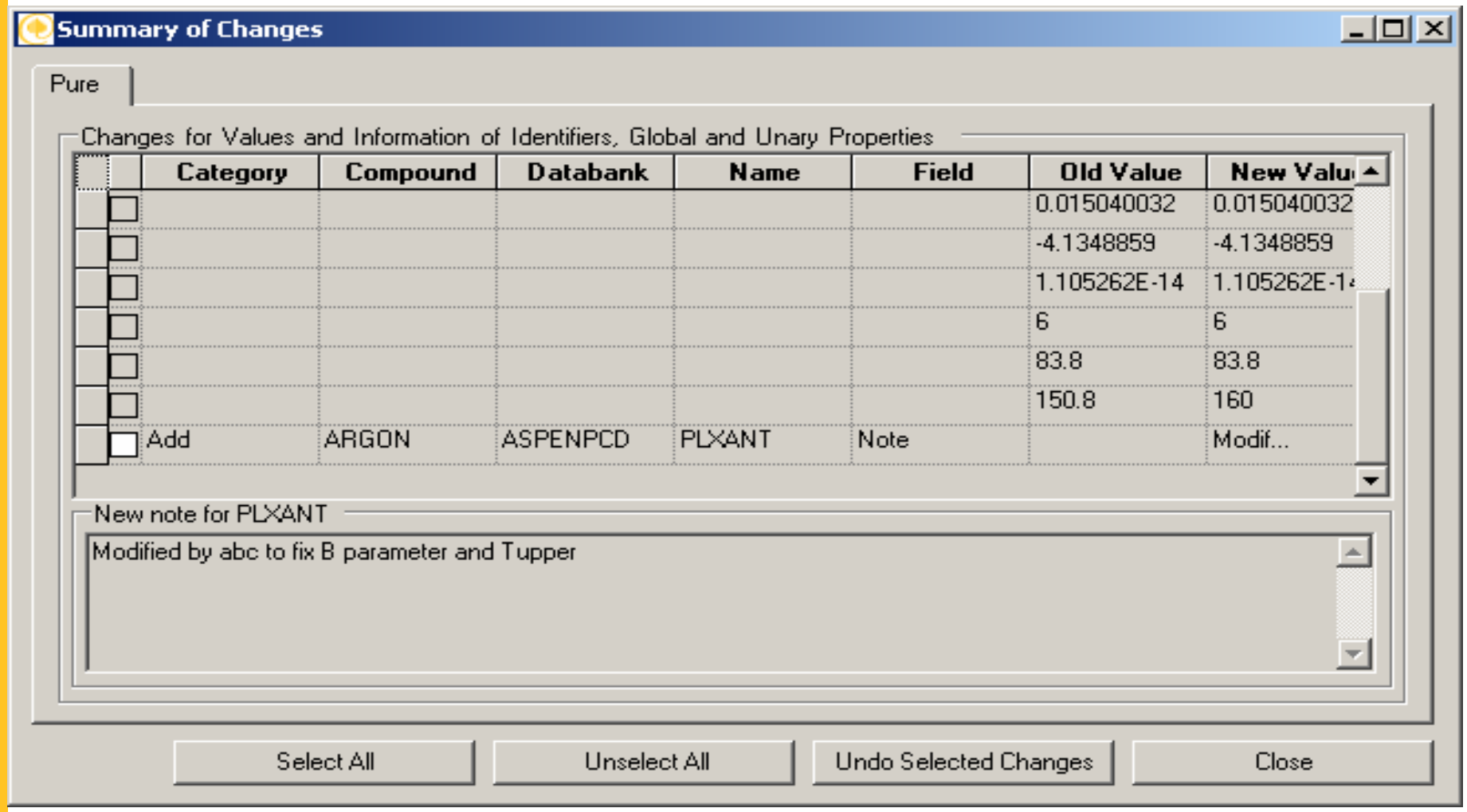
- The Database Manager:
  - Allows you to view and create databases for use with the Aspen Properties Enterprise Database and products that use it.
  - Is a database viewing and management tool. It is not intended to perform any property calculations.
  - You can create a new database by cloning an existing database, or by importing legacy data files of the following types:
    - DFMS input files
    - TBS input files used to customize the GUI
    - Optional DIPPR access database
    - Optional molecular structure information (compressed mole files) that have been stored in an access database

Aspen Properties Database Manager

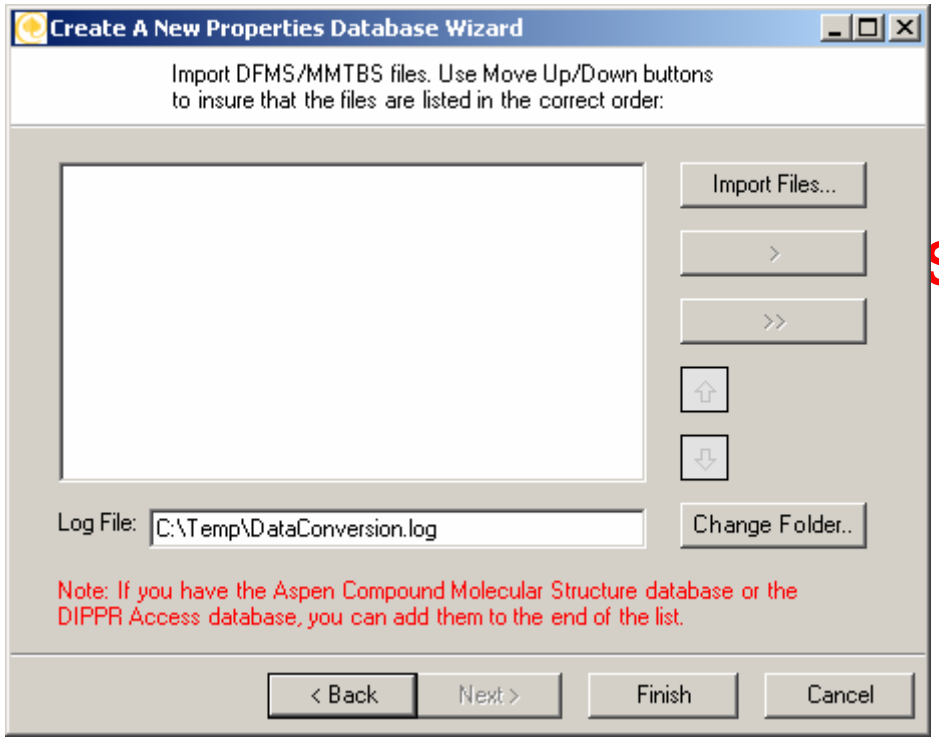




Click on View Change button shows the summary of changes



Importing Legacy Files



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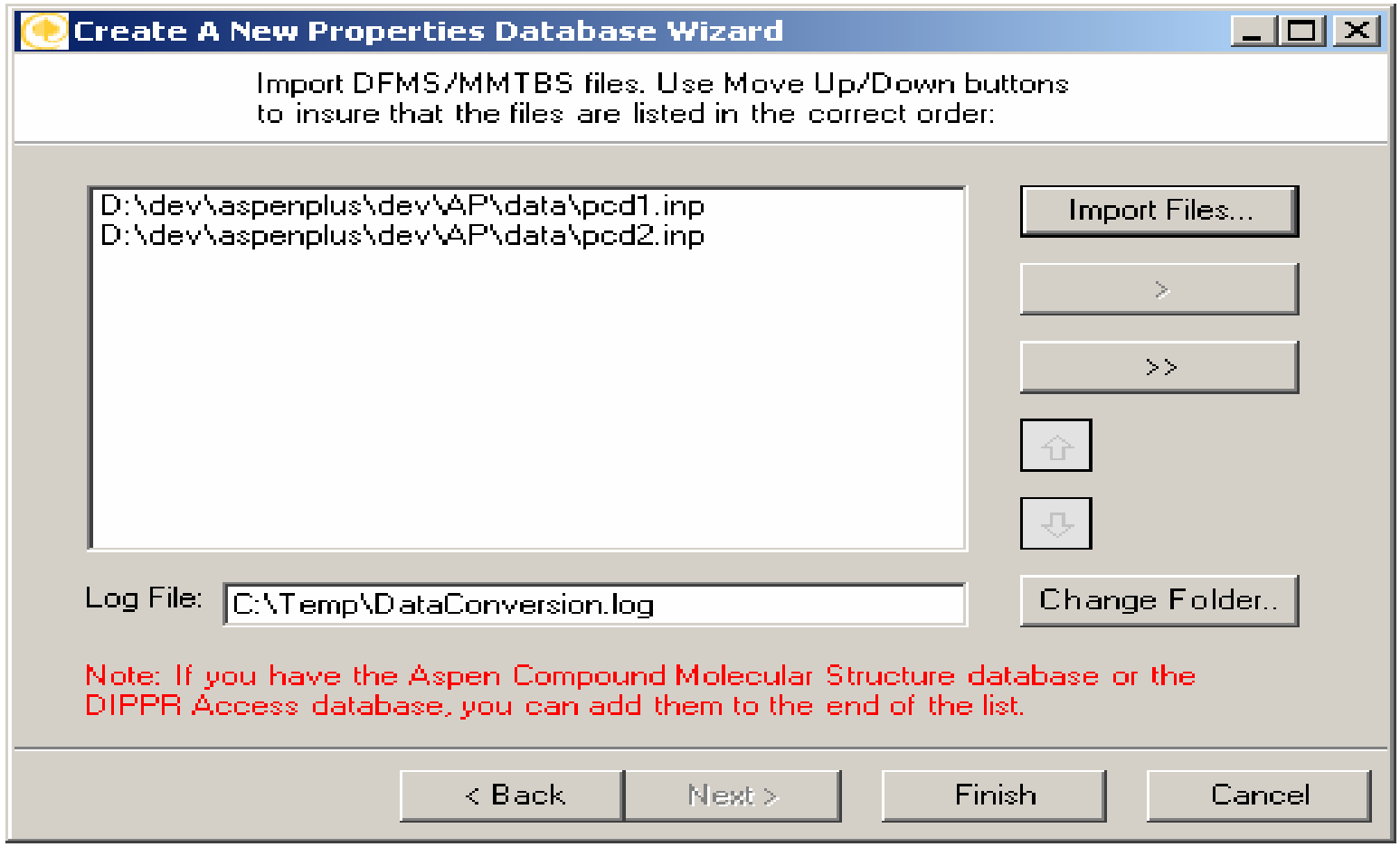

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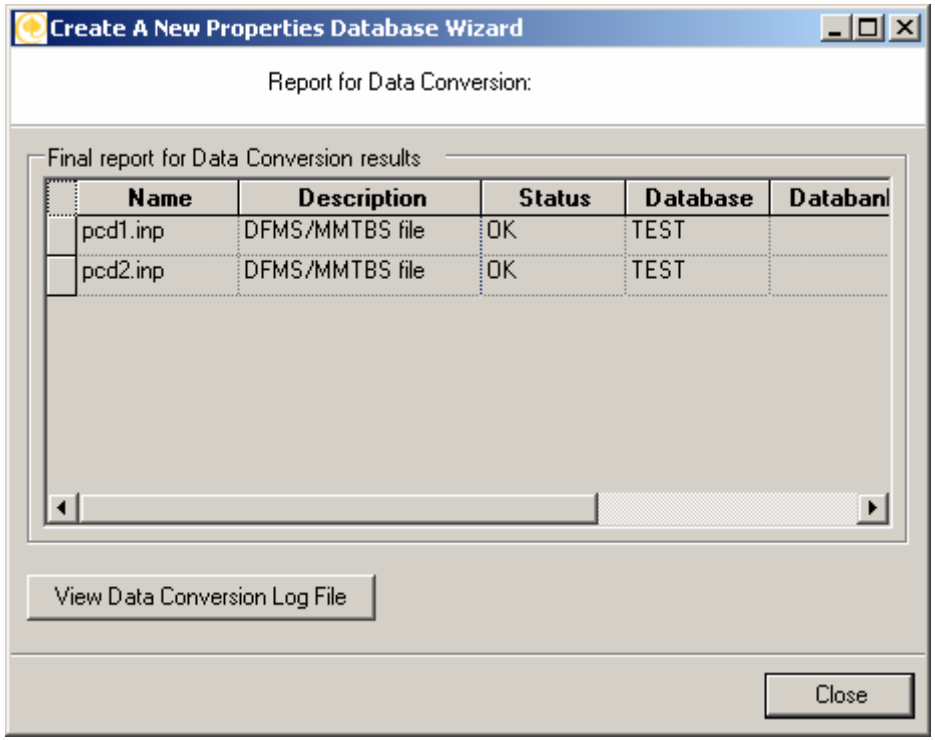

Questions?