

# CAPE-OPEN Update in PRO/II v10.1

CAPE-OPEN Property Package in compound Databank Search Order List

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# Agenda

**PRO/II v10.1 was released in June 2017**

**CAPE-OPEN Property Package Limitations  
with PRO/II v9.4 & v10.0**

**CAPE-OPEN Property Package behavior  
in PRO/II v10.1**

**Demo of PRO/II v10.1 - Property Package  
in compound Databank Search Order**

**Q&A**

# CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Limitations with PRO/II v9.4 and v10.0 :
  - The CO PP compounds are added as non-library compounds in PRO/II irrespective of whether the PP compounds are having CAS number or not.
  - Constant pure compound properties for the non-library compounds are taken from the CO PP.
  - This approach is having a limitation that user can't use PRO/II native thermo as the required temperature dependent properties are not filled for the non-library compounds.
  - The results of CO PP can't be compared with PRO/II native thermo in the same flowsheet.

# CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1 :
  - Both CO PP and PRO/II native thermo can co-exist in the same flowsheet and be used in parallel by unit operations within the flowsheet.
  - If PP compounds are having CAS numbers and matching CAS number is found in the SIMSCI or PROCESS libraries.
    - CO PP compounds are added as library compounds in PRO/II.
    - CO PP is made available in the compound databank search order list and will be first in the list with the “cascade” option checked by default.
    - Constant pure compound properties are taken from the CO PP, if it is first in the databank search order list.

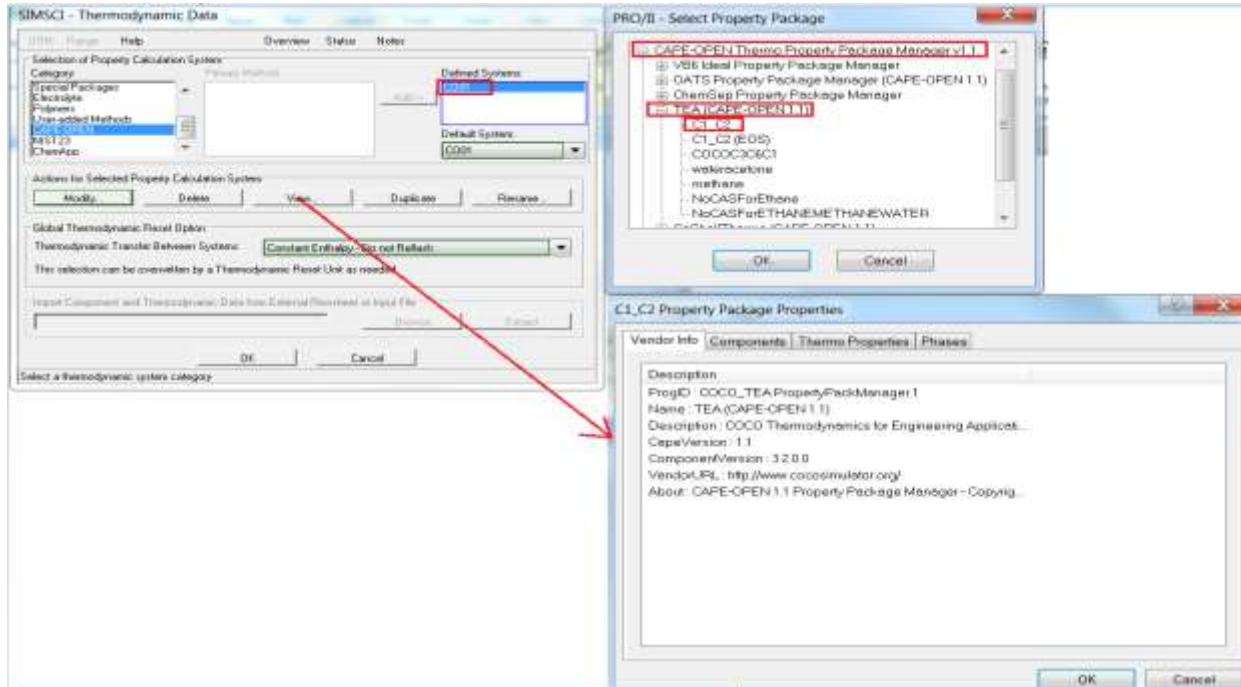
(contd...)

# CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1 :
  - The constant pure compound properties are disabled in PRO/II and user is not allowed to modify the properties, if they are taken from CO PP.
  - The temperature dependent properties (such as vapor pressure, thermal conductivity, viscosity, Ideal Gas Enthalpy, Surface Tension etc.) are not taken from the PP and they are always filled from SIMSCI or PROCESS libraries.
  - User is allowed to change the global databank search order list or for each individual compound.
- Multiple CO PP in a flowsheet are allowed. Each newly added PP will have its corresponding databank inserted at the top of the search order.

# CO PP in compound Databank Search Order List in PRO/II v10.1

## Selecting CO PP in PRO/II



# CO PP in compound Databank Search Order List in PRO/II v10.1

The image shows two overlapping windows from the PRO/II software. The left window, titled "PRO/II - Component Selection", displays a table of components and their search orders. The right window, titled "Component Selection - Databank Search Order", shows the configuration for the search order, including a list of available databanks and the current search order list.

**PRO/II - Component Selection**

UOM	Range	Help	Overview	Status	Notes
					Component Name/Alias    Databank Search Order
					1    METHANE    CURRENT
					2    ETHANE    CURRENT

**Component Selection - Databank Search Order**

Databank Type: Pure Component    Thermo Data Manager...

Available Databanks:

- Bio-Lib\_10.1: BIOETHNL
- Bio-Lib\_10.1: BIOFUELS
- DIPPR\_2016: DIPPR
- PROII\_10.1: OLLIB
- PROII\_10.1: PSRKTCCP

Current Search Order:

- CO:CO01
- PROII\_10.1: SIMSCI
- PROII\_10.1: PROCESS

Buttons: Move Up, Move Down, Restore Current Search Order to Installation Default, Set Search Order for All Components to Current, Cascading option for Component Properties: Use Cascading Search Order for All Component Properties, OK to PFD, OK, Cancel, Cancel to PFD.

Exit the window after saving all data

# CO PP in compound Databank Search Order List in PRO/II v10.1

**PRO/II - Component Selection**

UDM Range Help Overview Status Notes

Component Name/Alias	Databank Search Order
1 METHANE	CURRENT
2 ETHANE	CURRENT

Reorder List: Top, Up, Down, Bottom, NBP, MW, Internal

Edit List: Delete, Rename..., Databank...

Component Selection: From System or User-generated Databank, Component: [ ], Add->, Select from Lists..., Petroleum..., User-defined..., Polymer..., Databank Hierarchy..., Component Phases...

OK Cancel

Push to modify the databank search order of the selected components

**Individual Component Selection – Databank Search Order**

UDM Range Help

Databank Type: Pure Component Thermo Data Manager...

Specify Databank Search Order for Selected Components METHANE.

Use Cascading Search for Component Properties

Available Databanks: Bio-Lib\_10.1:BIOETHNL, Bio-Lib\_10.1:BIOFUELS, DIPPR12016:DIPPR, PROII\_10.1:OLILIB, PROII\_10.1:PSRKTCP

Insert Before Insert After Remove

Current Search Order: CO:CO01, PROII\_10.1:SIMSCI, PROII\_10.1:PROCESS

Move Up Move Down

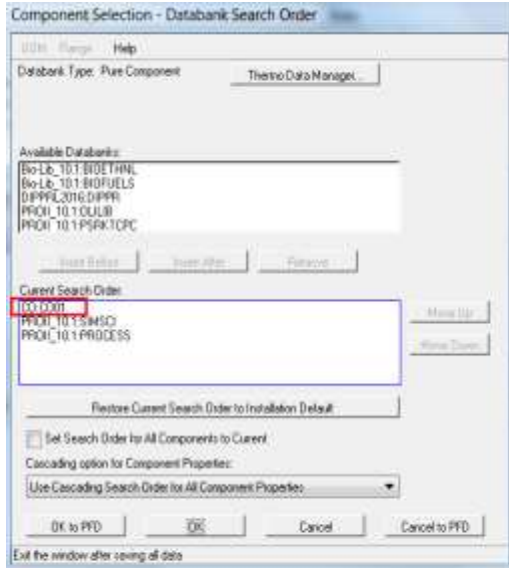
Restore Search Order to Current

OK to PFD OK Cancel Cancel to PFD

Mark this box to apply Databank Search Order only to Selected Components



# CO PP in compound Databank Search Order List in PRO/II v10.1



Component Properties - Fixed Properties

	Molecular Weight	Standard Liquid Density	Normal Boiling Point	Critical Temperature	Critical Pressure	Critical Volume	Critical Compressibility Factor	Acentric Factor
Comp								
Point	METHANE	16.042	217.30 AP	-258.69 F	-118.69 F	62.02 cm <sup>3</sup> /mol	0.286	0.011
Reset	ETHANE	30.07	289.07 AP	127.48 F	89.91 F	706.62 cm <sup>3</sup> /mol	0.270	0.000

Buttons: OK to PFD, OK, Cancel, Cancel to PFD

# CO PP in compound Databank Search Order List in PRO/II v10.1

Component Selection - Databank Search Order

LCM File Help

Databank Type: Plus Component Thermo Data Manager

Available Databanks:

- BIO-LG-10-1-BIOETHANL
- BIO-LG-10-1-BIOFUELS
- CAPPAC-2016-DAPPR
- PRO-II-10-1-OLUB
- PRO-II-10-1-PSRKTDC

Current Search Order:

- PRO-II-10-1-SHRSQ
- PRO-II-10-1-PROCESS
- CO-PP**

Buttons: OK to PFD, OK, Cancel, Cancel to PFD

Exit the window after saving all data

Component Properties - Fixed Properties

LCM File Help

	Molecular Weight	Standard Liquid Density	Normal Boiling Point	Critical Temperature	Critical Pressure	Critical Volume	Critical Compressibility Factor	Acentric Factor
Copy								
Paste	METHANE	16.0426	249.17 AP	-250.98 F	0.11835 F	0.07200 m <sup>3</sup> /kmol	0.285	0.0115478
Reset	ETHANE	30.0696	256.85 AP	-127.49 F	88.91 F	0.20652 m <sup>3</sup> /kmol	0.279	0.099493

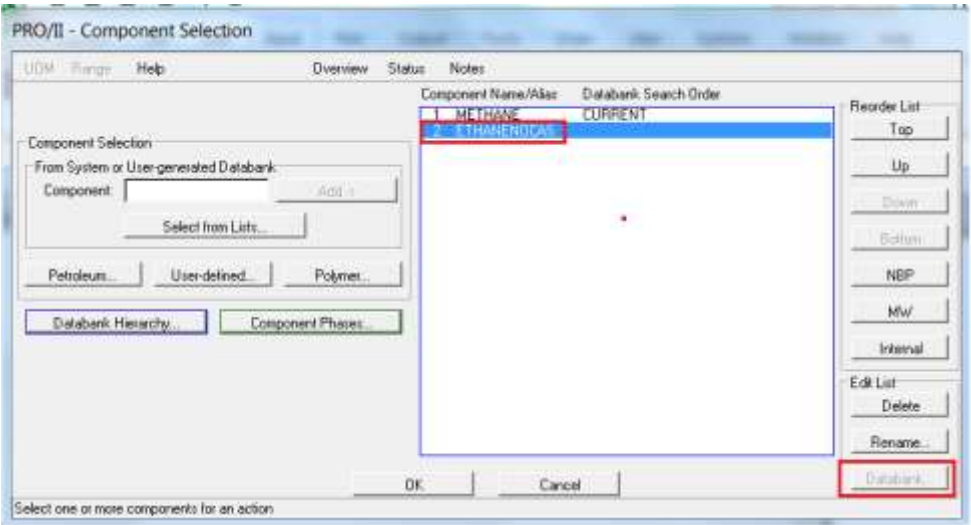
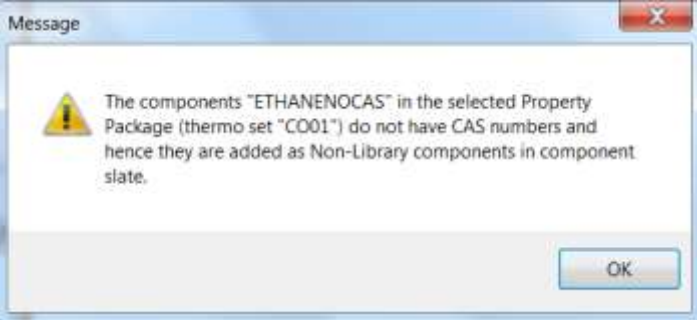
Buttons: OK to PFD, OK, Cancel, Cancel to PFD

Exit the window after saving all data

# CO PP in compound Databank Search Order List in PRO/II v10.1

- CO PP Behavior in PRO/II v10.1
  - If PP compounds are not having CAS numbers or matching CAS number is not found in the SIMSCI or PROCESS libraries
    - CO PP compounds are added as non-library compounds in PRO/II.
    - The constant pure compound properties are taken from the CO PP.
    - The temperature dependent properties are not filled from the CO PP.
    - Compound Databank Search Order is not available for non-library compounds

# CO PP in compound Databank Search Order List in PRO/II v10.1



# CO PP in compound Databank Search Order List in PRO/II v10.1

- If user deletes CO PP in PRO/II, the corresponding CO thermoset is deleted from the databank search order. The compounds associated with that PP are either deleted or retained in the PRO/II compound slate based on conditions.



- If user renames CO thermoset, the databank search order list having the CO thermoset should be renamed accordingly.
- If CO PP supports persistence and user modifies the constant pure compound properties by editing the CO PP, the updates values are reflected in PRO/II.

# CO PP in compound Databank Search Order List in PRO/II v10.1

Demo of CO PP in compound Databank Search Order in PRO/II v10.1

# CO PP in compound Databank Search Order List in PRO/II v10.1

Q&A

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