

# CAPE-OPEN Update in PRO/II v9.2 - Part 2

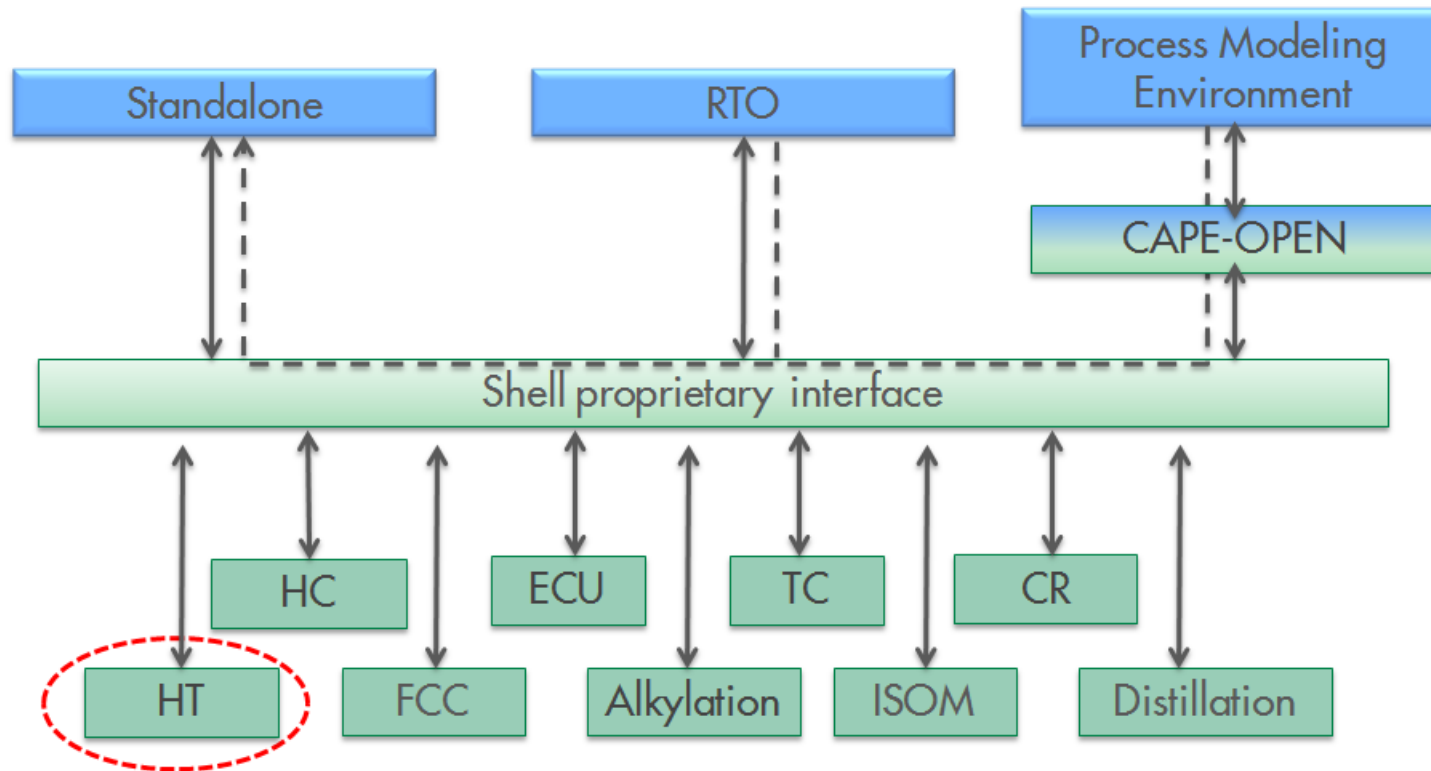
Support for CAPE-OPEN Petroleum Fractions specification

Jasper Van Baten & Krishna Murthy Penukonda

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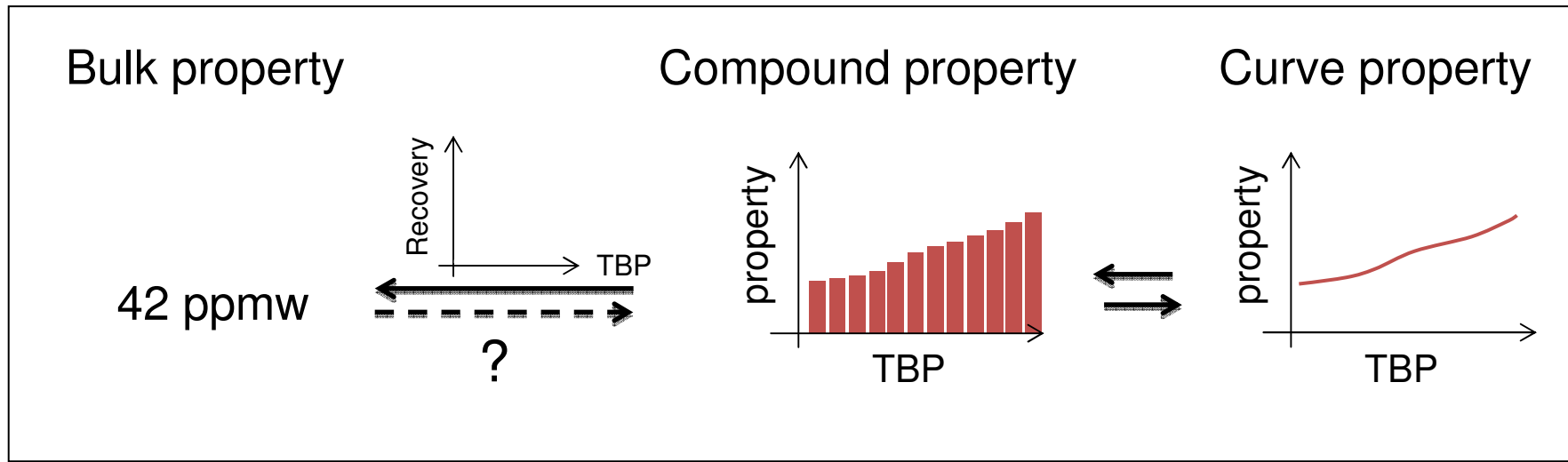
# PROCESS MODELING FRAMEWORK



R. Baur et al., presentation given at the 244th ACS National Meeting, Pennsylvania, August 19-23, 2012.

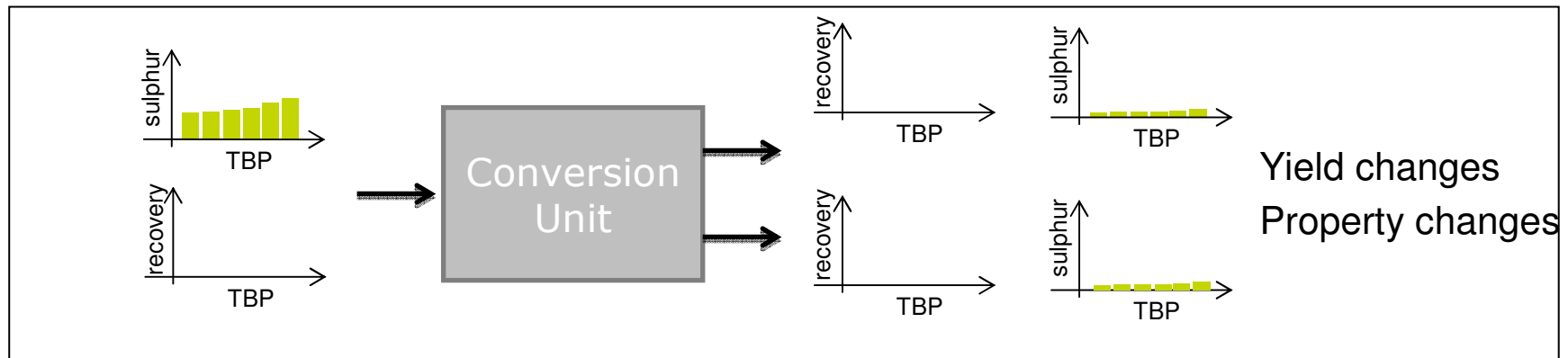
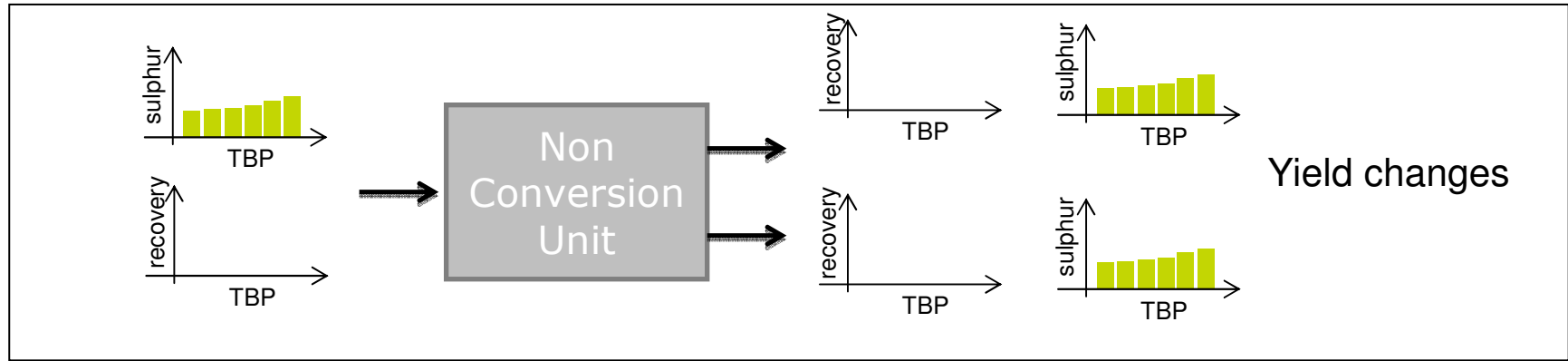
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# CAPE-OPEN Refinery Reactor SIG (2006-2008):



Property bases: mass, mole, volume, (none)  
Example: aromatic content kg/kg, mol/mol, m<sup>3</sup>/m<sup>3</sup>

# Conversion & non-conversion units



The unit decides which properties need to be modified at the outlet streams

# ***CAPE-OPEN Petro Property requirements***

- Standard list of properties?
- Which property values are known by default?
- Which properties are set by the unit operation?
- Which properties are affected?

Work flow:

Copy from source → Set properties → “Complete”

## *Copy from source* → *Set properties* → *"Complete"*

- **PMC copy feed to product**
  - PMC decides which product is populated from which feed
- **PMC sets product composition, compound density and bulk sulphur**
  - PMC should provide finest granularity, e.g. compound sulphur if it can
  - PMC should not make conflicting specifications, so not both bulk and compound sulphur
- **PMC calls "Complete"**
  - PME now knows which properties have been modified and which other properties will be affected.
  - PME calculates recharacterization and compound sulphur. Note: PME decides on best way to convert bulk sulphur to compound sulphur

# *Copy from source* → *Set properties* → **"Complete"**

When to call "Complete"?

Complete must be called before

- Flash calculation  
All product streams must be flashed by the PMC
- Property calculations  
PMC may require intermediate property calculations (e.g. to close enthalpy balance)

# CAPE-OPEN Implementation

List of properties

Method summary

- Pseudo? GetCompoundConstant("Type")
- CopyPetroProperties(source material)
- Get/SetPetroBulkProp(property, basis, value)
- Get/SetPetroCompoundProp(property, comps, basis, value)
- Get/SetPetroCurveProp(property, X-basis, Y-basis, X-values, Y-values)
- CompletePetroProperties()

IDL/TLB available



## *Implementation at SimSci (Pro/II)*

- **Support for the following bulk and compound properties:**  
Asphaltenes, BromineNumber, CetaneIndex, CetaneNumber, CloudPoint, ColdFilterPlugPoint, ConradsonCarbon, CriticalPressure, CriticalTemperature, CriticalVolume, FinalBoilingPoint, FlashPoint, FreezePoint, HydrogenContent, InitialBoilingPoint, IsoParafins, KinematicViscosity, LiquidDensity, MercaptanSulphur, MolecularWeight, MON, Napthenes, Nickel, Nitrogen, NormalBoilingPoint, Olefins, PourPoint, RefractiveIndex, ReidVaporPressure, RON, SmokePoint, Sulphur, Vanadium, ViscosityIndex, WatsonK
- **Support for the following curve properties:**  
CutPointCurve, D1160AtmCurve, D1160VacCurve, D86Curve, TBPCurve

## ***Implementation at SimSci (Pro/II)***

- **Support for the following functions:**  
GetListPetroBulkProp, GetListPetroCompoundProp,  
GetListPetroCurveProp, GetPetroBulkProp,  
GetPetroCompoundProp, GetPetroCurveProp,  
SetPetroCompoundProp, CopyPetroProperties,  
CompletePetroProperties
- **No support yet for setting curve properties:**  
SetPetroCurveProp
- **Currently, properties are only available in the basis in which they are defined**  
Example: if Sulphur is configured in a thermo set using a mass based blend rule, Sulphur can only be set and retrieved in mass basis

***Live demonstration by***

***Krishna Murthy***

# SIMSCI Petro Test Unit

The screenshot displays the SIMSCI Petro Test Unit interface. At the top, a process flow diagram shows a unit labeled 'CO1' with an inlet stream '1' and an outlet stream '2'. A context menu is open over the unit, listing options such as 'Delete', 'Produce Report', 'Data Entry...', 'CAPE-OPEN Settings', 'Notes...', 'Cut', 'Copy', 'Goto', 'Break Before', 'Break After', 'Collapse', 'Exclude Unit', 'Rotate', 'Flip', 'Restore Icon Size', 'Restore Label Position', 'Center in View', 'Add Bookmark...', and 'Lock'. An orange arrow points from the 'CAPE-OPEN Settings' option to a dialog box titled 'PRO1B - CAPE-OPEN Unit'. This dialog box contains fields for 'Unit' (CO1) and 'Description', and two tables: 'CAPE-OPEN Unit Ports' and 'CAPE-OPEN Unit Parameters'. The 'CAPE-OPEN Unit Ports' table has columns for Name, Direction, Stream, and Thermodynamic System. The 'CAPE-OPEN Unit Parameters' table has columns for Name, Mode, Value, and UOM. To the right of the dialog box is a data table with columns for Stream Name, Stream Description, Phase, and two columns labeled '1' and '2'. The data table contains various physical and chemical properties for two mixed streams.

Stream Name	Stream Description	Phase	1	2
		Mixed		
Temperature		F	450.0000	450.0000
Pressure		PSIG	14.0000	14.0000
Enthalpy		MM BTU/HR	070.5884	070.5884
Molecular Weight			235.3241	235.3241
Vapor Weight Fraction			0.1818	0.1818
Liquid Weight Fraction			0.8181	0.8181
Total Mass Rate		LB/HR	3723021.188	3723021.188
Total Weight Comp. Rates		LB/HR		
H2			0.0000	0.0000
H2S			0.0000	0.0000
N2			0.0000	0.0000
H2O			0.0000	0.0000
C1			0.0000	0.0000
C2			1902.8880	1902.8880
C3			4261.3519	4261.3519
HC4			7188.8731	7188.8731
			17211.8390	17211.8390
			45030.0283	45030.0283
			0.0000	0.0000
			0.0000	0.0000
			0.0000	0.0000
			0.0000	0.0000
			0.0000	0.0000
			0.0000	0.0000
			2289.8058	2289.8058
			17200.5118	17200.5118
			28232.8872	28232.8872

# SIMSCI Petro Test Unit

The screenshot displays the SIMSCI software interface. The main window is titled 'SIMSCI - Thermodynamic Data' and shows a 'Selection of Property Calculation System' dialog. Below this, the 'Thermodynamic Data - Modification' window is open, showing a list of properties and their current methods. A 'Refinery Inspection Properties...' button is highlighted. A secondary dialog box, 'Thermodynamic Method Selection for Refinery Inspection Properties', is overlaid on top, showing a table of property methods and their associated units and bases. An orange arrow points from the 'Refinery Inspection Properties...' button in the main window to the secondary dialog box. Another orange arrow points from the 'OK' button in the secondary dialog box to the 'Thermodynamic Data - Modification' window.

**Thermodynamic Method Selection for Refinery Inspection Properties**

Out	Property	Method	Base	Fill	Blending	
Insert	1 Kinematic Viscosity	SIMSD	Weight	No Fill	Mixing	Data...
Reset	2 Cloud Point Temperature	SIMSD	Liq.Vol	No Fill	Mixing	Data...
	3 Pour Point Temperature	Index	Liq.Vol	No Fill	Mixing	Data...
	4 Flash Point Temp./Open Cup	Index	Weight	No Fill	Mixing	Data...
	5 Sulfur Content	Summation	Weight	No Fill	Mixing	Data...
	6 Cetane Number	Summation	Liq.Vol	No Fill	Mixing	Data...
	7 Smoke Point	Summation	Liq.Vol	No Fill	Mixing	Data...

OK Cancel

Do not close this window after saving all data

# SIMSCI Petro Test Unit

The screenshot displays the SIMSCI Petro Test Unit software interface. The main window is titled "PRO/E - Stream Data" and shows the "Stream Data - Flowrate and Assay" dialog box. The "Fluid Flowrate" is set to 12075 tpd/hr. The "Define/Edit Assay..." button is highlighted with an orange arrow.

The "Stream Data - Assay Definition" dialog box is also visible, showing the "Assay curve data for stream 1" section. The "TBP Basis" is set to "Liquid Volume". The "Pressure" is set to -0.00013628 psig. The "Assay Curve" table is shown below:

Cut	Percent Distilled	Temperature F
1	3.00	97.00
2	5.00	149.00
3	10.00	208.00
4	20.00	330.00
5	30.00	458.00
6	40.00	580.00
7	50.00	690.00
8	60.00	770.00
9	70.00	865.00
10	80.00	960.00

The "Assay Property Selection for Refinery Inspection Properties" dialog box is also visible, showing a table of properties to be entered:

Cut	Property Name	Enter Data...
1	Sulfur Content	Enter Data...
2	Nitrogen (Total)	Enter Data...
3	Bronine Number	Enter Data...
4	Refractive Index (I20)	Enter Data...
5	Corrosion Carbon Residue	Enter Data...
6	Aniline Point	Enter Data...
7	Cloud Point Temperature	Enter Data...
8	Cetane Number	Enter Data...
9	Cold Filter Plug Point	Enter Data...
10	Freeze Point Temperature	Enter Data...

# SIMSCI Petro Test Unit

Report Properties ✖

Feed stream name: 1

Description: Calculation Option (0, 1, 2): 0

Components:

Name	compound...	casRegistr...	molecular...	criticalTem...	criticalPres...	criticalVolu...	criticalCom...	acent
H2	0	1333-74-0	2.0158801...	33.189998...	1313000	6.4147002...	0.3050000...	-0.215
H2S	0	7783-06-4	34.081878...	373.52999...	8962910.1...	9.8499998...	0.2840000...	9.416
NH3	0	7664-41-7	17.030559...	405.64999...	11280000	7.2470001...	0.2419999...	0.252
H2O	0	7732-18-5	18.015279...	647.13000...	22055000	5.5947799...	0.2290000...	0.344

All Properties: activityCoefficient, boilingPointTemperature, compressibilityFactor, density, dewPointPressure, dewPointTemperature, enthalpy, enthalpyF, entropy

Phases: Overall, Liquid, Vapor

Mole

Calc ->

Available Properties and Values:

Name	Overall	Liquid
enthalpy	127995	158433
fraction		
H2	0	0
H2S	0	0
NH3	0	0
H2O	0	0

Petroleum Bulk Properties:

Name	Value
AnilinePoint	523.218
Asphaltenes	9.52413e-006
BromineNumber	3.00146
ConradsonCarbon	0.00106108
CetaneIndex	44.5103
CetaneNumber	49.5913
ColdFilterPlugPoint	357.51
CloudPoint	655.373
FinalBoilingPoint	1110.15
FlashPoint	346.341

Petroleum Curves:

Fraction	CutPointCurve	D1160AtmCurve	D1160
0.01	0.01	123.603	86.326
0.05	0.05	325.108	234.64
0.1	0.1	369.386	268.65
0.15	0.15	389.067	284.90
0.2	0.2	423.66	312.21
0.25	0.25	466.222	345.59
0.3	0.3	509.805	380.06
0.35	0.35	548.767	411.55
0.4	0.4	582.661	439.61

Petroleum Fractions:

Name	Acentricity	CriticalPressure	CriticalTemperat...	CriticalVolume	LiquidDensity	MolecularWt
NBP 98	0.190012	3.95618e+006	487.332	0.000287045	10088.7	69.4972
NBP 109	0.198527	3.85475e+006	494.393	0.000296825	9784.27	72.1298
NBP 129	0.214034	3.68646e+006	506.941	0.000314701	9276.91	76.9461
NBP 151	0.231348	3.5185e+006	520.582	0.000334861	8769.56	82.3855
NBP 173	0.249181	3.36283e+006	534.305	0.000355926	8300.2	88.0785
NBP 192	0.264996	3.2367e+006	546.236	0.000374902	7918.01	93.2599

OK Cancel

# Conclusions

- CAPE-OPEN unit that implements ICapeThermoPetroFractionsII can be plugged in to PRO/II9.2 and use this functionality.
- The petro property should be specified in the PRO/II Thermo set. Returns error if the unit request the petro property which is not selected in Pro/II Thermo set.
- The basis (if applicable) of the petro property selected in PRO/II should be same. Returns error if the unit request the petro property with a basis which is not the same selected in Pro/II Thermo set.
- Set petro compound property: PRO/II doesn't allow to set the compound petro property for real compounds. Returns error if the compound petro property for real compounds is set by the unit.
- Set petro bulk property: PRO/II do not scale up/down the property for real compounds but adjust its contribution in pseudo compounds. In this way the set value will match with calculated and get value.
- Set petro curve property: Not supported in PRO/II.



***Thank you...***

**Q&A?**