

# Status and Future Perspectives of the Refinery Reactors SIG

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# Outline

- ◆ Motivation
- ◆ Refinery Units/Reactors
- ◆ Petroleum Fractions Interfaces
  - ◆ Changes
  - ◆ Unit Type Identification
  - ◆ Petroleum Properties: basis, list
- ◆ Future

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# Motivation

- ◆ Global CAPE-OPEN project defined a number of specialized CO interfaces:
  - ◆ Petroleum Fractions interface (ICapeThermoPetroFractions)
  - ◆ Never went beyond prototyping
  - ◆ Perceived as incomplete?
- ◆ Simulation vendors are extending petroleum fraction support and extended oil property capabilities into their products (RefSys, Proll, Unisim Design)
- ◆ Interest in having CO-based interfaces to integrate *refinery units* (PMCs) in simulation environments (PMEs)



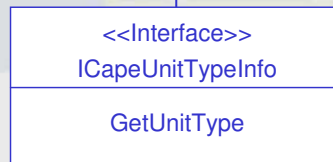
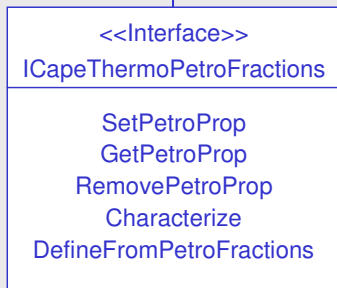
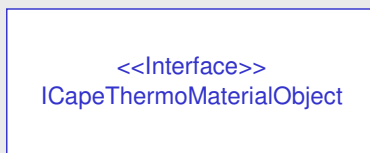
# Refinery Units/Reactors

- ◆ What is a *refinery unit* in this context?
- ◆ Unit Operation interacting with compounds defined by modifiable (petroleum) properties
  - ◆ Sulfur, viscosity, RON, TBP, metals content, etc
  - ◆ REFINERY REACTOR is used in the SIG name for historic reasons
  - ◆ Examples of refinery units:
    - ◆ Conversion *reactors* (reformer, FCC, hydrocracker, etc)
    - ◆ Property *calculators/setters*
    - ◆ Assay manipulators, basis changers, lumpers/delumpers
    - ◆ Separators and distillation columns are NOT refinery units in this context

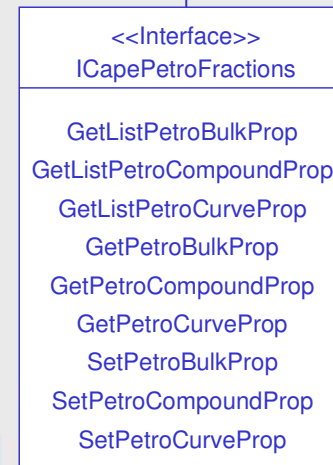
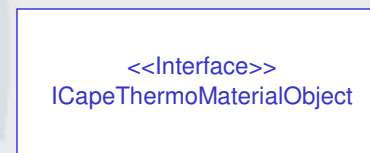


# Petroleum Fractions Interfaces

v1.0



Proposed:



# Interface changes

<b>v1.0</b>	<b>Proposed</b>
One get, and one set methods for all properties	One get, one set, and one list methods for each property type
RemovePetroProp method	Eliminated
DefineFromPetroProps method	Superseded by CopyFromMaterial in thermo v1.1 Can be done manually with list/set methods
Characterize method	Removed from current version PMC's responsibility Should be addressed in future



# Unit Type Identification

- ◆ Material Object needs to know if a unit operation supports the petroleum fraction interface; if it is a *refinery unit*
- ◆ Two possibilities:
  - ◆ ICapeUnit interface to have ICapeUnitTypeInfo interface with method GetUnitType (v1.0)
  - ◆ Information added to registry entry for unit

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# Bulk Petroleum Properties

## ◆ GetListPetroBulkProp:

- ◆ Out: `CapeArrayString*` *propertyID*

## ◆ GetPetroBulkProp:

- ◆ In: `CapeString` *propertyID*

- ◆ In: `CapeString` *basis*

- ◆ Out: `CapeDouble*` *value*

## ◆ SetPetroBulkProp:

- ◆ In: `CapeString` *propertyID*

- ◆ In: `CapeString` *basis*

- ◆ In: `CapeDouble*` *value*



# Compound Petroleum Properties

- ◆ **GetListPetroCompoundProp**
  - ◆ Out: **CapeArrayString\* *propertyID***
  
- ◆ **GetPetroCompoundProp**
  - ◆ In: **CapeString *propertyID***
  - ◆ In: **CapeString *compID***
  - ◆ In: **CapeString *basis***
  - ◆ Out: **CapeDouble\* *value***
  
- ◆ **SetPetroCompoundProp**
  - ◆ In: **CapeString *propertyID***
  - ◆ In: **CapeString *compID***
  - ◆ In: **CapeString *basis***
  - ◆ In: **CapeDouble\* *value***

# Curve Petroleum Properties

- ◆ **GetListPetroCurveProp**
  - ◆ Out: **CapeArrayString\* *propertyID***
  
- ◆ **GetPetroCurveProp**
  - ◆ In: **CapeString *propertyID***
  - ◆ In: **CapeString *basis***
  - ◆ Out: **CapeDouble\* *cutValues***
  - ◆ Out: **CapeDouble\* *propValues***
  
- ◆ **SetPetroCurveProp**
  - ◆ In: **CapeString *propertyID***
  - ◆ In: **CapeString *basis***
  - ◆ In: **CapeDouble\* *cutValues***
  - ◆ In: **CapeDouble\* *propValues***



# Property Basis

- ◆ **Basis for property values:**
  - ◆ **Existing (from Thermo): mass, mole**
  - ◆ **Other:**
    - ◆ **Volume @ *standard conditions***
    - ◆ **Volume basis widely used, especially in US refining**
    - ◆ **Which standard conditions?**
      - ◆ **Multiple options:**
        - ◆ **Temperature: 0 °C, 15 °C, 20 °C, 25 °C, 60 F**
        - ◆ **Pressure: 1 atm, 100 kPa, ...**
      - ◆ **Can convert from mass/mole if std liq volume/density is a defined property**
  - ◆ **Proposal: optional volume basis**
    - ◆ **60 F, 1 atm (std US refining)**



# List of Properties

- ◆ Basic list of properties to be supported
  - ◆ Not final list
- ◆ Need to support user-defined properties
  - ◆ Define at PME/MO level
  - ◆ Unit awareness through GetListXProp interfaces
  - ◆ But, how to identify?
    - ◆ E.g. RON\_BP user property to be used by unit as RON

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# Basic Bulk Properties

propID	Description
WatsonK	Watson K
TrueVaporPressure	True Vapor Pressure
ReidVaporPressure	Reid Vapor Pressure
FlashPoint	Flash Point
PourPoint	Pour Point
CloudPoint	Cloud Point
FreezePoint	Freeze Point
AnilinePoint	Aniline Point
SpecGravity	Specific Gravity
APIGravity	API Gravity
ViscosityAt100F	Viscosity At 100F
ViscosityAt210F	Viscosity At 210F
RefractiveIndex	Refractive Index
NParafinsIndex	Normal Parafins Index
CetaneIndex	Cetane Index

propID	Description
RON	RON
MON	MON
Paraffins	Paraffins Content
Olefins	Olefins Content
IsoParafins	IsoParafins Content
Napthenes	Napthenes Content
Aromatics	Aromatics Content
Asphaltenes	Asphaltenes Content
Sulphur	Sulphur Content
MercSulphur	Mercaptan Sulphur Content
Nickel	Nickel Content
Nitrogen	Nitrogen Content
Vanadium	Vanadium Content
ConCarbon	Conradson Carbon Content



# Basic Compound Properties

<b>propID</b>	<b>Description</b>
TC	Critical Temperature
PC	Critical Pressure
VC	Critical Volume
Acentric	Acentric Factor
MW	Molecular Weight
StdLiqDens	Standard Liquid Density
NBP	Normal Boiling Point
IBP	Initial Boiling Point
FBP	Final Boiling Point



# Basic Curve Properties

propID	Description
TBPCurve	TBP Curve
D86Curve	D86 Curve
D86CorrectedCurve	D86 Corrected Curve
D1160VacCurve	D1160 Vacuum Curve
D1160AtmCurve	D1160 Atmospheric Curve
TCCurve	Critical Temperature Curve
PCCurve	Critical Pressure Curve
AcentricCurve	Acentric Factor Curve
MWCurve	MW Curve
SpecGravityCurve	Specific Gravity Curve
MassDensCurve	Mass Density Curve

propID	Description
ParaffinCurve	Paraffins Content
OlefinCurve	Olefins Content
IsoParaffinCurve	IsoParafins Content
NaptheneCurve	Napthenes Content
AromaticsCurve	Aromatics Content
SulphurCurve	Sulphur Content

# Future

- ◆ End of 2008
  - ◆ Volume basis
  - ◆ List of properties
    - ◆ User properties
- ◆ 2009
  - ◆ Update prototypes
- ◆ Longer term
  - ◆ Characterize method
  - ◆ Decide on future interface support/development
  - ◆ Commercial support, especially from PMEs



# Thanks

- ◆ CO-LaN Refinery Reactors SIG members
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