# Exporting Custom Properties

# to CAPE-OPEN

## CAPE-OPEN 2022 Annual Meeting

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**&**

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# Overview

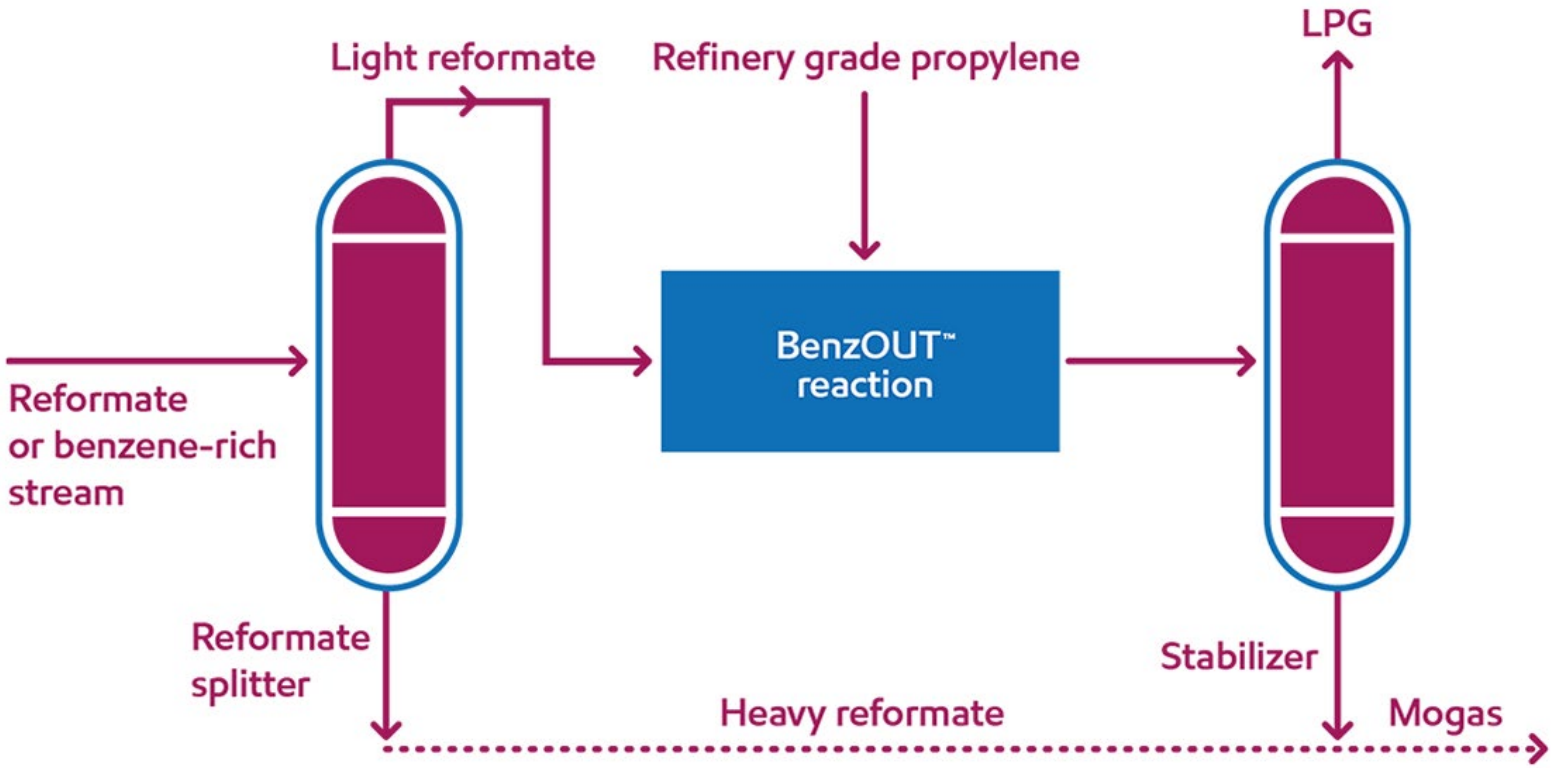
- Desire to expose petroleum properties in ChemSep via CAPE-OPEN Property Package
- Though these properties may be covered by the petroleum properties standard, adoption of that standard takes time
- Thermodynamic standard allows for “custom” properties to pragmatically add any property
- We used custom properties to export petroleum properties, accepting that they may not be universally understood
- Such properties can be ‘private’ between Unit Operation and CAPE-OPEN Property Package (COPP)

# History of ChemSep LITE

- ChemSep standalone distributed to universities
- 2005: v5.0: ChemSep LITE first *CAPE-OPEN* version, demonstrated as UnitOp in Pro/II & Aspen+
- 2006: v6.0: integrated CAPE-OPEN from wrapper into GUI and added adaptive icons (in COCO)
- 2015: v7.0: ChemSep CAPE-OPEN property packages
- 2018: v8.0: Parallel Column Model for DWC
- **2022: v8.3: Export of Additional Properties**

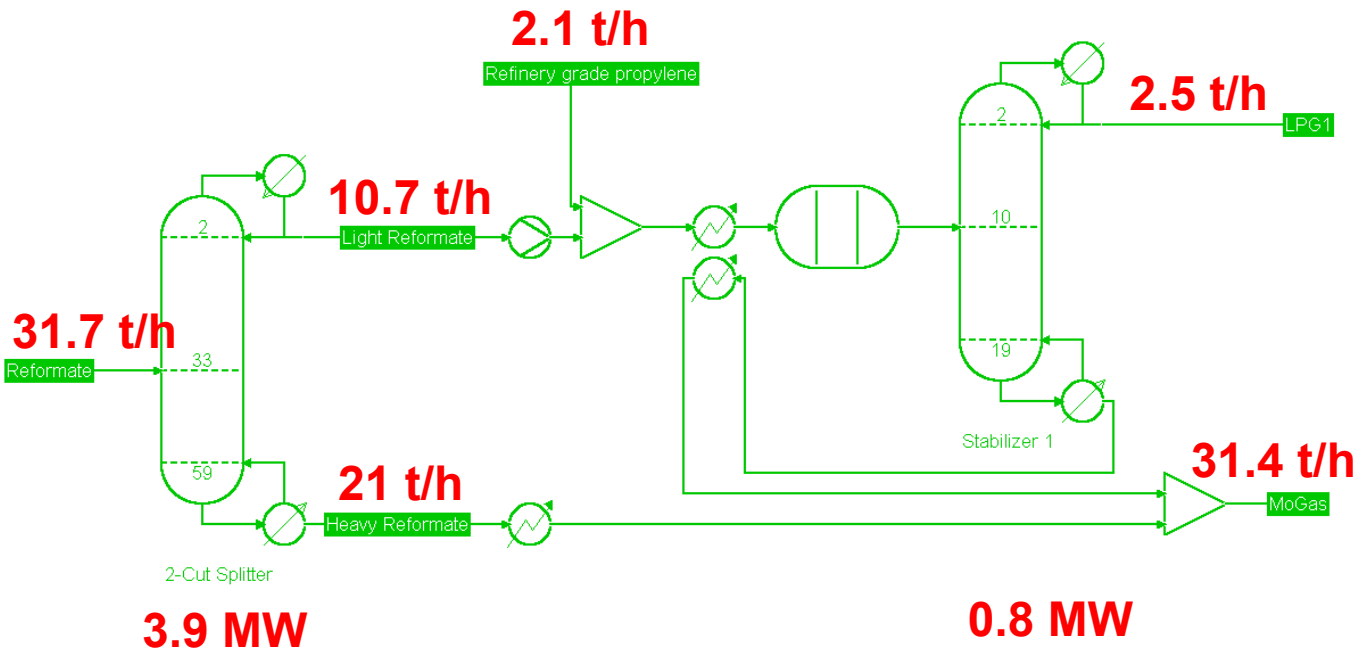
# Example: EXXON-Mobil BenzOUT

- Reduce Benzene in gazoline (Mogas) by reacting with Propylene without causing a loss in octane#
- Includes stabilizer to maintain low vapor pressure
- Patented process US 8,395,006 B2:



# Example: EXXON-Mobil BenzOUT

- Process needs to fulfill petroleum properties specs:
  - Minimize drop in octane number
  - Maintain low Reid Vapor Pressure of product




| Stream | Reformate | MoGas | Unit |
|---|---|---|---|
| Pressure | 3.5 | 2.5 | bar |
| Temperature | 100 | 71.0902 | °C |
| Flow rate | 343 | 335.349 | kmol / h |
| Mole frac n-butane | 0.0309038 | 0.00909843 | |
| Mole frac isopentane | 0.0819242 | 0.0835314 | |
| Mole frac n-pentane | 0.0580175 | 0.0592973 | |
| Mole frac 2-methylpentane | 0.0862974 | 0.0882657 | |
| Mole frac n-hexane | 0.045481 | 0.0465187 | |
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| Mole frac 1,3,5-trimethylbenzene | 0.0594752 | 0.0608322 | |
| Mole frac 1,4-diethylbenzene | 0.0116618 | 0.0119279 | |
| Mole frac Propane | 0 | 6.03384e-07 | |
| Mole frac Propylene | 0 | 6.69168e-07 | |
| Mole frac Cumene | 0 | 0.0595601 | |
| Mole frac P-diisopropylbenzene | 0 | 0.0320708 | |
| OCTN | 100.404 | 98.3165 | - |
| RVP | 0.414281 | 0.315115 | bar |
| TVP100 | 0.427999 | 0.333599 | bar |

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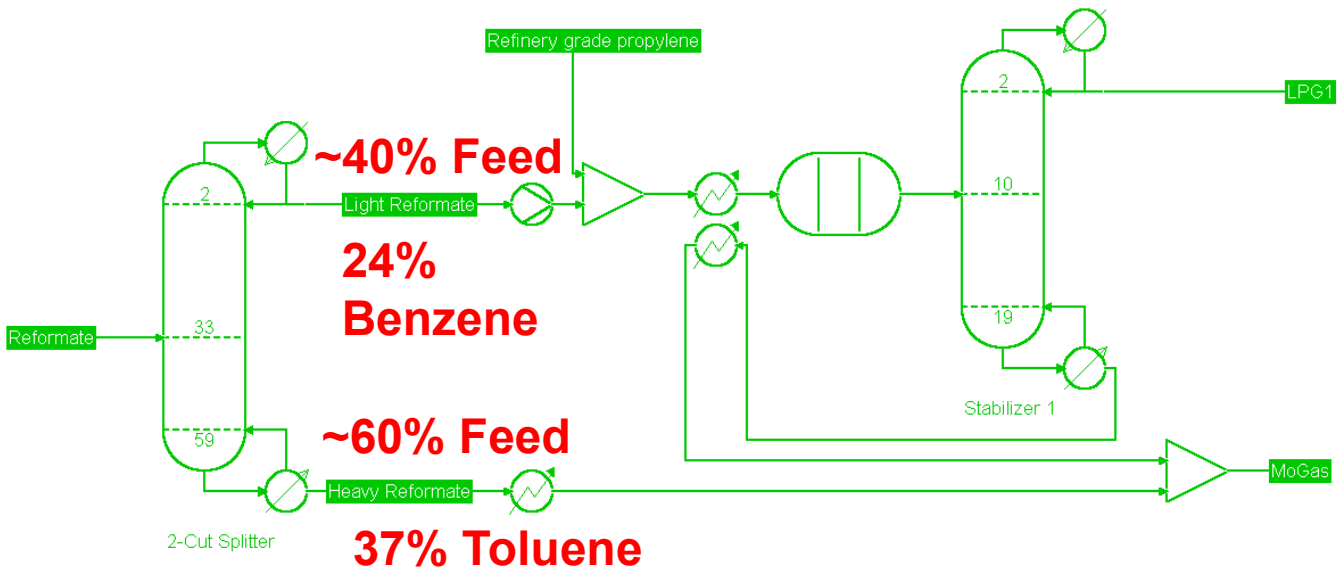


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| Mole frac o-xylene | 0.0478134 | 0.0489043 | |
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| Mole frac Cumene | 0 | 0.0595601 | |
| Mole frac P-diisopropylbenzene | 0 | 0.0320708 | |
| Liquid phase | | | |
| OCTN | 100.404 | 98.3165 | - |
| RVP | 0.414281 | 0.315115 | bar |
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# Example: EXXON-Mobil BenzOUT

Can we improve the economics of this process while maintaining performance in OCTN & RVP?

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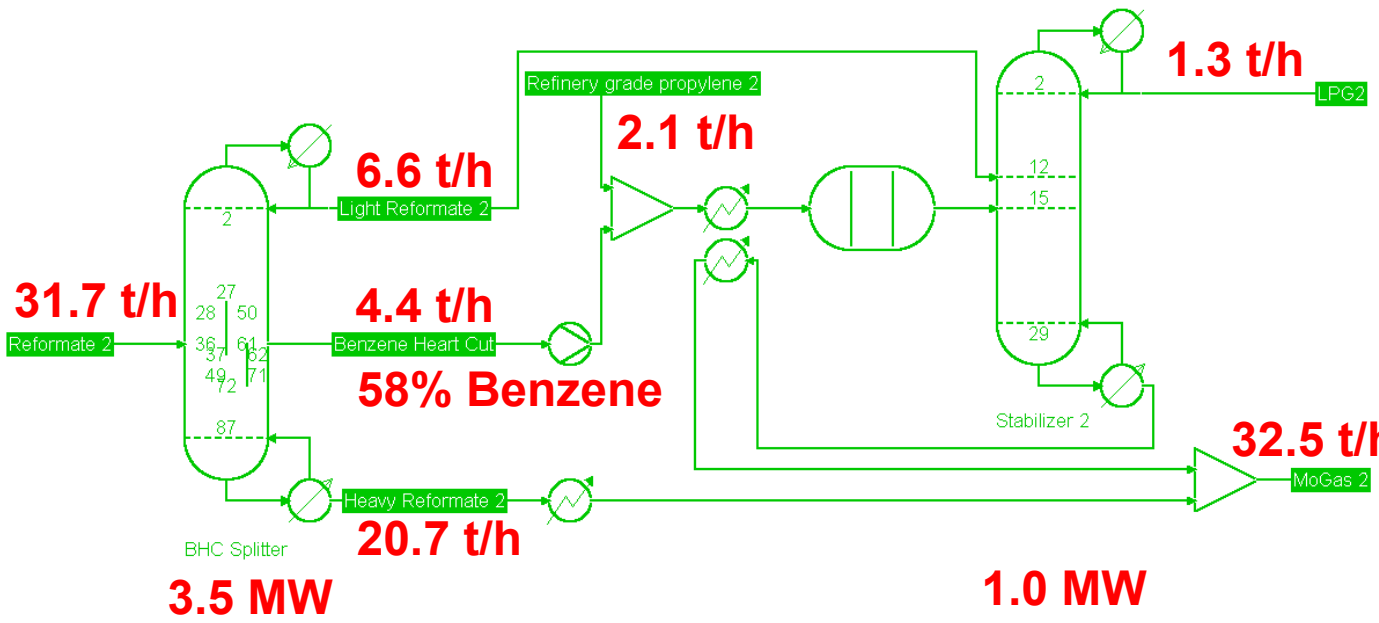
Can we improve the economics of this process while maintaining performance in OCTN & RVP?

- Produce “heart-cut” product in which >99% of the Benzene is recovered, only send this to the reactor: Reduces flow through reactor & stabilizer by 2x
- Use Dividing Wall Column (DWC) technology to revamp the reformate splitter in the same column

# Example: EXXON-Mobil BenzOUT

- Advantages:
  - Smaller reactor + stabilizer: TAC -30%
  - No difference in OCTN or RVP
  - 5% lower duty




| Stream | Reformate 2 | MoGas 2 | Unit |
|---|---|---|---|
| Pressure | 3.5 | 2.5 | bar |
| Temperature | 100 | 71.3644 | °C |
| Flow rate | 343 | 334.936 | kmol / h |
| Mole frac n-butane | 0.0309038 | 0.0115992 | |
| Mole frac isopentane | 0.0819242 | 0.0805443 | |
| Mole frac n-pentane | 0.0580175 | 0.0587449 | |
| Mole frac 2-methylpentane | 0.0862974 | 0.0883696 | |
| Mole frac n-hexane | 0.045481 | 0.0465759 | |
| Mole frac benzene | 0.101458 | 0.0120102 | |
| Mole frac 3-methylhexane | 0.0186589 | 0.0191081 | |
| Mole frac toluene | 0.248397 | 0.254377 | |
| Mole frac ethylbenzene | 0.0306122 | 0.0313493 | |
| Mole frac p-xylene | 0.0370262 | 0.0379177 | |
| Mole frac m-xylene | 0.106122 | 0.108678 | |
| Mole frac o-xylene | 0.0478134 | 0.0489646 | |
| Mole frac m-ethyltoluene | 0.0361516 | 0.037022 | |
| Mole frac 1,3,5-trimethylbenzene | 0.0594752 | 0.0609072 | |
| Mole frac 1,4-diethylbenzene | 0.0116618 | 0.0119426 | |
| Mole frac Propane | 0 | 2.02693e-06 | |
| Mole frac Propylene | 0 | 2.25938e-06 | |
| Mole frac Cumene | 0 | 0.0597255 | |
| Mole frac P-diisopropylbenzene | 0 | 0.0321599 | |
| Liquid phase | | | |
| OCTN | 100.404 | 98.3402 | - |
| RVP | 0.414281 | 0.318967 | bar |
| TVP100 | 0.427999 | 0.337995 | bar |

# Example: EXXON-Mobil BenzOUT

Other advantages:

- Flexible co-production of 58% Benzene product

Can we further optimize?

# Example: EXXON-Mobil BenzOUT

Other advantages:

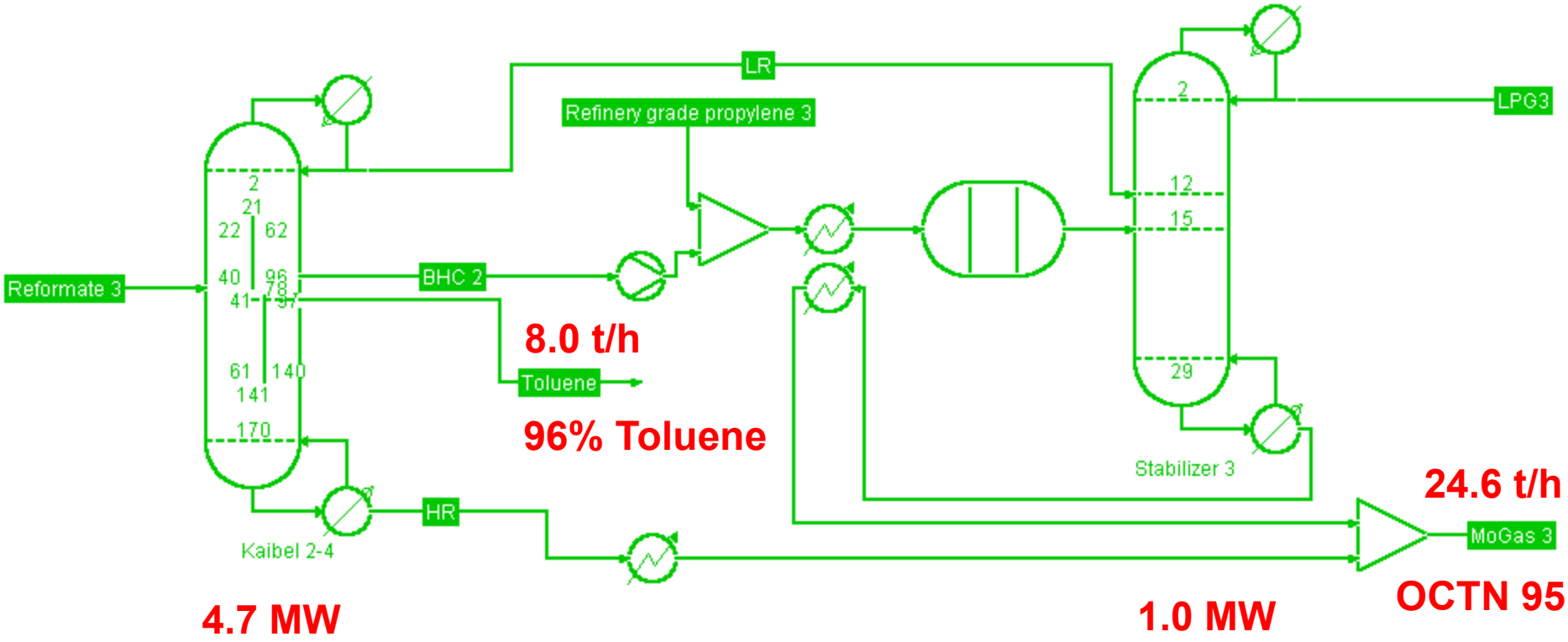
- Flexible co-production of 58% Benzene product

Can we further optimize?

- Extra duty enables co-production of >96% Toluene as separate product with Kaibel configuration
- Maintaining OCTN 95 Mogas

# Example: EXXON-Mobil BenzOUT

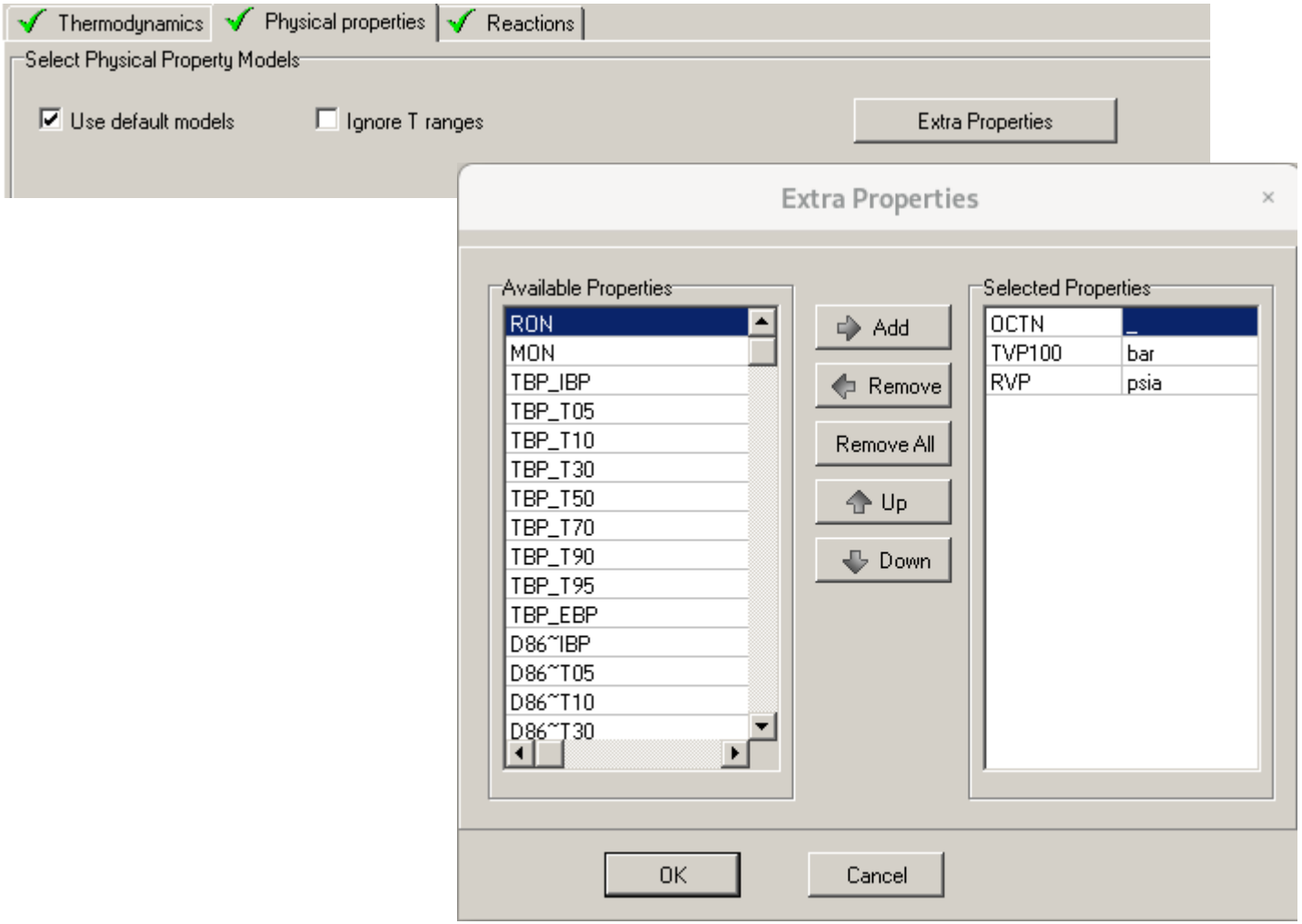
- Existing reformate splitters can be revamped using sloped-wall DWC designs, see Dejanovic *et al.**




* Dejanović, I., Matijašević, L., Jansen, H., Olujić, Ž., 2011. Designing a Packed Dividing Wall Column for an Aromatics Processing Plant. Industrial & Engineering Chemistry Research 50, 5680–5692. https://doi.org/10.1021/ie1020206

# Selection of Extra Properties

As part of the physical properties models selection



# Extra Properties Methods

RON & MON: Table values / Estimated from groups or Tb & SG

OCTN: Posted Octane Number = RON/2+MON/2

Flash Point: Riazi (eqn. 3.114/3.115)

TVP100: Antoine vapor pressure model at 100 F
(with Ambrose or Riedel as back-up)

RVP: Approximation using the TVP100, mixtures per Riazi p. 132

TBP: Spline interpolation

D86: Riazi-Daubert 1986 on TBP

API density

K Watson

More to come...

# RON & MON Estimation

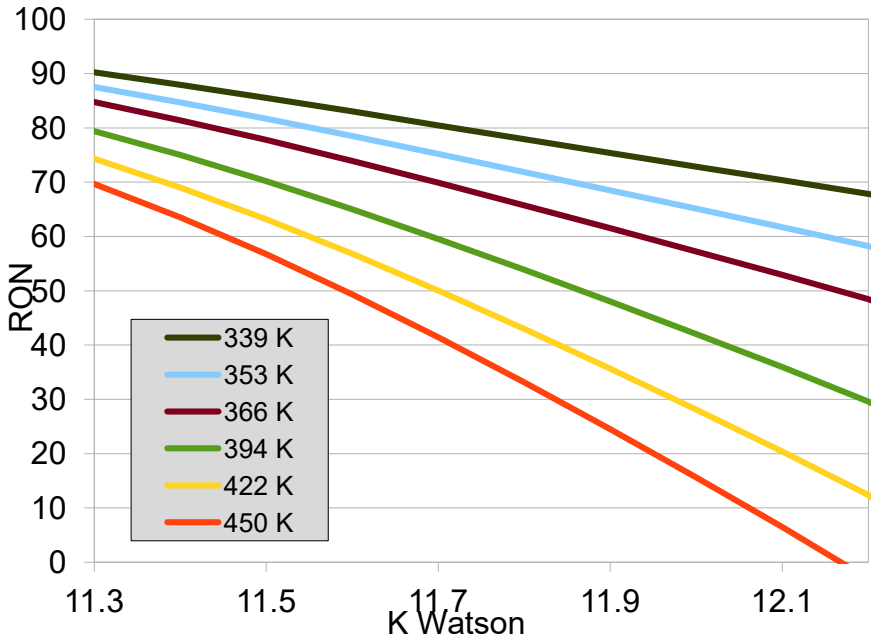
**RON**:

- UNIFAC groups: Albahri (*Ind.Eng.Chem.Res.* (2003) 42, pp. 657-662 + (2004) 43, p. 7964) and new -OH/=O/-O- groups
  average error 8.8%

- Pseudo's: Nelson (1969) as *f*(Kw,Tb) for Naphtha's

**MON**:

Jenkins (1968)
average error 8%



# Extra Properties Results

Clarkson UNIVERSITY defy convention

## Internal Thermo: Show as part of stream table output

| Stream | Feed1 | L.Feed1 | Top | Bottom | Sidestream |
|---|---|---|---|---|---|
| Stage | 37 | 37 | 1 | 88 | 61 |
| Pressure (psia) | 50.7632 | 49.5838 | 39.1602 | 56.7596 | 50.8737 |
| Vapour fraction (-) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Temperature (K) | 373.218 | 373.220 | 338.862 | 455.119 | 391.402 |
| Enthalpy (J/kmol) | -2.212E+07 | | -1.970E+07 | -8.930E+06 | -1.622E+07 |
| Entropy (J/kmol/K) | -36044.6 | | -50096.6 | -2814.91 | -38012.1 |
| Total molar flow (kmol/s) | 0.0952834 | 0.0952834 | 0.0255687 | 0.0576599 | 0.0120548 |
| Total mass flow (kg/s) | 8.81370 | 8.81370 | 1.92960 | 5.89568 | 0.988422 |
| Vapour std.vol.flow (m3/s) | | | | | |
| Liquid std.vol.flow (m3/s) | 0.0111053 | 0.0111053 | 0.00302690 | 0.00681101 | 0.00126738 |
| Liquid: | | | | | |
| Mole weight (kg/kmol) | 92.4999 | 92.4999 | 75.4672 | 102.249 | 81.9941 |
| Density (kg/m3) | 716.579 | 716.563 | 587.747 | 700.750 | 676.010 |
| Std.density (kg/m3) | 793.649 | 793.649 | 637.483 | 865.610 | 779.892 |
| Viscosity (N/m2.s) | 2.3365E-04 | 2.3365E-04 | 1.6713E-04 | 1.4136E-04 | 1.8449E-04 |
| Heat capacity (J/kmol/K) | 200600 | 200601 | 188257 | 237046 | 189124 |
| Thermal cond. (J/s/m/K) | 0.104216 | 0.104211 | 0.0959115 | 0.0931280 | 0.102774 |
| Surface tension (N/m) | 0.0160580 | 0.0160577 | 0.0113389 | 0.0115046 | 0.0134855 |
| Extra: | | | | | |
| OCTN ( ) | 100.382 | 100.382 | 74.6569 | 114.685 | 84.9530 |
| TVP100 (bar) | 0.428177 | 0.428177 | 1.20952 | 0.0510031 | 0.316488 |
| RVP (psia) | 6.01158 | 6.01158 | 17.1398 | 0.651681 | 4.12011 |

# Extra Properties Results

## CS/COPP: As part of the stream table output in COCO

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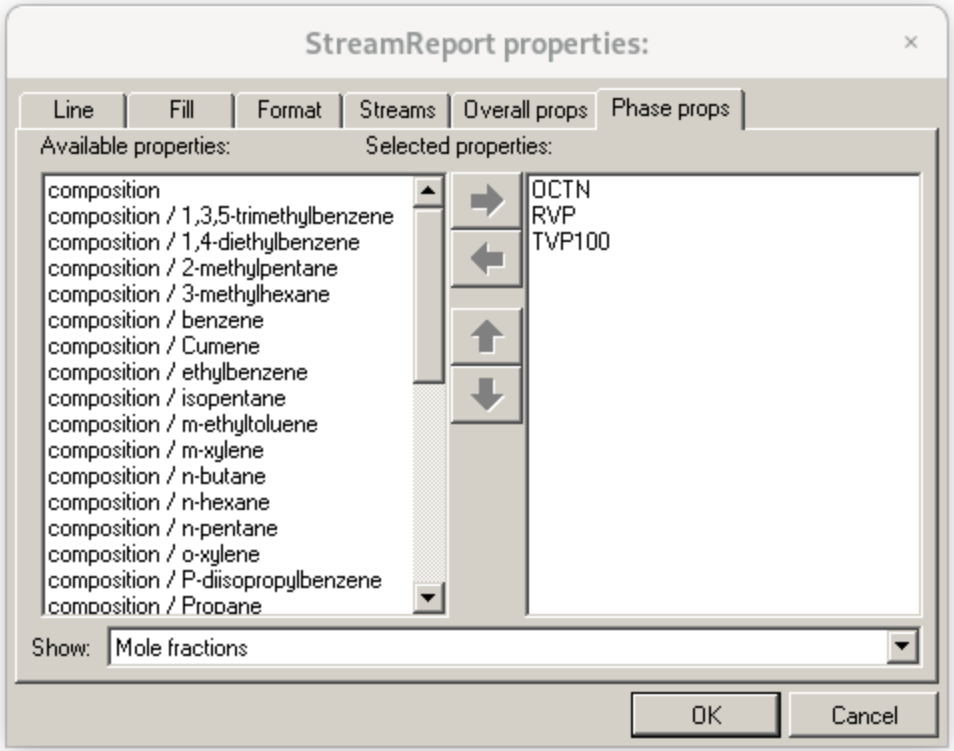

# Extra Properties Results

## Units of Measure – Allows conversion of units

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| Liquid phase | | | |
|---|---|---|---|
| OCTN | 100.404 | 98.3165 | - |
| RVP | 6.00864 | 4.57036 | psi |
| TVP100 | 6.2076 | 4.83844 | psi |

# Code to get the Extra Properties?

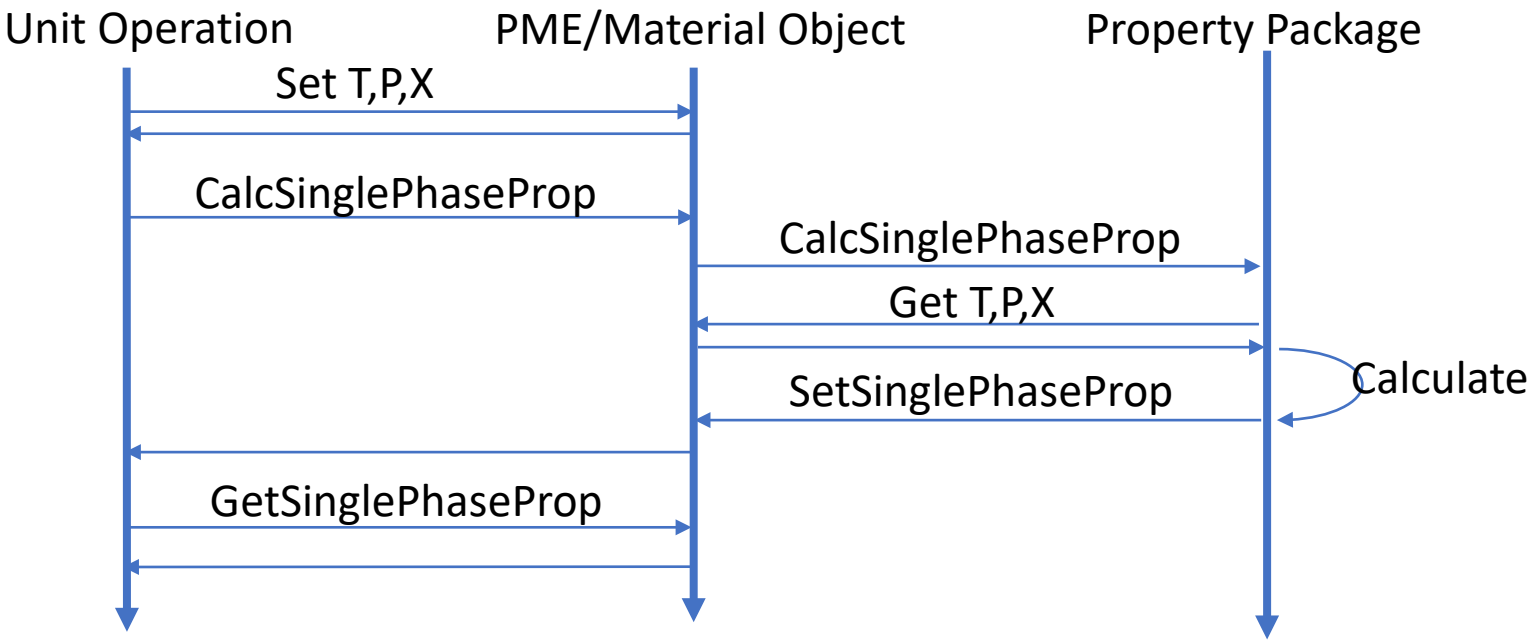
Call to Fortran DLL:

```
nex = NumberExtraProps()
do j=1,nex
 i = idExtraProperty(j)
 call EPname (i, Cname)
 call EPdesc (i,iDmns,Desc)
 call EProp (i, Cvalue, T, p, Ffeed, Z, nc, ncmax, iErr)
 if (iErr .eq. 0) then
  write(io,*) Cvalue, ' '//Cname
 else
  write(io,*) 'error calculating '//Cname
 end if
end do
```

- See the back-up slides for a description of the function arguments

# Extra Properties Calculation

Calling Sequence:



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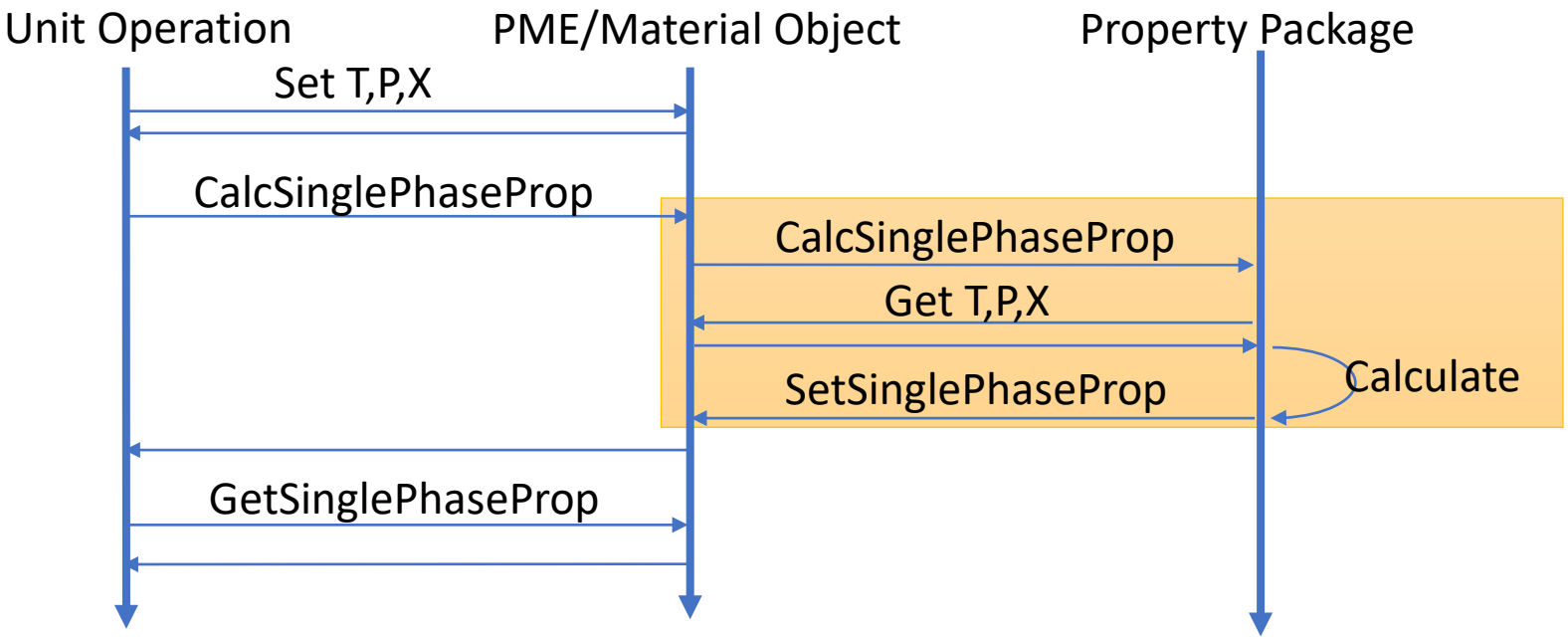
Calling Sequence:




PME can also access the property by itself!

# Summary

- CAPE-OPEN Custom Properties (COCP) are useful
- ChemSep uses COCP for Petroleum Properties Drawback: Overall properties are missing, exposed as liquid properties
- COCP definition (ChemSep ↔ COCO) via private API Drawbck: No support by other PMEs

# Questions?

# Backup slides

# Code to get the Extra Properties?

integer **NumberExtraProps**()

*Returns the number of Extra Properties in the COPP*

integer **idExtraProperty**(j)

*Returns the type of the $j^{th}$ Extra Property. Each type has its own number*

subroutine **EPname** (i, Cname)

*Returns the name for the $i^{th}$ Extra Property as string in Cname*

subroutine **EPdesc** (i,iDmns,Desc)

*Returns the description Desc as string and dimensions array Dmns for the $i^{th}$ Extra Property*

Subroutine **EProp** (i, Cvalue, T, p, Ffeed, Z, nc, ncmax, iErr)

*Integer i, nc, ncmax, iErr; double Cvalue, T, p, Ffeed; double array Z*

*Returns the value Cvalue for the $i^{th}$ Extra Property using T,p,Ffeed,Z()*

# How to Get the Extra Properties?

C/C++ Getting the DLL entry points:

- NumberExtraProps=(F_NUMBEREXTRAPROPS)GetProcAddress(dllHandle,"numberextraprops_");
- if (!NumberExtraProps) { throw COException(L"Unable to load NumberExtraProps function from ChemSep DLL"); }
- idExtraProperty=(F_IDEXTRAPROPERTY)GetProcAddress(dllHandle,"idextraproperty_");
- if (!idExtraProperty) { throw COException(L"Unable to load idExtraProperty function from ChemSep DLL"); }
- EPdesc=(F_EPDESC)GetProcAddress(dllHandle,"epdesc_");
- if (!EPdesc) { throw COException(L"Unable to load EPdesc function from ChemSep DLL"); }
- EProp=(F_EPROP)GetProcAddress(dllHandle,"eprop_");
- if (!EProp) { throw COException(L"Unable to load EProp function from ChemSep DLL"); }

# How to Get the Extra Properties?

CS/COPP DLL calls in C/C++:

- int nex=(*NumberExtraProps)();
- for (int i=1;i<=nex;i++) {
- int id=(*idExtraProperty)(&i);
- char propName[101];
- propName[100]=' ';
- int dimension[7];
- (*EPdesc)(&id,dimension,propName,100);
- for (int j=100;j>=0;j--) { if (propName[j]!=' ') {propName[j+1]=0; break; }
- }
- UTF8toUTF16 pName(propName);
- propMap[pName]=PropDetails::make((PropertyID)(PropID_EXTAPROP0+id),0,Deriv_None,massBasisDependent,SinglePhaseProperty,pName);
- propList1p.emplace_back(pName);
- }

# RON & MON Text-Files

ComponentList RON & MON Applications in Energy and Combustion Science 5 (2021) 100018

CAS Number
RON
MON

1
74-84-0
115
99

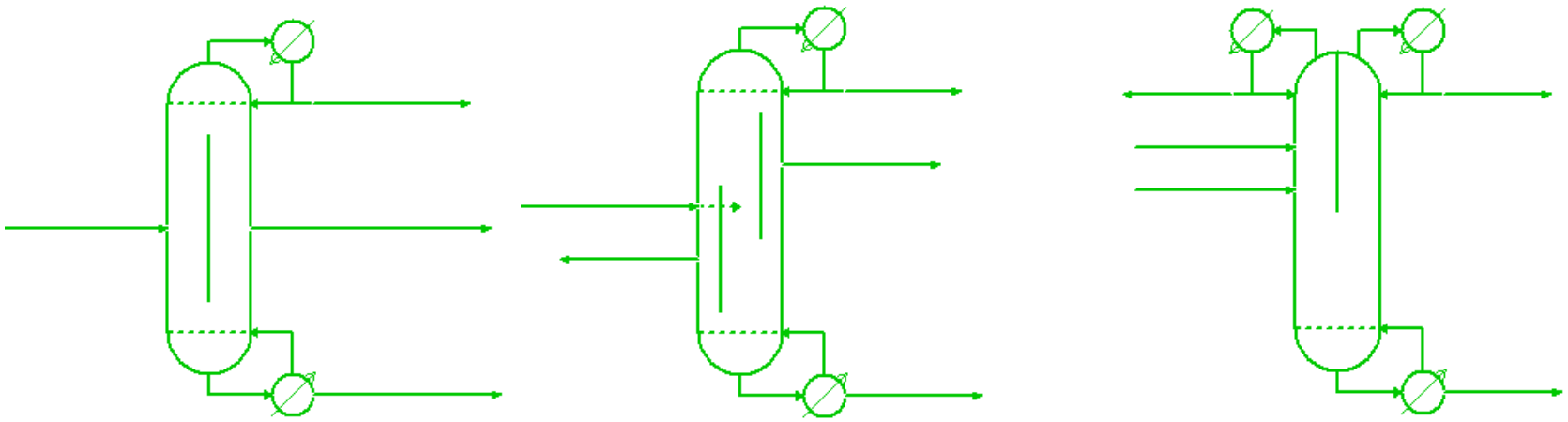
2
74-98-6
111
97

3
106-97-8
94
89

...

# DWC Process Simulation in ChemSep

- Parallel Column Model for CAPE-OPEN compliant systems
- Does not require any guesses for streams
- Predefined configurations with single & multiple walls, selection from drop-down list
- Icons reflect actual configuration (in COCO)
- Rapid tray/packing internals design of each column section with selection of any modern type internal
- Column sizing include auxiliaries: CAPEX & OPEX
- Connection to vendor rating tools



Icons in COCO (www.cocosimulator.com)