



# Beyond Compliance

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# Assuring CAPE-OPEN Adoption

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- A set of standardized interfaces are in place and have been implemented by multiple vendors
- Widespread adoption/use of these interfaces will depend upon more than technical feasibility and availability



# Adoption Issues

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- Quality of implementation in Process Modeling Environment (PME)
- PME interface capabilities
- Interface experience

***Ideally user should not even notice that CAPE-OPEN interfaces are being used.***



# Implementation Quality

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- Implementation should be as seamless as possible
  - Maximize existing knowledge of PME
- Exploit capabilities of PME



# Implementation Quality (HTRI)

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- Implemented Unit Operation interface for three most used *Xchanger Suite* modules
  - Xist (Shell and Tube)
  - Xace (Air-coolers/Economizers)
  - Xphe (Plate and frame)
- Implemented Thermodynamic interface within *Xchanger Suite*
- Tested against multiple process simulators and property packages



# Implementation Quality (HTRI)

- *Xchanger Suite* calculation modules evolved as stand alone engines
  - Optimized for rigor instead of calculation speed
    - Fluid property handling modified
    - Known versus unknown duty
  - Significant input/runtime problems result in diagnostic messages and end of calculations
  - Process condition handling not consistent with most process simulators
    - HTRI based on property grid
    - Simulators provide temperature and vapor fraction which may be inconsistent with interpolated conditions

# Property Options

Property Generation

Generate new properties during run

Number of pressure sets  Temperature increment method

Number of temperature points  Flash type

Adjust calculated points

Insert bubble point if in temperature range

Insert dew point if in temperature range

Generate component fractions

Supercritical Conditions

Critical pressure  psia

Supercritical phase

Starting Temperature

Use inlet temperature

Use temperature  F

Starting Pressure

Use inlet pressure

Use pressure  psia

Ending Temperature

Use opposite stream inlet temperature

Use calculated outlet temperature

Temperature estimate  F

Use temperature  F

Ending Pressure

Use calculated pressure

Pres. drop estimate  psi

Use pressure  psia

Use pressure drop  psi



# PME Capabilities

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- Reporting
- Unit operation interface



# Reporting (Native)

17	<b>PARAMETERS</b>					
18						
19	<b>Exchanger Design (End Point)</b>					
20						
21	Tube Side DeltaP:	0.6895 kPa *	Shell Side DeltaP:	68.95 kPa *	Passes:	---
22	UA:	845.7 kJ/C-h	Tolerance:	1.0000e-04 *		
23	Tube Side Data			Shell Side Data		
24	Heat Transfer Coefficient	---	Heat Transfer Coefficient	---		
25	Tube Pressure Drop	0.69 kPa *	Shell Pressure Drop	68.95 kPa *		
26	Fouling	0.00000 C-h-m <sup>2</sup> /kJ *	Fouling	0.00000 C-h-m <sup>2</sup> /kJ *		
27	Tube Length	1.00 m *	Shell Passes	1		
28	Tube O.D.	20.00 mm *	Shell Series	1 *		
29	Tube Thickness	2.0000 mm	Shell Parallel	1 *		
30	Tube Pitch	50.0000 mm *	Baffle Type	Single		
31	Orientation	Horizontal	Baffle Cut(%Area)	20.00 *		
32	Passes Per Shell	1 *	Baffle Orientation	Horizontal		
33	Tubes Per Shell	80 *	Spacing	800.0000 mm *		
34	Layout Angle	Triangular (30 degrees)	Diameter	530.0259 mm *		
35	TEMA Type	A E L	Area	5.03 m <sup>2</sup>		
36	<b>SPECS</b>					
37						
38		Specified Value	Current Value	Relative Error	Active	Estimate
39	Heat Balance	0.0000 kJ/h	1.279e-010 kJ/h	-3.553e-014	On	On
40	UA	---	845.7 kJ/C-h	---	On	On
41						
42	<b>Detailed Specifications</b>					
43	<b>Heat Balance</b>					
44	Type: Duty	Pass: Error		Spec Value: 0.0000 kJ/h		
45	<b>UA</b>					
46	Type: UA	Pass: Overall		Spec Value: ---		

# Reporting (CAPE-OPEN)

The screenshot shows the 'CO-100' unit configuration window. The 'General properties' section includes:

- Unit Type: HtriCO100.Xist
- Unit Name: CO-100
- Unit description: CAPE-OPEN (1-0-0) for HTRI's Xist shell and tube heat exchanger program
- Report to be integrated in the HYSYS Report: Output Summary
- Report result from LAST unit execution

The 'Performance' section displays the following data:

Performance	
Overdesign, %	6.120e-2
Overall U, W/m2-K	158.77
Required U, W/m2-K	158.67
Duty, MegaWatts	5.4213
Shellside h, W/m2-K	611.46
Tubeside h, W/m2-K	231.44
Shellside delta P, kPa	15.840

The window has tabs for 'Material Connections', 'Unit Variables', 'General' (selected), and 'Thermo'. A green bar at the bottom indicates the unit is 'Solved', and a 'Show Unit GUI' button is present.



# Reporting

1		Case Name:	E:\Cape-Open\Samples\Sample Xist CO Case .hsc
2	<b>Honeywell</b> HONEYWELL Calgary, Alberta CANADA	Unit Set:	SI
3		Date/Time:	Sunday Feb 12 2006, 10:16:07
4			
5			
6	<b>CAPE-OPEN Unit 1.0 Operations: CO-100</b>		
7			
8	( No Datasheets exist for this unit operation )		
9			
10			
11			
12			
13			
14			
15			
16			
17			
18			

Can CAPE-OPEN access the native reporting mechanisms?



# Unit Operation Interface

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- Access allowed to native unit operation interface
  - Required for complete control of unit operation
- Allows population of parameters in PME
  - Necessary for PME access to unit operation parameters

# Unit Operation Interface (CAPE-OPEN)

CO-100

Unit Specific Data and Public Variables

Name	Type	Mode	Lower bound	Upper bound	Value	Va
Input shell inside diameter, m	Real	IN	0	1E+35	1	
Input duty, J/s	Real	IN	0	1E+35	0	
Shell inside diameter, m	Real	OUT	0	1E+35	0.99999994136982	
Baffle spacing, m	Real	OUT	0	1E+35	1.399999991081953	
Tube passes	Real	OUT	0	1E+35	1	
Tube diameter, m	Real	OUT	0	1E+35	001014746726E-02	
Tube pitch ratio	Real	OUT	0	1E+35	1.24999889731631	
Tube length, m	Real	OUT	0	1E+35	6.09592616729736	
Tube wall thickness, m	Real	OUT	0	1E+35	999955956265E-04	
Shellside pressure drop, Pa	Real	OUT	0	1E+35	15843.1952070794	
Tubeside pressure drop, Pa	Real	OUT	0	1E+35	1693.93267464606	
Shellside coefficient, J/m2-K	Real	OUT	0	1E+35	611.393741699219	
Tubeside coefficient, J/m2-K	Real	OUT	0	1E+35	231.445079202271	
Area, m2	Real	OUT	0	1E+35	355.874785226074	
U, J/m2-K	Real	OUT	0	1E+35	158.763096513367	
EMTD, K	Real	OUT	0	1E+35	96.0103344901794	
Duty, J/s	Real	OUT	0	1E+35	0.000000000000000	

Reset Parameters

Material Connections    **Unit Variables**    General    Thermo

**Solved**    Show Unit GUI

# Unit Operation Interface (Native)

**L/R Exch**

**Rating**

**Sizing**

Parameters

Sizing Data

Overall  Shell  Tube  Accept any input data

Configuration

Number of Shell Passes	1
Number of Shells in Series	1
Number of Shells in Parallel	1
Tube Passes per Shell	1
Exchanger Orientation	Horizontal
First Tube Pass Flow Direction	Counter
Elevation (Base)	0.0000

TEMA Type

Calculated Information

Shell HT Coeff [kJ/h-m <sup>2</sup> -C]	<empty>
Tube HT Coeff [kJ/h-m <sup>2</sup> -C]	<empty>
Overall U [kJ/h-m <sup>2</sup> -C]	168.2
Overall UA [kJ/C-h]	845.7
Shell DP [kPa]	68.95
Tube DP [kPa]	0.6895
Heat Trans. Area per Shell [m <sup>2</sup> ]	5.027
Tube Volume per Shell [m <sup>3</sup> ]	1.608e-002
Shell Volume per Shell [m <sup>3</sup> ]	0.1955

Design **Rating** Worksheet Performance Dynamics HTFS - TASC

Delete    Ignored

# Unit Operation Interface (Extension)

The screenshot displays the 'L/R Exch' software window. On the left is a navigation pane with 'Design' selected. The main area shows a schematic of a heat exchanger with blue arrows indicating flow directions. A dropdown menu is open over the 'Heat Exchanger Model' section, listing options like 'Exchanger Design (End Point)', 'Exchanger Design (Weighted)', 'HTRI Xist Heat Exchanger', 'Steady State Rating', and 'Dynamic Rating'. The 'Shell Side' section shows 'Delta P' as 68.95 kPa and 'UA' as 845.7 kJ/C-h. The 'Heat Leak/Loss' section has 'None' selected. The 'Exchanger Geometry' section has 'Calculate Ft Factor' checked. A table at the bottom shows the following data:

Tube Passes per Shell	Shell Passes	Shells In Series	First Pass	Shell TEMA Type
1	1	1	Counter	E

At the bottom, there are tabs for 'Design', 'Rating', 'Worksheet', 'Performance', 'Dynamics', and 'HTFS - TASC'. Below the tabs are buttons for 'Delete', 'OK', 'Update', and 'Ignored'.

Can CAPE-OPEN allow access to native unit operation interface?



# Interface Experience

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- Unit Operation interface tested against HYSYS, ASPEN Plus, PRO/II, and UniSim Design
- Property package interface tested against ASPEN Plus, PPDS, Simulis, and UniSim Design





# Interface Experience

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- Successful interface with one software package does not guarantee it will work with other packages
- Interface required modification for each new package tested
- Requires software packages to be available for testing and interaction between companies

***Overall experience was  
successful in that common  
code used for all packages!***



# Interface Experience

- Most problems have been related to properties
- For example overall enthalpy:
  - Software A: Calculated automatically via CalcFlash
  - Software B: Must be specified in the CalcFlash property list
  - Software C: Due to a bug CalcFlash throws an exception when property list supplied
  - Software D: Not calculated by CalcFlash, must be determined from phase properties
- Makes code more complex than necessary



# Interface Experience

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- Examples of some other problems
  - Volume property calculated instead of Density. Modified HTRI software to detect this and use the available property.
  - IDispatch Invoke method not supported. Modified HTRI software to never use Invoke.
  - IPersistStorage interface not supported. Other vendors implemented IPersistStorage.



# Interface Experience

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- Improved documentation
  - Flexibility interferes with standardization. Allowing both Volume or Density makes things more difficult not less
  - More specific mechanisms (e.g., overall enthalpy)
  - Required/recommended properties
- Better testing software



# Testing Software

- Vendors could supply
  - Program specific testers
    - Allows testing of compatibility with particular software without requiring access to vendor software
    - Could be available to CAPE-OPEN members on website
  - Sample code
    - Provides additional examples beyond Mixer/Splitter block
    - Jump start for new members
- CAPE-OPEN could supply
  - Reference implementation
    - Would require multi-vendor support
    - Substantial amount of work



# Summary and Conclusions

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- Simply providing technically correct interfaces is not sufficient
- Vendors should optimize software for use in PME
- Additional work in PME could enhance adoption
- CAPE-OPEN could enhance documentation in some areas
  - Details of physical property handling
- Vendor specific testing tools/example code would be useful