

Industrial case study

Updating an existing interface to CAPE-OPEN standards

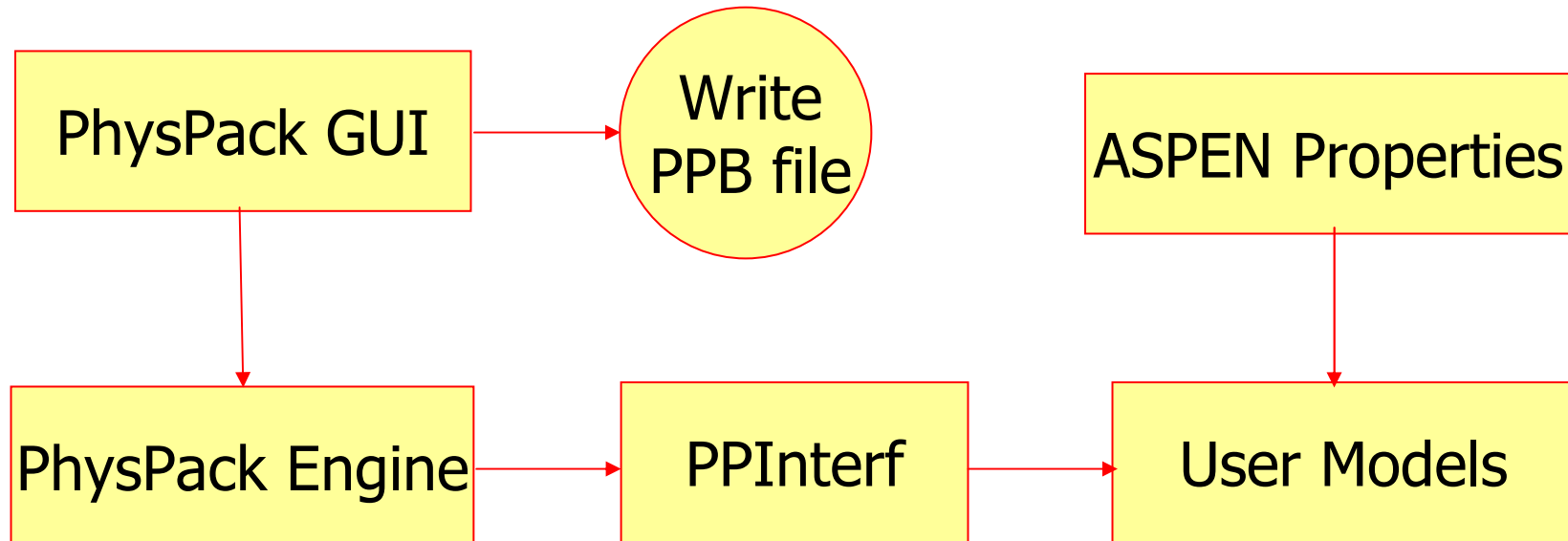
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- Review of PPDS CO status
- Description of case study
- Results of case study / demonstration

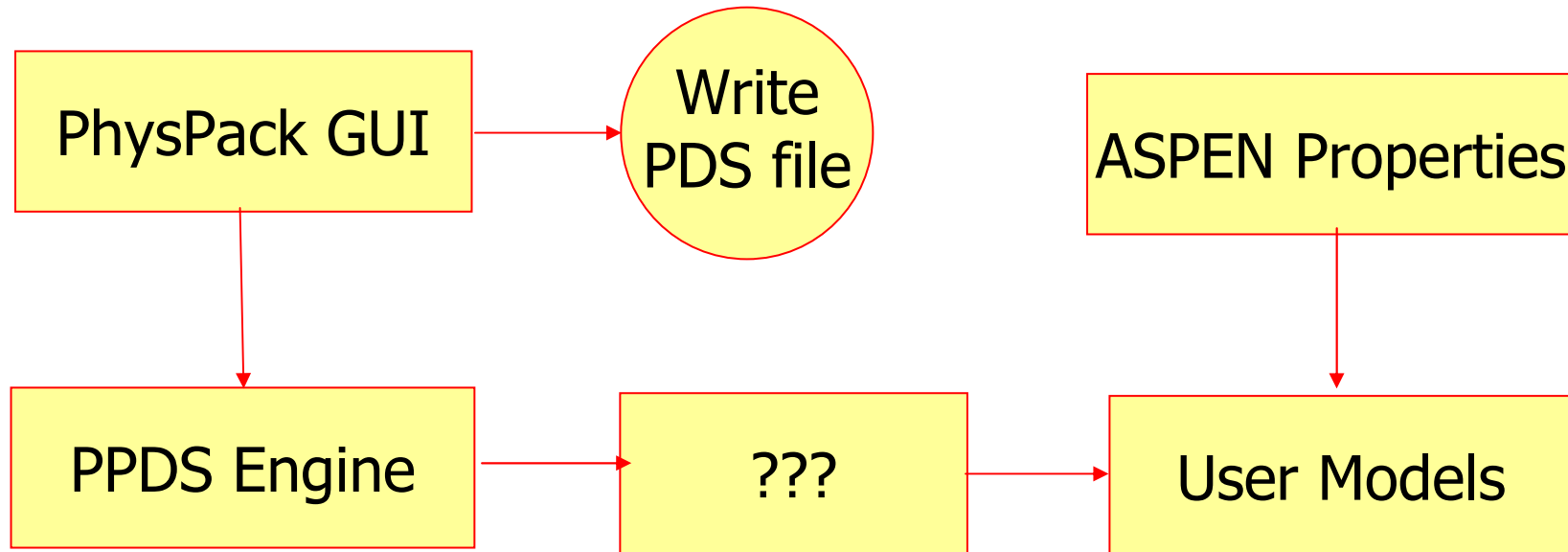
- PPDS v3.1.x has CO v1.0 Thermo plug available for testing
 - PPDS ThermoServer
 - PPDS Standalone Packages
- PPDS v4.0 for release 2006Q2 will contain property package manager
- Upgrade to Thermo v1.1 planned for late 2006

Case study modules

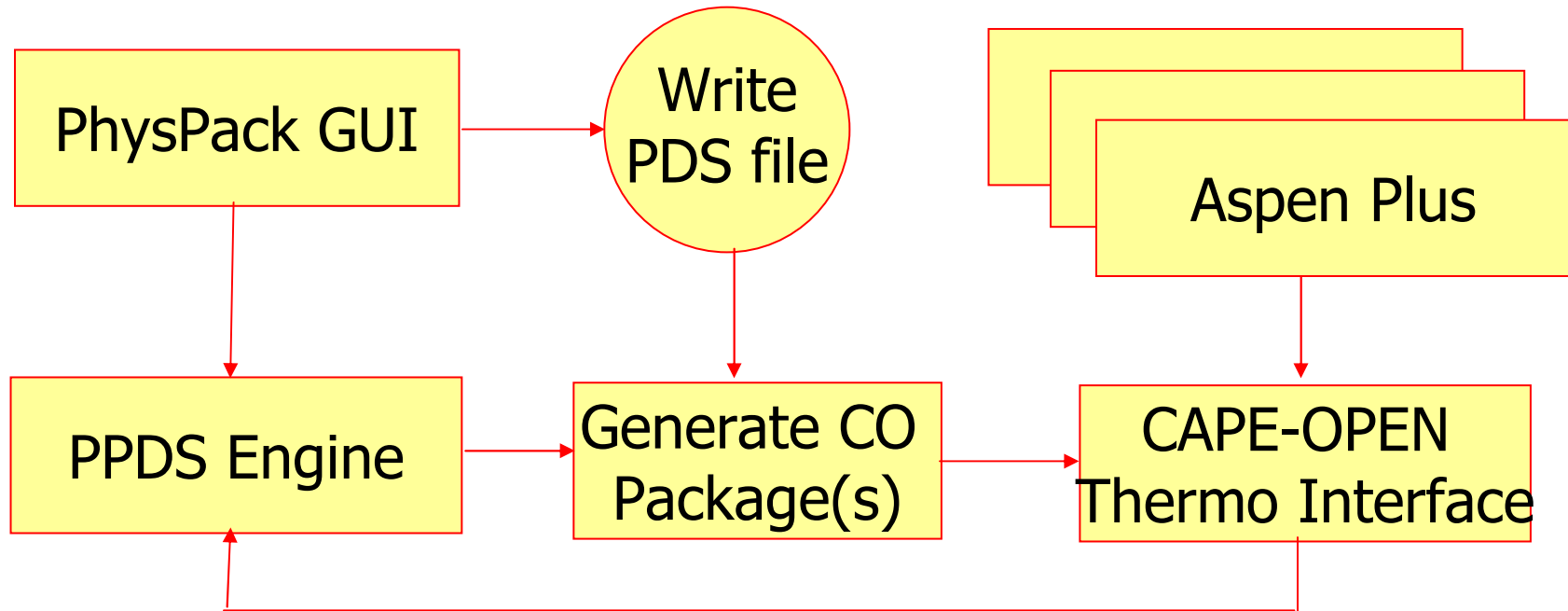
- PPDS flash/property calculator from TUV NEL
 - v3.1.4.2
- PhysPack flash/property calculator from ABB
 - v3.6.3
- Aspen Plus simulator from AspenTech
 - v2004.1
- PRO/II simulator from Invensys Process systems
 - v7.1.0



- Maintenance difficult
- Needs updating for each new release of Aspen Plus
- Currently used with ASpen Plus v10/11



- New interface required?
- Needs updating for each new release of Aspen Plus?

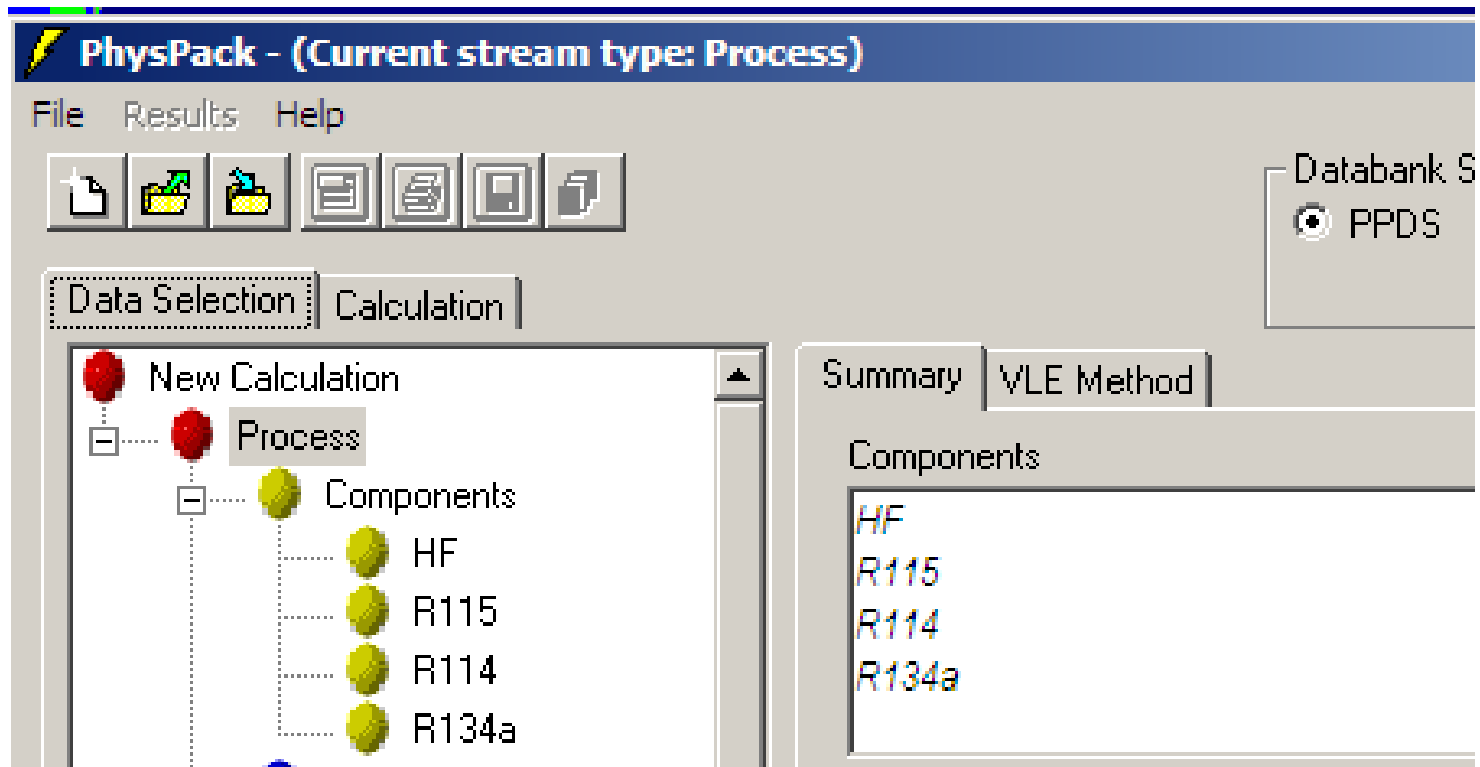


- Flexible system, easy to maintain
- Can be used with any CO simulator / package

Case study summary

- Run PhysPack standard calculation for given stream and model set
- Create new CO package from PPDS with chemical compounds and models
- Start Aspen Plus, use new CO package and run same calculation
- Start PRO/II, use new CO package and run same calculation
- Get same answer in each case!

Stream definition



- Refrigerant test problem with 4 components
- Model set is VPA (vapour) / Wilson-O (liquid)

Input compositions

PhysPack - (Current stream type: Process)

File Results Help

Databank System
 PPDS Aspen

Data Selection Calculation

- Conditions
- Feed
- Properties
- Advanced
- Units
- Calculate

	Mol Wt	Molar (kmol)	M Fra
1. HF	20.0080	10.0000	0.0
2. R115	154.4670	10.0000	0.0
3. R114	170.9210	10.0000	0.0
4. R134a	102.0320	10.0000	0.0
Avg Mol Wt/Totals	111.8565	40.0000	1.0

- Equimolar mixture

Problem conditions

The screenshot shows the PhysPack software interface. The title bar reads "PhysPack - (Current stream type: Process)". The menu bar includes "File", "Results", and "Help". Below the menu bar is a toolbar with icons for file operations. On the right, the "Databank System" is set to "PPDS". The "Data Selection" pane on the left has "Conditions" selected. The "Calculation" pane shows "Calculation Type" set to "Mixture (Equilibrium)". The "At:" dropdown is set to "Pressure" and the "And:" dropdown is set to "Molar Vapour Fraction". Below these, there are two input fields: the first is set to "10.000" with "Range" and "List" radio buttons, and the second is set to "0.9000" with "Range" and "List" radio buttons. "Get last calc values" buttons are present next to each input field.

- Input pressure 10 bar
- Constant vapour fraction = 0.9

Calculation results

PhysPack - (Current stream type: Process)

File Results Help

Databank Syst
 PPDS

Data Selection Calculation

Stream Pressure bar	Stream Molar VF	Stream Temperature C	Stream Mass Vap Fr	Vapour Enthalpy J/kmol
10	0.9	48.6645	0.878638	-139487

Conditions
 Feed
 Properties
 Advanced
 Units
 Calculate
 Messages

- Equilibrium temperature = 48.66 C

CO package setup

	A	B	
1	Name	VPA_test_package	
2	Description	Test PP for VPA model (Wilson-E)	
3	Model	VPA/Wilson-O	
4	NumSets		1
5	NumComps		4
6			
7	Comps		396 HF
8			436 R115
9			435 R114
10			885 R134A
11			
12			
13			
14			

Save CO Package

- New entry point in PPDS dual interface library

Available Property Packages

Property Packages	Name	PPDS.CapeThermoSystem.1
<ul style="list-style-type: none"> [-] PPDS.CapeThermoSystem.1 <ul style="list-style-type: none"> [...] Hydrocarbon_test_package [...] Chemical_test_package [...] INDISS_test_package <li style="background-color: #e0e0e0;">[...] VPA_test_package [+] Aspen Properties [+] Standalone Property Packages 	Description	
	About	

- New VPA_test_package in list

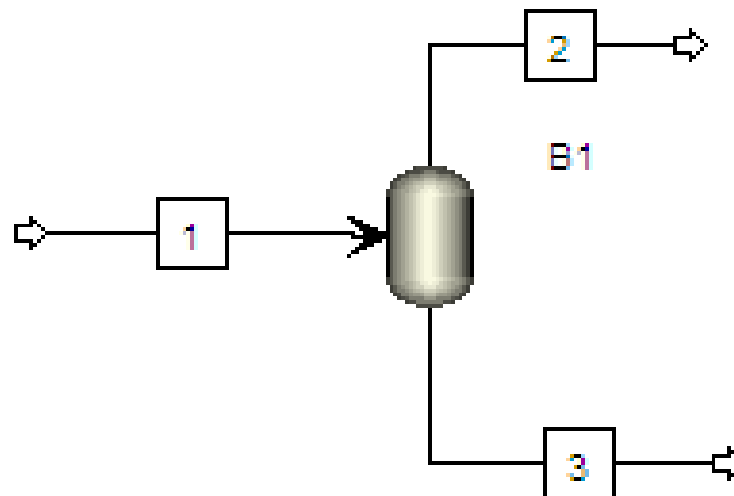
Component list

Package: VPA_test_package in PPDS.CapeThermoSystem.1

Components		Available Properties and Phases		
iupacName	Component	casRegistryNumber	chemicalFomula	nomalBoilingPoint
1,1,1,2-TETRAFL...	R134A	811-97-2	C2H2F4	247.000
1,2-DICHLORO-1,...	R114	76-14-2	C2Cl2F4	277.060
CHLOROPENTA...	R115	76-15-3	C2Cl1F5	234.010
HYDROGENFLU...	HF	7664-39-3	F1H1	292.690

- Set of four refrigerants

Simple flash simulation



- Conditions as per PhysPack example

Flash input conditions

Specifications Flash Options PSD Component Attr. EO Options

Substream name: MIXED Ref Temperature

State variables

Temperature: 100 C

Pressure: 10 bar

Total flow: 40 kmol/hr

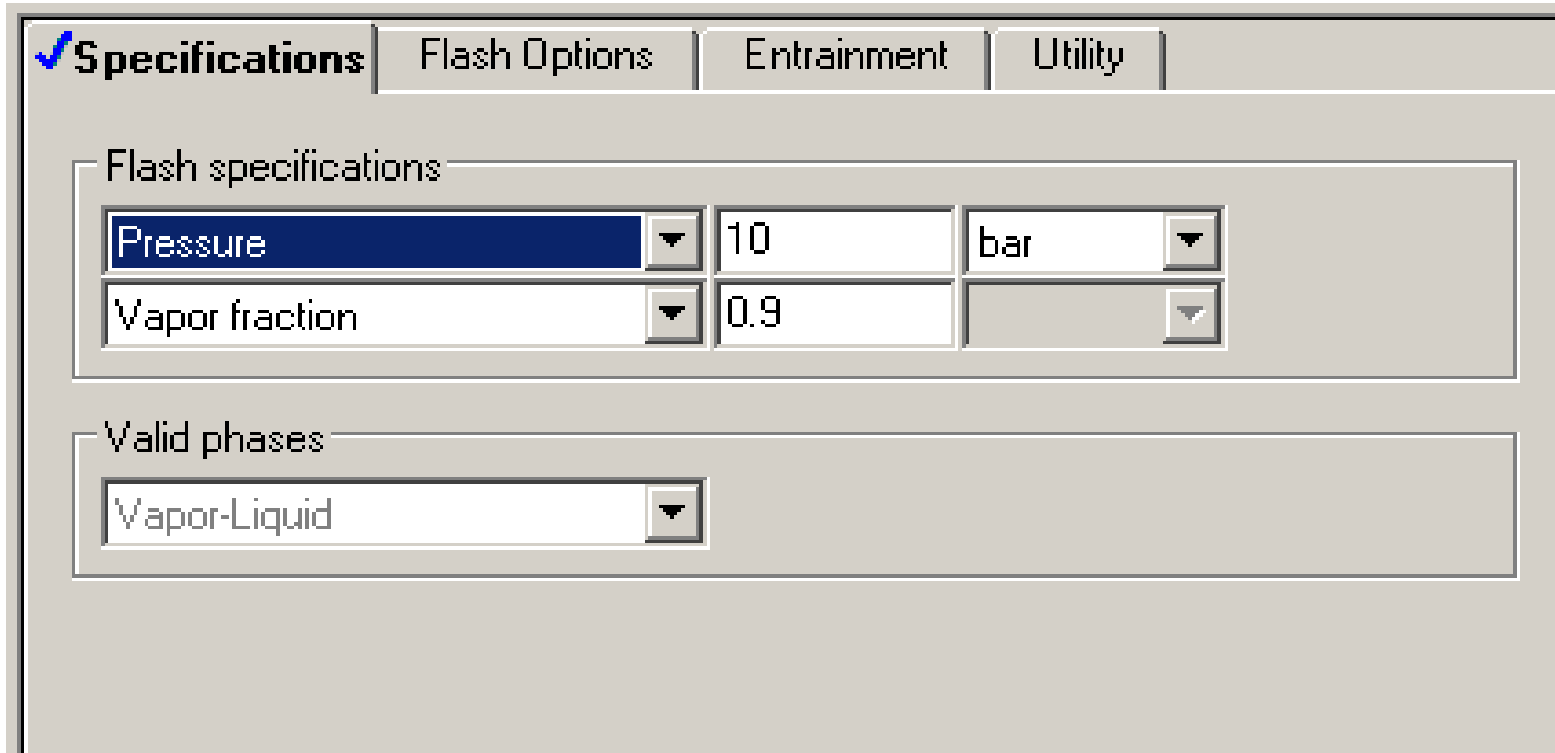
Solvent:

Composition

Mole-Flow: kmol/hr

Component	Value
HF	10
R114	10
R115	10
R134A	10

- Equimolar feed



Specifications | Flash Options | Entrainment | Utility

Flash specifications

Pressure	10	bar
Vapor fraction	0.9	

Valid phases

Vapor-Liquid

- As per PhysPack example

Material							
	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petro. Curves	Poly. Curves
Display:	All streams	Format:	GEN_M	Stream Table			
	1	2	3				
Temperature C	100.0	73.9	73.9				
Pressure bar	10.000	10.000	10.000				
Vapor Frac	1.000	1.000	0.000				
Mole Flow kmol/hr	40.000	36.000	4.000				
Mass Flow kg/hr	4474.255	4076.198	398.057				
Volume Flow cum/hr	124.100	103.883	0.312				
Enthalpy MMkcal/hr	-7.598	-6.976	-0.658				
Mole Flow kmol/hr							

- Using standard model gives $T = 73.9 \text{ C}$

Material | Heat | Load | Work | Vol.% Curves | Wt. % Curves | Petro. Curves | Poly. Curves

Display: All streams | Format: GEN_M | Stream Table

	1	2	3	
Temperature C	100.0	48.7	48.7	
Pressure bar	10.000	10.000	10.000	
Vapor Frac	1.000	1.000	0.000	
Mole Flow kmol/hr	40.000	36.000	4.000	
Mass Flow kg/hr	4474.255	3931.248	543.007	
Volume Flow cum/hr	110.839	70.515	0.432	
Enthalpy MMkcal/hr	0.055	-0.024	-0.016	
Mole Flow kmol/hr				

- Using CO model gives $T = 48.7$ C as before

PRO/II results

*** PROBLEM SOLUTION REACHED

STREAM 'S1'

	TOTAL	VAPOR	LIQUID
	-----	-----	-----
RATE, KG-MOL/HR	18.1437	16.3293	1.8144
TEMPERATURE, C	48.66	48.66	48.66
PRESSURE, BAR	10.00	10.00	10.00
MOLECULAR WEIGHT	111.8551	109.7132	131.1324
FRACTION		0.9000	0.1000
ENTHALPY, KJ/KG-MOL	-4199.1715	-2805.4227	-16742.9105
CP, KJ/KG-C	0.0000	0.0000	0.0000
MOLAR FLOWRATES, KG-MOL/HR			
1 - HF	4.5359	4.3491	0.1868
2 - R114	4.5359	4.1946	0.3414
3 - R115	4.5359	3.6852	0.8507
4 - R134A	4.5359	4.1004	0.4355

Acknowledgements

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