

Using two fluid packages in Aspen HYSYS 7.3 using OLI

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Overview

There are many times when a user wishes to use a traditional fluid package (such and Peng-Robinson) in one part of the HYSYS flowsheet and then to use the OLI fluid package in another part of the flowsheet. The user may not care to use the rigorous electrolytes (and the potentially large computational overhead) in all of the flowsheet but needs the rigor in only a portion. There are two major issues when attempting to do this in HYSYS.

The first issue is that HYSYS permits only one fluid package per flowsheet section. If you need to use a second fluid package, you must create a sub-flowsheet. The second issue is that the component names between fluid packages may not be the same.

In this example we are going to use the Peng-Robinson fluid package in the main flowsheet and the OLI Fluid package in a sub-flowsheet. The following table illustrates the component name differences between the Peng-Robinson (hereafter referred to as "PR") and the OLI fluid package that we are using in our example.

Component	Peng Robinson Name	OLI Name	
Hydrogen	Hydrogen	H2	
Nitrogen	Nitrogen	N2	
Carbon Monoxide	CO	СО	
Argon	Argon	Ar	
Oxygen	Oxygen	02	
Methane	Methane	CH4	
Carbon Dioxide	CO2	CO2	
Carbonyl Sulfide	COS	COS	
Ammonia	Ammonia	NH3	
Hydrogen Cyanide	HCN	HCN	
Water	H2O	H2O	

As you can see the naming system is not consistent between the two fluid packages. In fact, HYSYS considers the species to be completely different even if the names are the same (e.g., H2O).

Assumptions

We make the following assumptions:

- 1. The user knows how to start and operate HYSYS 2006 or later. This example was created in 7.3 but should be applicable to all versions since 2006.
- 2. The user has OLI properly installed
- 3. The user has a familiarity with aqueous chemistry

The Example

Simulation Basis Manager: Peng-Robinson Basis-1

Start Aspen HYSYS 7.3. This should display the Simulation Basis Manager

4 Simulation Basis Manag	er					
Component Lists Master Component List	View Add Delete Copy Import Export Refresh Re-import					
Components Fluid Pkgs	Hypotheticals	Oil Manager	Reactions	Component Maps	User Properties	
					Enter Simulation	n Environment

OLI finds it easier to start on the Fluid Pkgs tab. Click that tab

rrent Fluid Packages		Flowsheet - Fluid Pkg Ass	sociatio <u>n</u> s	
	View	Flowsheet	Fluid Pkg To Use	
		Case (Main)	<empty></empty>	
	Add	-		
	Delete			
	Сору			
		Default Fluid Pkg		~
	Import	Fluid Pkg for New Sub-Fl	owSheets	
	Export	⊙ Use Default Fluid Pl ◯ Use Parent's Fluid P		
Components Fluid Pkgs Hy	potheticals Oil Manager	Reactions Component M	laps User Propertie	

We need to add a fluid package. We will start with the PR fluid package. Click the Add... button.

Property Package Sele	ction		
Kabadi-Danner Lee-Kesler-Plocker MBWR NBS Steam Neotec Black Oil NRTL OLI_Electrolyte Peng-Robinson PR-Twu PRSV	 Property Package Filter All Types EOSs Activity Models Chao Seader Models Vapour Press Models Miscellaneous Types 	ß	
Component List Selecti Component List - 1	View		
Set Up Parameters	sBinary CoeffsStabTestPhase Or	der Rxns Tabular Notes	

Scroll down and highlight the *Peng-Robinson* fluid package.

By-default the name of the component list is *Component List* -1 we will use the default name. Click the *View* button next to *Component List* -1

Components Traditional Electrolyte Hypothetical Other Understein	Add Component	Selected Components		-Components Avai	lable in the Component Library	
Wethane C1 CH4 Wethane C2 C2H6 Propane C3 C3H8 Wathane iButane C4 C4H10 Wathane iButane iC4 C4H10 Wathane iButane iButane iButane Wathane iButane C3 C3H8 Wathane iButane C4 C4H10 Wathane iButane iButane C4 Wathane C5 C5H12 Wathane Wathane C6 C6H14 nHetwane Nonane C9 C9H20 nOctane Nonane C9 C9H20 nC1 C10H22 NC11 C11 C11H24 nC13 C13H28	Electrolyte				O Full Name / Synonym	
Remove→ iPentane iC5 C5H12 Remove→ 05 Pentane n-C5 C5H12 Sott List n-Heptane C6 C6H14 n-Heptane C7 C7H16 Nonane C8 C8H18 n-Decane C10 C10H22 n-C12 C11 C11H24 n-C13 C13 C13H28				Ethane Propane i-Butane	C2 C3 i-C4	C2H6 C3H8 C4H10
Sort List n-Nonane C9 C9H20 n-Decane C10 C10H22 Nc11 C11 C11H24 n-C12 C12H26 n-C13				hi-Pentane No-Pentane n-Hexane	i-C5 n-C5 C6	C5H12 C5H12 C6H14
n-C13 C13 C13H28				n-Nonane n-Decane n-C11	C9 C10 C11	C9H20 C10H22 C11H24
Show Synonyms Cluster		[View Component]		C13		
				Show Synony	ms Cluster	

There are several types of components. For the PR fluid package we will select the *Traditional* components. We have also selected the *Sim Name* radio button.

Add the components displayed in the list below.

Component List Vie	ew: Component List - 1				
Add Component	Selected Components	Components A	vailable in the Component Library		-1
Components Traditional Electrolyte	Hydrogen Nitrogen CO Argon	Match Sim Name	e O Full Name / Synonym	View Filters	
— Hypothetical — Other	Oxygen Methane CO2 COS Ammonia H2O	CAdd Pure Ethane Propane i-Butane i-Butane i-Pentane	C2 C3 i-C4 i-C4 i-C5	C2H6 C3H8 C4H10 C4H10 C5H12	
		Remove> n-Pentane n-Hexane n-Heptane n-Detane n-Nonane	n-C5 C6 C7 C8 C9	C5H12 C6H14 C7H16 C8H18 C9H20	
		Sort List n-Decane n-C11 n-C12 n-C13 n-C14	C10 C11 C12 C13 C14	C10H22 C11H24 C12H26 C13H28 C13H30	~
		Show Sync	onyms 🗌 Cluster		
Selected Compor	nent by Type				
Delete		Name Component List - 1			

Click on the "X" in the upper right-hand corner to close this dialog.

urrent Fluid Packages	the second se	Flowsheet - Fluid Pkg Ass	ociatio <u>n</u> s	
Basis-1 NC: 10 PP: Peng-Robins	on View	Flowsheet	Fluid Pkg To Use	
		Case (Main)	Basis-1	
	Add			
	Delete			
	Сору			
		Default Fluid Pkg	Basis-1	~
	Import	Fluid Pkg for New Sub-Flo	owSheets	
	Export	⊙ Use Default Fluid Pk ○ Use Parent's Fluid P		
Components Fluid Pkgs Hypot	heticals 0il Manager	Reactions Component M	aps User Propertie	25

We now have our first fluid package defined. By default this is named *Basis-1*.

Simulation Basis Manager: OLI Electrolytes Basis-2

We now need to add the OLI fluid package. Click the *Add...* button. Scroll down to find the *OLI_Electrolyte* package.

Lee-Kesler-Plocker Margules	~	Property Package Filt
		O EOSs
NBS Steam		O Activity Models
Neotec Black Oil NBTL		Chao Seader Mod
OLI_Electrolyte		Vapour Press Mod
Peng Robinson	1	Miscellaneous Typ
PR-Twu	-	O miscelidricous ryp
PBSV		C
Sour PR	~	Launch Property W

Immediately after selecting the fluid package, a warning about incompatible components will be displayed.

Incompatible Components			
Ammonia Argon		ts are not available for use age you have selected.	
CO CO2 COS	Desired Prop Pkg:	OLI_Electrolyte	1
H2O Hydrogen Methane Nitrogen Oxygen	Action If you continue, I w the listed compone		

This message seems strange. Essentially the PR fluid package does not understand about the OLI fluid package and thinks that all of the species listed above do not exist in the OLI fluid package. From a computational point of view this is correct although thermodynamically this is not correct. Since this is a computer program we need to resolve this limitation. We will accept the action *"If you continue, I will delete the listed components."* This sounds a bit dramatic and somewhat personal. It is ok to accept this action.

Click the OK button.

Property Package Selection	n	Initialize Electrolyte	s Environment
Glycol Package Grayson Streed Infochem Multiflash Kabadi-Danner Lee-Kesler-Plocker Margules MBWR NBS Steam	 All Types EOSs Activity Models Chao Seader Models Vapour Press Models Miscellaneous Types 	Phase Option Solid Vapour Vapour Exclu	d Option ude All Solids caling Tendency
Neotec Black Oil NRTL OLI Electrolyte	Launch Property Wizard	Redox Options	ubsystem Selection
Component List Selection		View Electrolyte Reacti	on in Trace Window
Component List - 2	View		
Set Up Parameters	Binary Coeffs StabTest Phase (rder Rxns Tabular Notes	

A new basis is created (*Basis-2*) and a new component list is created (*Component List – 2*). As before, click the *View...* button next to *Component List – 2*.

Add Component	Selected Components		Components Availa	able in the Component Library		
Components Traditional			Match	Add	itional Database	
Electrolyte			O Sim Name	💽 Full Name / Synonym	O Formula	
— Hypothetical 以 — Other		<add pure<br=""><-Substitute-> Remove></add>	CL2ET12 CL2FL2ETH CL2FL2ETHS CL2PNTAN15 CL2PROL1 CL2PRPEN23 CL2PRPN11 CL2TBUYN13	1,2-Dichloroethane 1,2-Dichloro-1,1-difluoroethane 1,2-Dichloro-1,2-difluoroethane 1,5-Dichloropentane 2-Chloro-1-propanol 2,3-Dichloropropane 1,1-Dichloropropane alpha-1,3-Dichloro-2-butene	C2H4Cl2 C2H2Cl2F2 C2H2Cl2F2 C5H10Cl2 C3H7Cl0 C3H4Cl2 C3H6Cl2 C4H6Cl2 C4H6Cl2	
		Sort List View Component	CL3ACETAC CL3ACETAL CL3ACETCL CL3BNZ135 CL3ET111 CL3ET112 CL3FL4ET	Trichloroethanoic Trichloroacetaldehyde Trichloroacetyl 1.3.5-Trichlorobenzene 1.1.1-Trichloroethane 1.2.2-Tichloroethane 1.2-Dichlorotetrafluoroethane	C2HCI3O2 C2HCI3O C2CI4O C6H3CI3 C2H3CI3 C2H3CI3 C2H3CI3 C2CI2F4	~
Selected Compor	ient by Type	Name Compor	ent List - 2			

The OLI property package requires the use of *Electrolyte* components and you can see it highlighted above.

By default the *Full Name / Synonym* radio button is selected. It is recommended that you leave this button on. Enter the components below as displayed.

Component List Vie	ew: Component List - 2	
Add Component Components Traditional Electrolyte Hypothetical Other	Selected Components H2 N2 C0 AR 02 CH4 C02 C0S NH3 H20	Components Available in the Component Library Match I Additional Database Sim Name Full Name / Synonym ABIETICAC Abietic C20H3002 ACENAPHTHN 1,8-Ethylenenaphthalene C12H10 ACENAPHTHN 1,8-Ethylenenaphthalene C12H10 ACENAPHTHN 1,8-Ethylenenaphthalene C12H10 ACENAPHTHN 1,8-Ethylenenaphthalene C12H10 ACETALDE Acetic C2H402 ACETALDEHD Acetic C2H402 ACETANIDE Ethanamide C2H5N0 ACETANILD ACETANILD Nethylenenaphthalene C8H1402 ACETANILD ACETANILD ACETANILD ACETANILD ACETANILD ACETANILD ACETBR Acetyl C2H38r0 ACETONE ACETONE ACETPHENDN ACETPHENDN ACETYLENE Acetyl C2H38r0 ACETYLENE ACETYLENE Acetylene C2H2
Selected Compor	nent by Type	Name Component List - 2

Click the "X" in the upper right-hand corner to close this dialog

Simulation Basis Manager					
Current Fluid Packages		Flowsheet - Fluid Pkg Ass	ociations		
Basis-1 NC: 10 PP: Peng-Robinson Basis-2 NC: 10 PP: OLI_Electrolyte	View Add	Flowsheet Case (Main)	Fluid Pkg To Use Basis-1		
	Delete				
	Import	Default Fluid Pkg	Basis-1	~	
	Export	Fluid Pkg for New Sub-Flo O Use Default Fluid Pk O Use Parent's Fluid P	(g		
Components Fluid Pkgs Hypothetical	s Oil Manager	Reactions Component M		es	

We now have two basis's entered. Notice that in the *Flowsheet – Fluid Pkg Associations* we only have on association. We will leave this alone for the moment.

Click the *Enter Simulation Environment...* button.

Main-flowsheet

Here we have simply added a stream using the palate. The stream conditions are at 25 C and 1 atmosphere pressure. We are using 100 kgmole/hr as the molar flow. Notice that the stream is set to **Basis-1**.

Click the *Composition* category.

Worksheet	Stream Name	
Conditions	Vapour / Phase Fraction	Kemp
 Properties Composition K Value User Variables Notes 	Temperature [C]	25.
	Pressure [atm]	1.0
	Molar Flow [kgmole/h]	100
	Mass Flow [kg/h]	Kempt
	Std Ideal Liq Vol Flow [m3/h]	Kempt
	Molar Enthalpy [kJ/kgmole]	Kempt
Cost Parameters	Molar Entropy [kJ/kgmole-C]	Kempty
	Heat Flow [kJ/h]	Kempty
	Lig Vol Flow @Std Cond [m3/h]	Kempty
	Fluid Package	Basis-1
<		
Worksheet Att	achments Dynamics	

Now we will enter the composition of the stream. We will enter 0.01 mole fraction for each component except water which will be 0.91 mole fraction.

*1		
Worksheet		Mole Fractions
0.12	Hydrogen	<empty></empty>
- Conditions	Nitrogen	<empty></empty>
- Properties	CO	<empty></empty>
- Composition	Argon	<empty></empty>
- K Value	Oxygen	<empty></empty>
12 19 20 20 20 20 20 20 20 20 20 20 20 20 20	Methane	<empty></empty>
- User Variables	C02	<empty></empty>
Notes	COS	<empty></empty>
Cost Parameters	Ammonia	<empty></empty>
	H20	<empty></empty>
		operties Basis m Functionality
< <u>></u>		R
Worksheet Att.	achments Dynamics	
	Unknown Compositio	ons
Delete	Define from Other Stre	:am 🕈 🕈

	MoleFraction	Composition Basis
Hydrogen	0.0100	Mole Fractions
Nitrogen	0.0100	O Mass Fractions
CO	0.0100	
Argon	0.0100	Liq Volume Fractions
Oxygen	0.0100	Mole Flows
Methane CO2	0.0100	
COS	0.0100	O Mass Flows
Ammonia	0.0100	Lig Volume Flows
H2O	0.9100	
		Composition Controls
		Erase
	_	Normalize
		Cancel
Equalize Composi	tion Total 1.0000	ОК

Click on **OK** to close this dialog

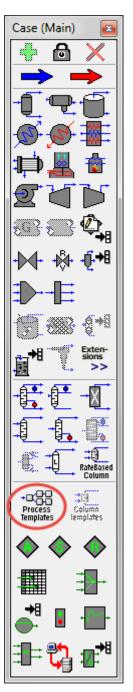
1		
Worksheet	CO CO	Mole Fractions
- Conditions	Argon	0.010000
Properties	Oxygen	0.010000
- Composition	Methane	0.010000
- K Value	C02	0.010000
Period and a state of the second	COS	0.010000
- User Variables	Ammonia	0.010000
- Notes	H20	0.910000
Cost Parameters		> >
	Total 1.	00000
	Edit Edit Prop	perties Basis
	Extend Stream	n Functionality
< <u>></u>		
Worksheet Att	achments Dynamics	
	OK.	
Delete	Define from Other Stream	m 🕈 🗭

The status bar has turned green indicating that the stream has converged.

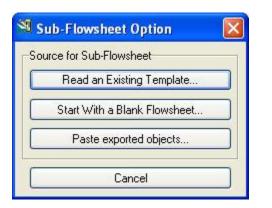
Click on the "X" in the upper right-hand corner to close the dialog.

Sub-flowsheet

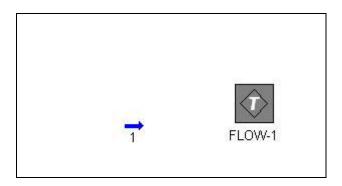
Next select the *Flowsheet* icon from the palate.



A Sub-flowsheet option dialog will appear.



For this example click the *Start With a Blank Flowsheet...* button



This will place the sub-flowsheet *FLOW-1* on the PFD.

Double-Click FLOW-1

This will display several options for the sub-flowsheet. The first option is to connect the streams going to and from the flowsheet (referred to as external streams) to the streams inside the flowsheet (referred to as internal streams).

Sub-Flowsheet Operation - FLOW	-1
Name FLOW-1	Tag TPL1
Injet Connections to Sub-Flowsheet	
Internal Stream	External Stream
** New **	<empty></empty>
Outlet Connections to Sub-Flowsheet	External Stream
** New **	<empty></empty>
Connections Parameters Transfer	Basis Transition Variables Notes pck

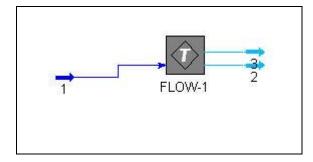
We will make life easy for ourselves and use the same numbers on the main-flowsheet as the subflowsheet. In small flowsheets this is ok but for large flowsheets you may get confused.

-1 Tag TPL1 ons to Sub-Flowsheet Internal Stream External Strea 1 J ** New **	am 1
Internal Stream External Strea 1	1
1 🛛	1
	1 <empty></empty>
** New **	<empty></empty>
ctions to Sub-Flowsheet	
Internal Stream External Strea	
2	2 3
3 ** New **	<empty></empty>
ns Parameters Transfer Basis Transition Varia	ibles Notes bok

Enter the *External Stream* 1. Notice that the internal stream is automatically created.

Repeat the process for the streams leaving the sub-flowsheet, Streams 2 and 3.

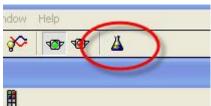
Click the "X" in the upper right-hand corner to close the dialog.



The main flowsheet now has the converged inlet stream "1" to the FLOW-1 sub-flowsheet and two unconverged outlet streams "2" and "3".

Changing the basis of the sub-flowsheet

By default the sub-flowsheet will have the same basis as the main-flowsheet. We need to change the basis of the sub-flowsheet.



Click the small flask in the button bar at the top of the PFD. It is usually located at the right-most position.

This will return you to the *Simulation Basis Manger*. Notice that under the *Flowsheet – Fluid Pkg Associations* that we have the name of the sub-flowsheet. Currently the fluid package assigned to the sub-flowsheet is *Basis-1*.

Simulation Basis Manager					
	View Add Delete Copy Import Export	Fluid Pkg ③ Use	t - Fluid Pkg Ass owsheet Cose (Main) IW-1 @Main ault Fluid Pkg for New Sub-Flo Default Fluid Pk Parent's Fluid Pk	Fluid Pkg To Use Bosis 1 Basis-1 Basis-1	
Components Fluid Pkgs Hypotheticals	Oil Manager	Reactions	Component M	aps User Properti	 onment

Hold your mouse over the box containing the word **Basis-1** and you will see that it becomes a drop-down arrow.

Fluid Pkg To Use
Basis-1
Basis-1 💌
h

Select *Basis-2* from the list. Remember that Basis-2 is the OLI Electrolyte fluid package.

Flowsheet	Fluid Pkg To Use
Case (Main)	Basis-1
Case (Main) FLOW-1 @Main	Basis-2
	N
	N

urrent Fluid Packages		Flowsheet - Fluid Pkg Ass	ociatio <u>n</u> s	
Basis-1 NC:10 PP:Peng-Robinson	View	Flowsheet	Fluid Pkg To Use	
Basis-2 NC: 16 PP: OLI_Electrolyte		Case (Main)	Basis-1	
	Add	FLOW-1 @Main	Basis-2	
	Delete			
	Сору			
		Default Fluid Pkg	Basis-1	×
	Import	Fluid Pkg for New Sub-Flo	owSheets	
	Export	 Use Default Fluid Pk Use Parent's Fluid P 		
Components Fluid Pkgs Hypotheti	cals 0il Manager	Reactions Component M	aps User Propertie	es l

We have now updated the fluid package for the sub-flowsheet. This may display a warning dialog.

LOW-1 @Main	Feed Stream	Basis	
	1	P-H Flash	
	** New **		
	Product Stream	Basis	
	2	P-H Flash	_
	3	P-H Flash	
	** New **		
Due to the differing enthalpy i the P-H Flash is not recomme You may change them here if	nded as a transfer basi		

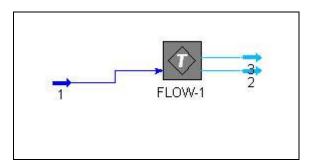
The major problem with using multiple fluid packages (OLI or some other package) is the reference point for enthalpy may be different. These differences in enthalpy can cause a temperature creep to occur between flowsheets. The default transfer basis is a P-H (pressure-enthalpy) calculation. In this we set the enthalpy to be constant and a new temperature is determined.

OLI recommends that the temperature be held constant (something that is easily measured) and so we select a T-P flash.

Position your mouse in each box and	d change the drop-down box to T-P flash.
-------------------------------------	--

1 T-F ** New **	Flash
Product Stream B	asis
	' Flash ' Flash
** New **	

When done, click the *Return to Simulation Environment*.



Mapping components from one basis to another

We can see that the diagram has not changed except for repositioning of the lines.

Double-click the *FLOW-1* sub-flowsheet.

Once again we are returned to the sub-flowsheet options. We now need a method of transferring the data for our components from the main flowsheet to the sub-flowsheet. For example, the species Argon in the main-flowsheet is AR in the sub-flowsheet. This is called a *Transition*.

lame FLOW-1	Tag TPL1
Tame reown	Tag TPL1
Injet Connections to Sub-Flowsheet	
Internal Stream	External Stream
1	1
** New **	<empty></empty>
Outlet Connections to Sub-Flowsheet Internal Stream 2	External Stream 2
	External Stream 2 3
Internal Stream 2	2
Internal Stream 2	2 3
Internal Stream 2	2 3 <empty></empty>

Click the Transition tab

Streams	Transition	
1	Fluid Pkg Transition	
		View Transitio
its		
Streams	Transition	
2	Fluid Pkg Transition	
3	Fluid Pkg Transition	
		View Transitio
1		
erall Imbalance Into Sub-Flo	wsheet Overall Imbal	ance Out of Sub-Flowsh

We now need to create the transition of components for the inlet to the sub-flowsheet and do the same for the outlet of the sub-flowsheet. We wills start with the inlet stream (from the main-flowsheet) "1".

Position your mouse on "1" and then click the *View Transition* in the upper box.

This dialog has a lot of options. We can see that the inlet stream "1" has Basis-1 as its fluid package. Stream "1" in the sub-flowsheet is represented as "1@TPL1" and has Basis-2. We need a mapping of components from Basis-1 to Basis-2.

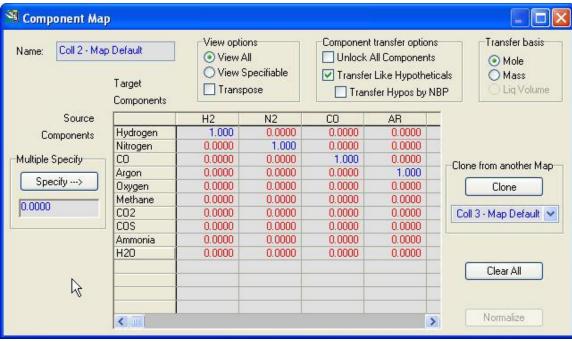
💐 Fluid Package T	ransition		
Inlet Stream Inlet Fluid Pkg	1 Basis-1	Outlet Stream Outlet Fluid Pkg	1 @TPL1 Basis-2
-Forward Component M	aps	Backward Component	Maps
Coll 2 - Map Default	View	Coll 3 - Map Default	View
	Add		Add
	Delete		Delete
Transfer Basis	2		
⊙ T-P Flash	◯ VF-T Flash	🚫 None Required	Active
O P-H Flash	○ VF-P Flash	O None Set	Imbalance
	No	t Solved	

Click the View... button in the Forward Component Maps box.

Name: Coll 2 · Map Default Target Components		View options View All View Specifiable Transpose		Component transfer options Unlock All Components Transfer Like Hypothetica Transfer Hypos by NB		s (O) Mole (O) Mass	
Source		H2	N2	CO	AR	-	
Components	Hydrogen	0.0000	0.0000	0.0000	0.0000		
	Nitrogen	0.0000	0.0000	0.0000	0.0000		
Multiple Specify	CO	0.0000	0.0000	0.0000	0.0000	Clone from another Ma	
	Argon	0.0000	0.0000	0.0000	0.0000		
Specify>	Oxygen	0.0000	0.0000	0.0000	0.0000	Clone	
0.0000	Methane	0.0000	0.0000	0.0000	0.0000		
0.0000	CO2	0.0000	0.0000	0.0000	0.0000	Coll 3 - Map Default	
	COS	0.0000	0.0000	0.0000	0.0000		
	Ammonia	0.0000	0.0000	0.0000	0.0000		
	H20	0.0000	0.0000	0.0000	0.0000		
						Clear All	

This displays a very busy box. The components listed going down the column are the Basis-1 (Peng-Robinson) components. The components listed across the columns are for Basis-2 (OLI). At the moment there are no mappings.

Find each cross-reference (e.g., Hydrogen – H2) and enter a 1.0. This maps every mole of the component Hydrogen in Basis-1 (Peng-Robinson) to a single mole of H2 in Basis-2 (OLI).



Here we cans see that we have a partially completed list. Scroll to the right to finish the list.

	COS	NH3	H20	H2C03	HN
Hydrogen	0.0000	0.0000	0.0000	0.0000	
Nitrogen	0.0000	0.0000	0.0000	0.0000	
CO	0.0000	0.0000	0.0000	0.0000	
Argon	0.0000	0.0000	0.0000	0.0000	
Oxygen	0.0000	0.0000	0.0000	0.0000	
Methane	0.0000	0.0000	0.0000	0.0000	
CO2	0.0000	0.0000	0.0000	0.0000	
COS	1.000	0.0000	0.0000	0.0000	
Ammonia	0.0000	1.000	0.0000	0.0000	
H20	0.0000	0.0000	1.000	0.0000	
<			1		>

Here the Peng-Robinson components (Basis-1) have been mapped to the corresponding OLI (Basis-2) components. Notice that there are no mapped components to a species such as H2CO3 (OLI, Basis-2). This component will be determined by the OLI solvers.

Click the "X" in the upper right-hand corner to close the dialog.

💐 Fluid Package T	ransition		
Inlet Stream Inlet Fluid Pkg	1 Basis-1	Outlet Stream Outlet Fluid Pkg	1 @TPL1 Basis-2
Forward Component M	laps	Backward Component M	Maps
Coll 2 - Map Default	View	Coll 3 - Map Default	View
	Add		Add
	Delete		Delete
Transfer Basis		-	
T-P Flash	◯ VF-T Flash	🚫 None Required	Active
O P-H Flash	OVF-P Flash	🚫 None Set	[Imbalance]
	(JK	

We can see that the status bar has turned green. This indicates that the transition was complete and the OLI solvers converged.

Click on the "X" in the upper right-hand corner to close the dialog.

Streams	Transition	
1	Fluid Pkg Transition	
		Non Transition
		View Transitio
s		
Streams	Transition	
	Fluid Pkg Transition	
2	Fluid Pkg Transition	
		View Transitio
		— N

We now have to map the OLI (Basis-2) components back to the PR (Basis-1) components).

Click on stream "2" and then click on *View Transition* in the lower box.

This dialog is similar to the inlet dialog. You can see that the internal stream "2" is actually referred to as 2@TPL1) and is set to Basis-2 (OLI). The outlet stream on the main-flowsheet is "2 and is set to Basis-1 (PR).

Inlet Stream	2 @TPL1	Outlet Stream	1000 - 100 - 100
Inlet Fluid Pkg	Basis-2	Outlet Fluid Pkg	Basis-1
Forward Component	Maps	Backward Component	Maps
Coll 3 - Map Defau	View	Coll 2 - Map Default	View
	Add		Add
	Delete		Delete
Transfer Basis			
T-P Flash	◯ VF-T Flash	🔘 None Required	Active
O P-H Flash	○ VF-P Flash	O Nue Set	Imbalance

Click the View... button in the Forward Component Maps box.

Name: Coll 3 - Maj	o Default Target Components	View opti View View Trans	All Specifiable	Unlock	transfer options All Components Like Hypothetica sfer Hypos by NBf	Sector Sector
Source		Hydrogen	Nitrogen	CO	Argon 🔨	
Components	H2	0.0000	0.0000	0.0000	0.0000	
Components	N2	0.0000	0.0000	0.0000	0.0000	
Multiple Specify	CO	30000	0.0000	0.0000	0.0000	CI
	AB	0.0000	0.0000	0.0000	0.0000	Clone from another Map
Specify>	02	0.0000	0.0000	0.0000	0.0000	Clone
0.0000	CH4	0.0000	0.0000	0.0000	0.0000	
0.0000	CO2	0.0000	0.0000	0.0000	0.0000	Coll 2 - Map Default 🗸
-	COS	0.0000	0.0000	0.0000	0.0000	L
	NH3	0.0000	0.0000	0.0000	0.0000	6
	H20	0.0000	0.0000	0.0000	0.0000	
	H2C03	0.0000	0.0000	0.0000	0.0000	Clear All
	HNH2CO2	0.0000	0.0000	0.0000	0.0000	
	NH42C03	0.0000	0.0000	0.0000	0.0000	
	NH44H2CO3	0.0000	0.0000	0.0000	0.0000 💌	Normalize

This brings up a similar dialog as before except this time OLI (Basis-2) is listed going down the column and PR (Basis-1) is listed across the top.

As before, enter a 1.0 to map the OLI component to the PR component. Do not map OLI species that do not appear as PR species.

Name: Coll 3 - Map	o Default Target Components	View opti View View View Trans	All Specifiable	Unlock .	transfer option All Components r Like Hypothet sfer Hypos by N	s 🧿 Mole icals 🔷 Mass
Source	1	Hydrogen	Nitrogen	CO	Argon 🗸	N
Components	H2	1.000	0.0000	0.0000	0.0000	
Componionio	N2	0.0000	1.000	0.0000	0.0000	
Multiple Specify	CO	0.0000	0.0000	1.000	0.0000	Class from smalles Man
	AR	0.0000	0.0000	0.0000	1.000	Clone from another Map
Specify>	02	0.0000	0.0000	0.0000	0.0000	Clone
0.0000	CH4	0.0000	0.0000	0.0000	0.0000	
0.0000	CO2	0.0000	0.0000	0.0000	0.0000	Coll 2 - Map Default 💌
	COS	0.0000	0.0000	0.0000	0.0000	
	NH3	0.0000	0.0000	0.0000	0.0000	10
	H20	0.0000	0.0000	0.0000	0.0000	
	H2C03	0.0000	0.0000	0.0000	0.0000	Clear All
	HNH2C02	0.0000	0.0000	0.0000	0.0000	
	NH42CO3	0.0000	0.0000	0.0000	0.0000	
	NH44H2C033	0.0000	0.0000	0.0000	0.0000	Normalize

Why not map OLI species such as "H2CO3" to PR species? You may be tempted to make the following conversion:

H2CO3 = CO2 + H2O

This means in the mapping columns under both CO2 and H2O there will be two entries with a 1.0, lined up with the component H2CO3.

When OLI and HYSYS were originally developed (back in version 3.2 of HYSYS) a convention was made that the OLI solvers will automatically map the moles of the electrolyte species (such as the ions) back to the same species originally entered (the Basis-2 components). If you do this same conversion here you will be double-accounting for the species and may introduce a mass imbalance. Let OLI manage the conversion and you should only map the components you actually entered in the *Simulation Basis Manager*.

Inlet Stream	2 @TPL1 Basis-2	Outlet Stream Outlet Fluid Pkg	Basis-1
Forward Component	Maps	Backward Component N	laps
Coll 3 - Map Defau	It View	Coll 2 - Map Default	View
	Add		Add
	Delete		Delete
Transfer Basis			
T-P Flash	🔘 VF-T Flash	🚫 None Required	Active
O P-H Flash	OVF-P Flash	O None Set	Imbalance

Click on the "X" to close the dialog.

You are returned to this dialog. Notice that the status bar is yellow (not solved). This is because we have not yet made a connection to the outlet streams inside the sub-flowsheet.

Click on the "X" to close the dialog.

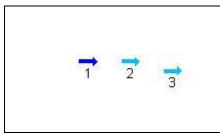
This returns you to the sub-flowsheet operation dialog.

Finishing the sub-flowsheet

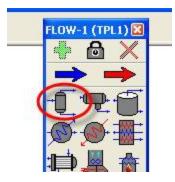
Streams	Transition	
1	Fluid Pkg Transition	
		View Transition
lets		
Streams 2	Transition	
Streams 2 3	Fluid Pkg Transition	_
2		View Transition
2	Fluid Pkg Transition	View Transition
2	Fluid Pkg Transition	
2	Fluid Pkg Transition	View Transition
2	Fluid Pkg Transition Fluid Pkg Transition	k
2	Fluid Pkg Transition Fluid Pkg Transition	

We are now ready to go.

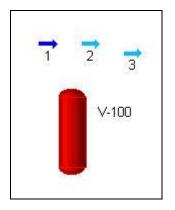
Click the *Sub-Flowsheet Environment*...Button.



You can see that the sub-flowsheet has disconnected streams. For this example we will introduce a 2-phase separator.



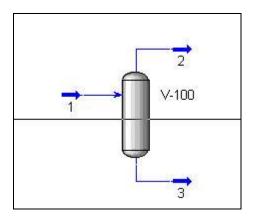
Select the 2-phase separator from the palate and place it on the sub-flowsheet PFD.



Double-click the V-100 unit operation to make the connections or use the connection tool.

€ V-100		
Design Connections Parameters User Variables Notes	Name V-100 Inlets Control of the second sec	Vapour Outlet 2
	Vessel Fluid Package Basis-2	Liquid Outlet
Design Read	tions <u>Rating</u> Worksheet Dynamics	Ignored

Once the connections are made the unit operation is converged. Click on the "X" to close the dialog.



We can see that the unit has converged. The vapor is leaving stream "2" and the aqueous liquid is leaving stream "3"

Click on Stream "3"

Worksheet	Stream Name	3
- Conditions	Vapour / Phase Fraction	0.0000
 Properties Composition K Value 	Temperature [C]	25.00
	Pressure [atm]	1.000
	Molar Flow [kgmole/h]	92.51
	Mass Flow [kg/h]	1685
- Electrolytes	Std Ideal Liq Vol Flow [m3/h]	<empty></empty>
User Variables	Molar Enthalpy [kJ/kgmole]	-2.850e+005
- Notes	Molar Entropy [kJ/kgmole-C]	71.65
 Cost Parameters 	Heat Flow [kJ/h]	-2.637e+007
	Liq Vol Flow @Std Cond [m3/h]	<empty></empty>
	Fluid Package	Basis-2
		1
<u> </u>		
Worksheet Att	achments Dynamics	
	Unknown Flow Rate	

You can see that there is molar flow of 92.51 kgmole/hr. The stream is "Yellow" because there is no "**Std Ideal Liq Vol Flow**" value. These values are not returned by the OLI solver and the error checking subroutines have identified a flash-failure. The stream is actually converged.

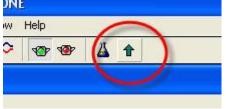
Click on the *Electrolytes* category.

Worksheet Conditions Properties Composition	True Species Info Properties Composition Phase O Aque O Solic		
	рН	8.6364	
K Value	Osmotic Pressure	20.662 atm	
Electrolytes	Ionic Strength	5.1741e-004 kgmol/kg	
User Variables	Heat Capacity	74.084 kJ/kgmole-C	
Notes	Viscosity	1.0211 cP	
Cost Parameters	Specific Electrical Conductivity	4.3854 S/m	
	Molar Electrical Conductivity	0.81069 S-m2/kgmole	
	R	5	
Worksheet Att.	achments Dynamics		
	Unknown Flow Rate		

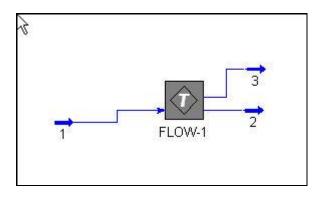
Here we can see that there is a pH of 8.6 which is a value returned by the OLI solvers.

Click on the "X" to close the dialog.

Once back on the sub-flowsheet we can return to the main flowsheet by locating the "UP Arrow". This is usually the right-most button on the button toolbar.



Click the UP Arrow



We are now returned to the main flowsheet. Notice that the streams "2" and "3" are reversed on the PFD. Please remember that one stream is a vapor and the other liquid as determined by the sub-flowsheet. Stream "3" was the liquid stream.

Click Stream "3".

Worksheet	Stream Name	3	
Conditions	Vapour / Phase Fraction	0.0080	
 Properties Composition K Value 	Temperature [C]	25.00	
	Pressure (atm)	1.000	
	Molar Flow [kgmole/h]	92.51	
	Mass Flow [kg/h]	1685	
- User Variables	Std Ideal Liq Vol Flow [m3/h]	1.706	
- Notes	Molar Enthalpy [kJ/kgmole]	-2.849e+005	
- Cost Parameters	Molar Entropy [kJ/kgmole-C]	55.25	
	Heat Flow [kJ/h]	-2.635e+007	
	Liq Vol Flow @Std Cond [m3/h]	1.664	
	Fluid Package	Basis-1	
	<	1	>
() >			
Worksheet Att	achments Dynamics		-
	ÖK		

Notice that the basis is now Basis-1 (PR). The molar flow is the same but the other flow rates have been calculated. Also notice that the category *Electrolytes* is not present. This is because the PR fluid package does not support electrolyte components. The aqueous electrolyte information is only contained in the sub-flowsheet.