

OLI Tips 72

Changing the Weighting factor in ESP

Introduction

The OLI ESP program works on a true-species basis rather than on an apparent-species basis. That means we consider the sodium ion (Na^+) and the chloride ion (Cl^-) in the solution rather than the apparent species NaCl. In ESP it is often desirable to display the species in apparent form rather than true form. The methodology to convert true-species into apparent-species is straightforward but may lead to undesirable apparent species being displayed. We have introduced a method of weighting the apparent species so you can better represent the solution.

Additional Links:

The difference between Apparent and True species.

<http://support.olisystems.com/TIPS/OLI-Tips19-Explaining-True-Apparent-Species.pdf>

Assumptions:

1. It is assumed that you have OLI ESP version 7.0 or later installed
2. This tip assumes you are already familiar with creating chemistry models and process files in OLI ESP.

Creating the Example Case

In this example we will create a chemistry model that contains the components H₂O, HCL, NAOH and NACL. We will then create a small process consisting of a single MIX block with the following inflow streams and outflow streams.

Inflow Stream: Acid

Temperature	25	C
Pressure	1	Atm
H ₂ O	55.508	Mol/hr
HCL	1.0	Mol/hr

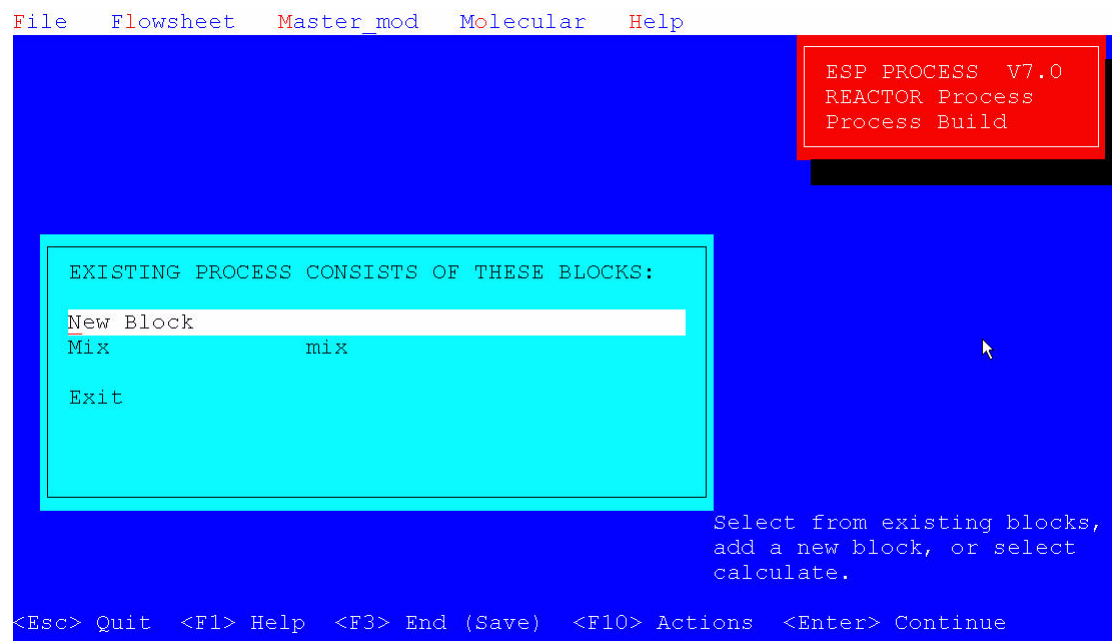
Inflow Stream: Base

Temperature	25	C
Pressure	1	Atm
H ₂ O	55.508	Mol/hr
NAOH	1.0	Mol/hr

Outflow Stream: Reacted

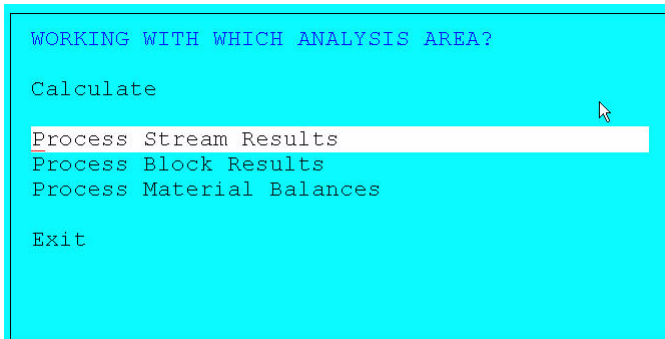
The MIX unit operation should be set to ISOTHERMAL at 25 C and 1 Atmosphere.

When done the Process Build Screen should look like this:

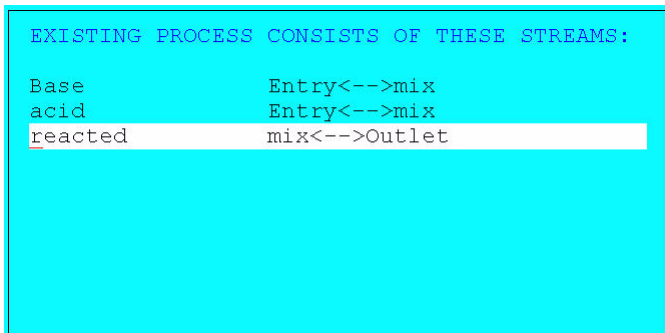


Exit this screen and then Select Process Analysis and calculate the case as normally done.

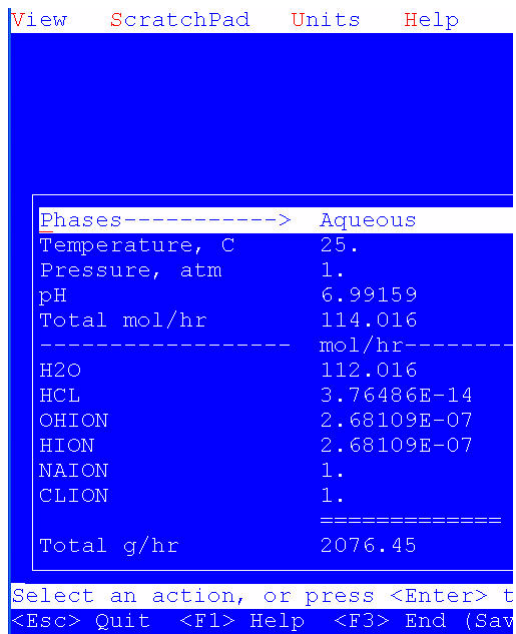
After the calculation has completed you should be returned to this screen.



Select Process Stream Results



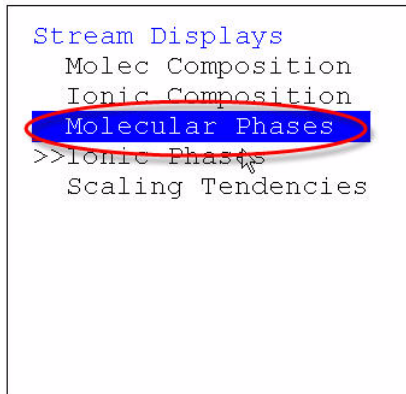
Now select the “reacted” stream.



This is a partial display of the stream "Reacted". As you can see it is in true-species format.



Select view from the menu line

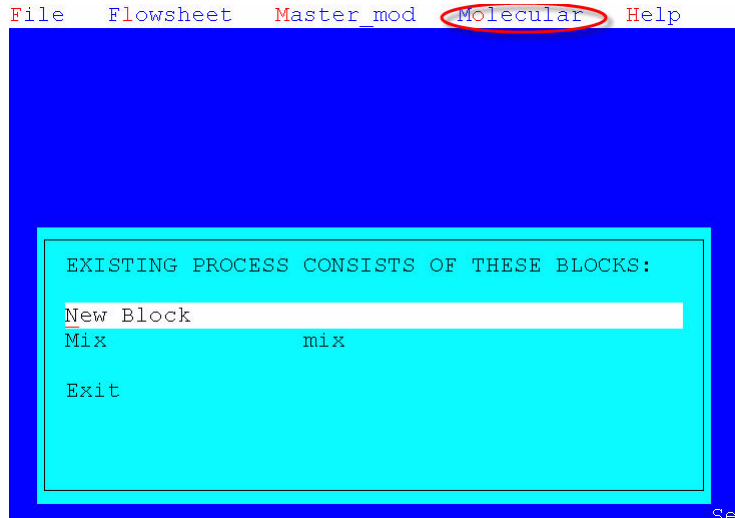


Select **Molecular Phases** from the **Stream Displays** menu.

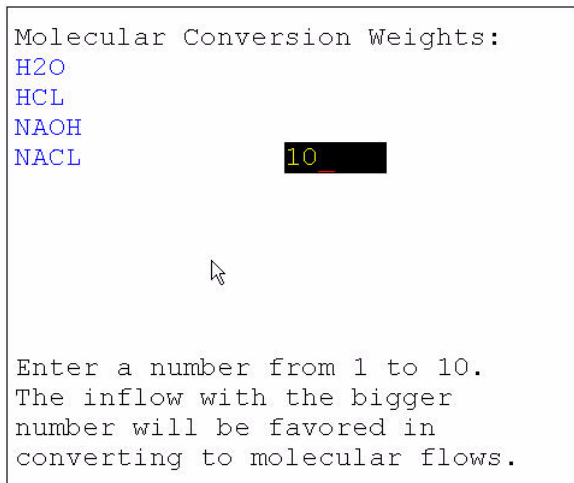
Phases-----> Aqueous	
Temperature, C	25.
Pressure, atm	1.
pH	6.99159
Total mol/hr	113.016
-----	mol/hr-----
H2O	111.016
HCL	1.
NAOH	1.
=====	
Total g/hr	2076.45
Volume, m3/hr	0.00204229
Enthalpy, cal/hr	-7.74938E+06
Density, g/m3	1.01672E+06

As you can see, the apparent species are H2O, HCL and NAOH. These are the same species we entered originally. There appears to be no reaction. Yet if you look at the pH it is nearly 7.0 indicating that the acid and base streams have fully reacted.

To change how this display shall look, we need to return to PROCESS BUILD.



Select the **Molecular** menu item.



Here we have set the weighting factor to 10 for the apparent inflow species NACL. This means that the program will attempt to place all the sodium ions and chloride ions into the apparent species NACL before sending any remaining species to the others.

This weighting factor is located in the BIN file. The process file must be recalculated to update the weighting.

Return to PROCESS ANALYSIS and then CALCULATE the process once more.

Select Process Stream Results and reselect the Reacted Stream.

View ScratchPad Units Help

Phases-----> Aqueous	
Temperature, C	25.
Pressure, atm	1.
pH	6.99159
Total mol/hr	114.016
----- mol/hr-----	
H2O	112.016
HCL	3.76486E-14
OHION	2.68109E-07
HION	2.68109E-07
NAION	1.
CLION	1.
=====	
Total g/hr	2076.45

You can see that the default true-species representation is exactly the same as before. Select View from the menu.

Then select Molecular Phases from the drop-down list.

Phases-----> Aqueous	
Temperature, C	25.
Pressure, atm	1.
pH	6.99159
Total mol/hr	113.016
----- mol/hr-----	
H2O	112.016
NACL	1.
=====	
Total g/hr	2076.45
Volume, m3/hr	0.00204229
Enthalpy, cal/hr	-7.74938E+06
Density, g/m3	1.01672E+06
Vapor fraction	0.0

You can see that we have weighted the apparent species towards NACL. This weighting factor also applies to the molecular output in Process Summary.