OLI Tips #54

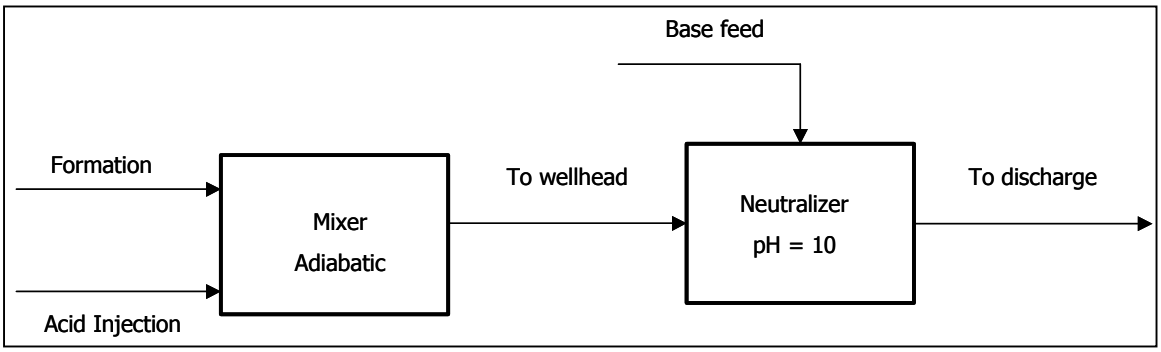
Using Multiple models in ESP.

Using Multiple Models in ESP version 7.0 and later.

Case 1: New Screens for Model Generation

The ability to use multiple chemistry models in ESP required some changes to the chemistry model generation screens. In this section, we will build a traditional aqueous model as follows;

An dolomite formation is treated with acid injection. This lowers the pH and reacts the dolomite solids. The pH is then increased using sodium hydroxide and new solids appear. One solid that appears is ordered dolomite which does not occur under most circumstances.



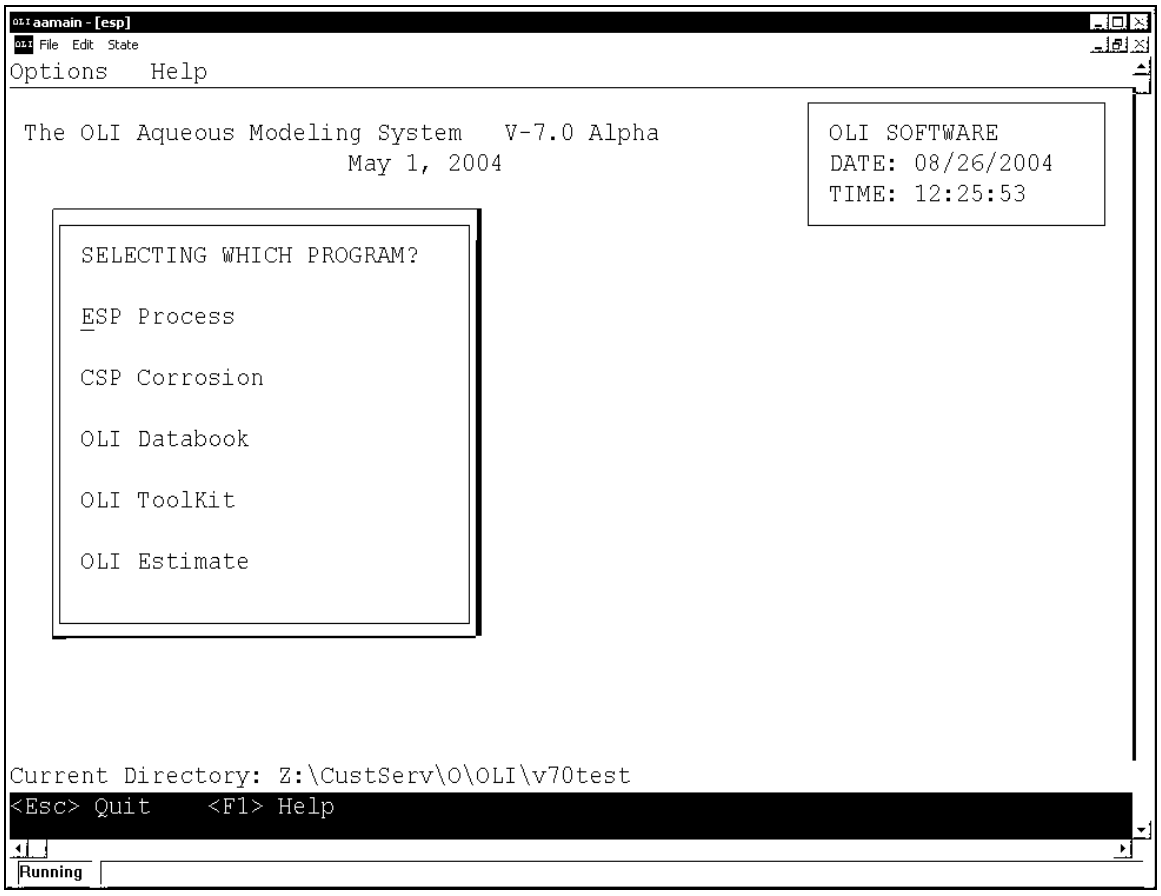
Compositions

	Formation	Acid Injection	Base Feed
Temperature ^{o}C	40	25	25
Pressure Atm	1.5	1.0	1.0
Total Flow mole	100	100	100
H2O mole	55.508	55.508	55.508
Dolomite mole	1	0	0
HCl	0	6	0
NaOH	0	0	10

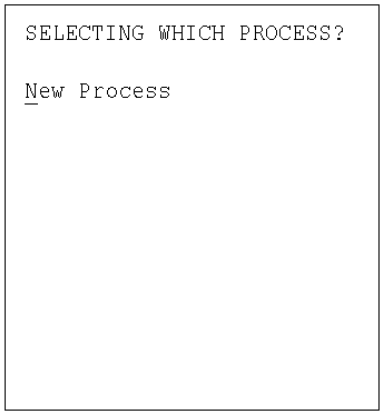
Step 1: Create a standard ESP chemistry model with the following inflow:
H2O
DOLOMITE
HCL
NAOH

The GeoChem database will have to be used.

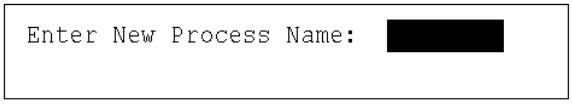
Start the ESP version 7.0 or later Software



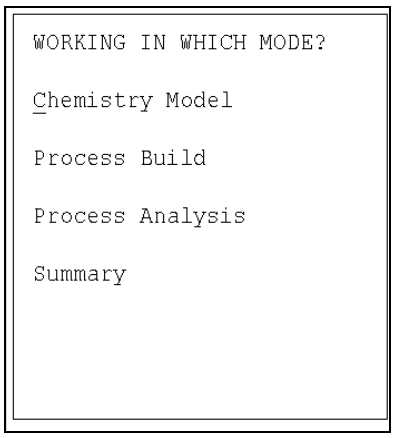
Select ESP Process



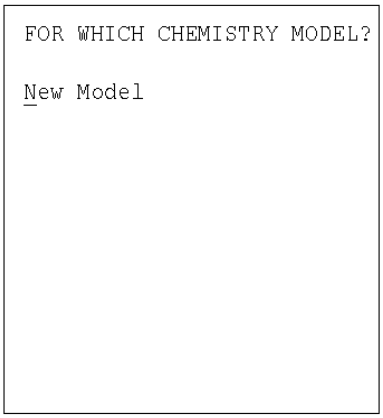
You may have more than one process in this folder. Select a new process



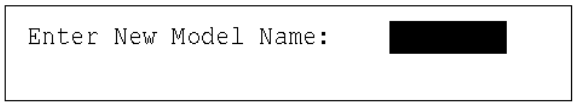
Enter the name of the new process ***ACIDINJ***



Select Chemistry Model

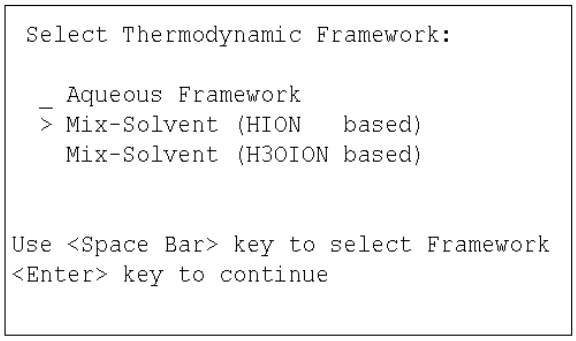


You may have more than one model in this folder. Please select New Model



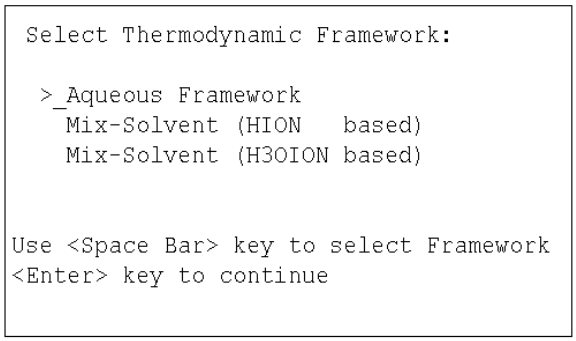
Please enter the name of the new model ***ACIDTEST***

Note this name is different than the process name.



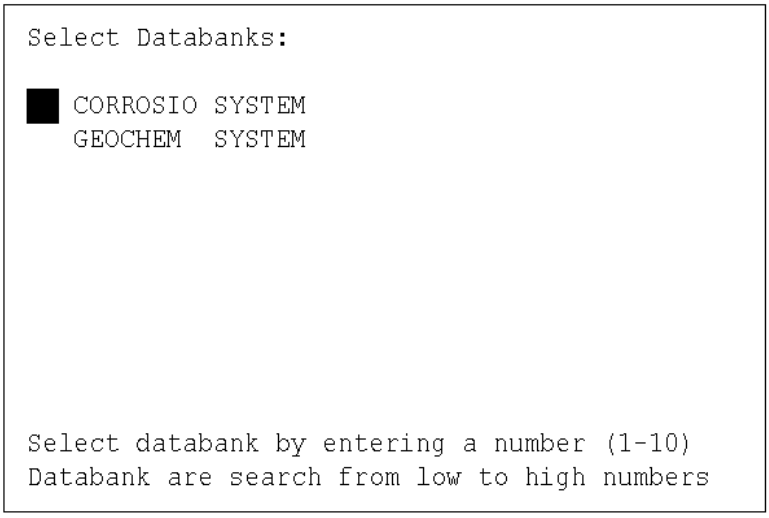
This is a new screen for model generation in version 7.0. With this release, OLI now has the ability to use two new thermodynamic frameworks other than the traditional aqueous framework. It is beyond the scope of this tip/tutorial to explain the differences in the thermodynamic models.

Please position the cursor bar on ***Aqueous Framework*** and press the ***Spacebar***.



This has moved the framework select arrow up to ***Aqueous Framework*****.**

Press the ENTER key to continue.

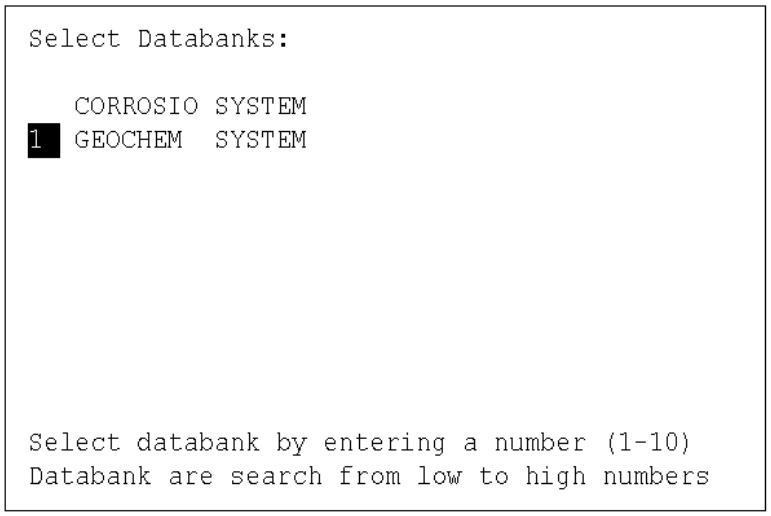


The specification of the databanks and their search order must be defined prior to entering any species. As you can see from the figure, the **CORROSIO** and **GEOCHEM** databases are available. These are system databases and are located in the following folder on your computer:

C:\Program Files\OLI Systems\ESP 7.0\Databanks

Any database you place in this folder will be available to all folders on your computer. Databases stored locally will be displayed with a different tag.

Please place a number “1” next to GEOCHEM.



Press ENTER to continue

This will display the standard ESP Chemistry Model generation dialogs. It is assumed that the user already knows how to create a model.

Add the species listed in Step 1 and finish the chemistry model.

Step 2: Build the Process

Build the ESP process as shown in the preceding diagram. Run the process after building it.

A summary of results are shown below:

Stream	Formation	Acid Injection	To Wellhead	Base Feed	To Discharge
Phase	Mixed	Aqueous	Mixed	Aqueous	Mixed
Temperature, C	40	25	39.1787	25	70.2276
Pressure, atm	1.5	1	1	1	1
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	98.23009	90.24517	188.4756	59.12905	247.6006
CO2	1.64E-04		3.539312		0.004703782
CAO	8.22E-05		1.769656		6.14E-04
MGO	8.22E-05		1.769656		1.78E-05
ORDDOL	1.769576				1.765574
HCL		9.754827	9.754808		9.754855
NA2O				4.886054	4.886062
CACO3					0.003476069
MGOH2					0.0040721
Total mol/hr	100	100	205.309	64.0151	264.02
Total g/hr	2095.98	1981.47	4077.45	1368.06	5445.51
Volume, m3/hr	0.0018977	0.00182583	0.0987188	0.00105678	0.00498489
Enthalpy, cal/hr	-7.67E+06	-6.54E+06	-1.42E+07	-4.77E+06	-1.90E+07
Vapor fraction			0.01815921		
Solid fraction	0.0176958				0.006715855
Organic fraction					

There are some issues with this output

1. We entered Dolomite (the naturally occurring species) in our **FORMATION** feed yet the program reports the species **ORDDOL** (ordered dolomite, a synthetic variety).
2. ORDDOL appears in the effluent. Dolomite is very slow to form. Under these acid stimulation conditions, we would expect to see calcium carbonate (calcite) and $Mg(OH)_2$ (brucite) to form.

Case 2: Removing dolomite solids from the neutralizer

Clearly we need to modify the process. Prior to version 7.0 of ESP, it was not possible to change models in different unit operations. Now we can.

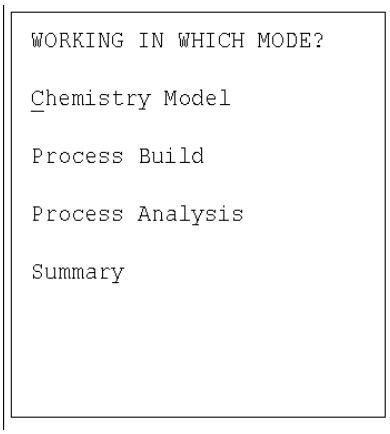
Step 1: Create a sub-model

We will now create a model that does not have dolomite solids present yet has the same inflow list. This brings up the concept of master and subordinate models.

Master Models

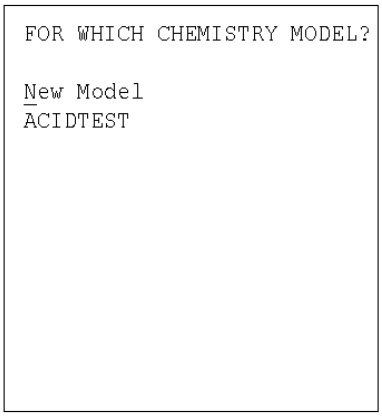
A master model contains all the species that you may find anywhere in the process. It does not have to contain all the phenomena such as reaction kinetics. Each subordinate model must contain a subset of the species in the master model

To create the sub-model, press the ESC key to return to this figure:



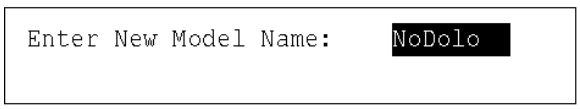
Select Chemistry Model.

By default, the cursor will be on the currently selected model. Press the Up Arrow key.

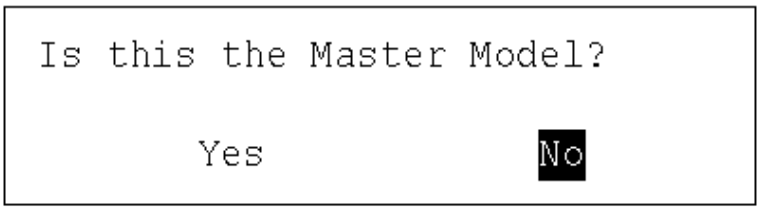


Select New Model

Enter the name of the new model **NODOLO**



Press the Enter key to continue

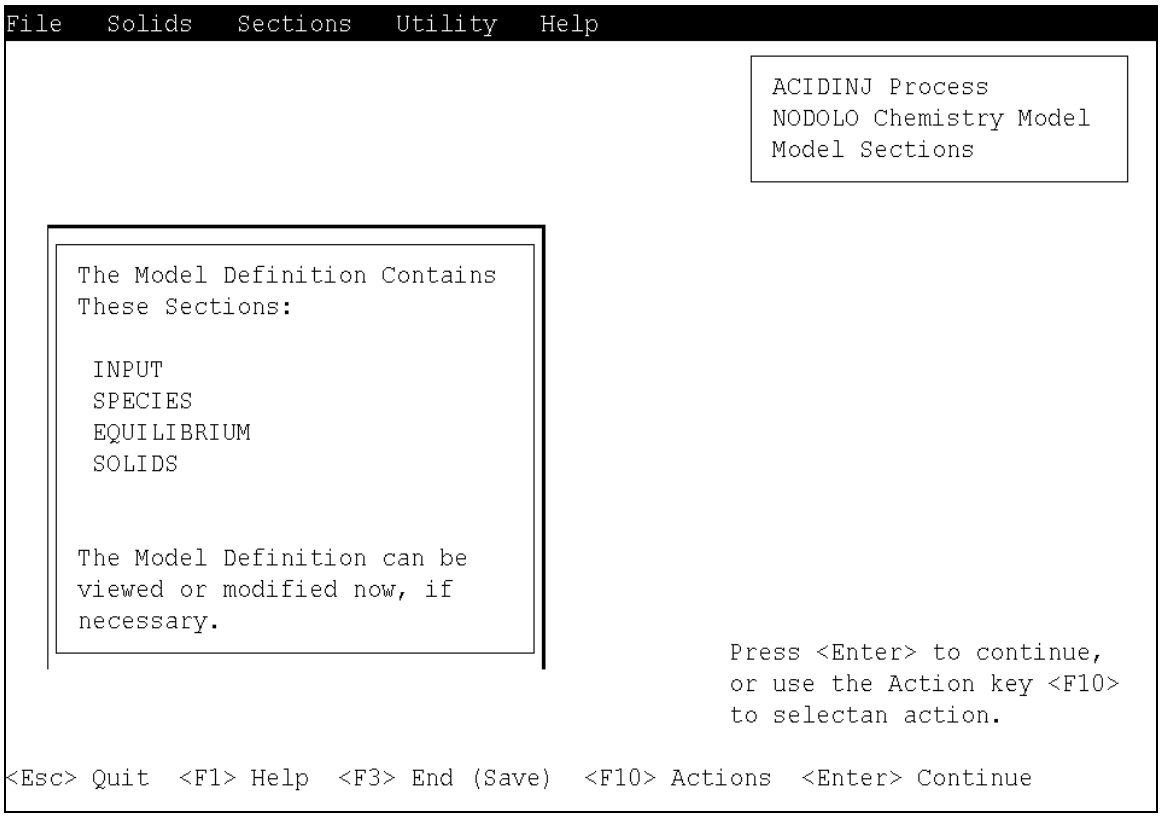


By default, any initial model for a process is designated a MASTER model. When a new model is added to a process, you have the choice to designate the model as a replacement MASTER model.

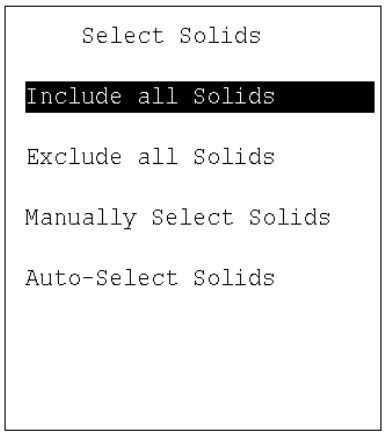
In this case, the new model is a subset so we will select NO.

As with the previous model, select the Aqueous Framework, the GeoChem database and the previously mentioned inflow list.

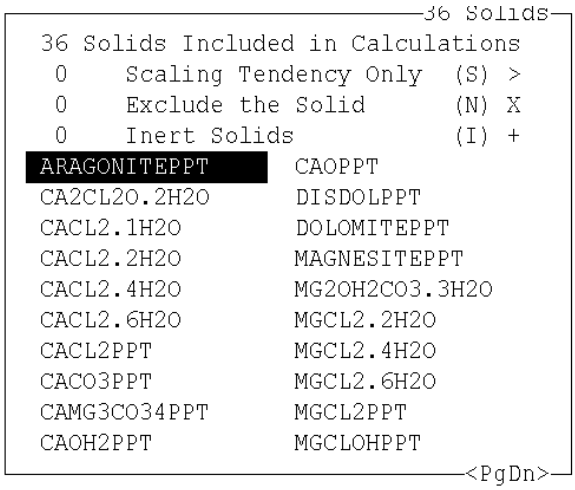
Generate the chemistry as normally done but stop on the following screen.



Use the action key and select **Solids** from the action line.



Select **Manually Select Solids**



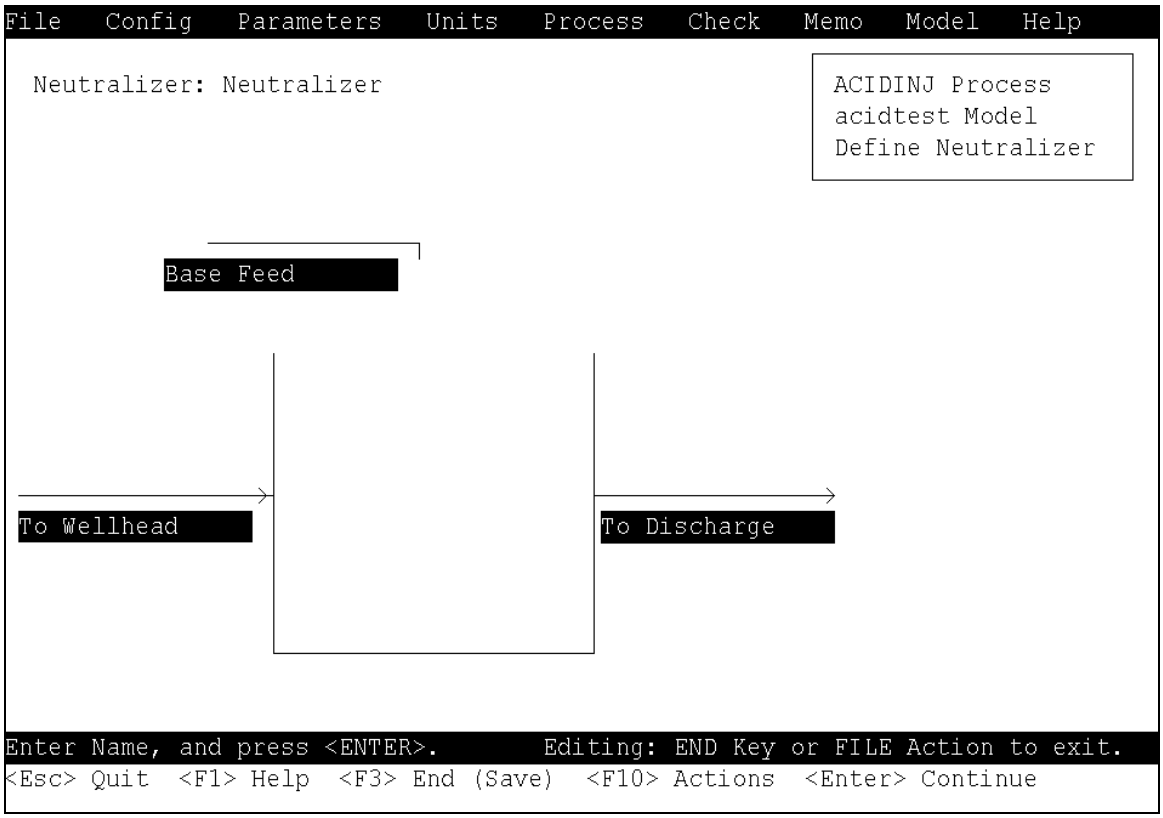
Position the cursor on the following solids and press the "S" key to allow the species to be effectively removed from the model. It's scaling tendency will be calculated. The selection is noted with the ">" symbol.

Remove the species **DISDOLPPT, DOLOMITEPPT,** and **ORDDOLPPT**

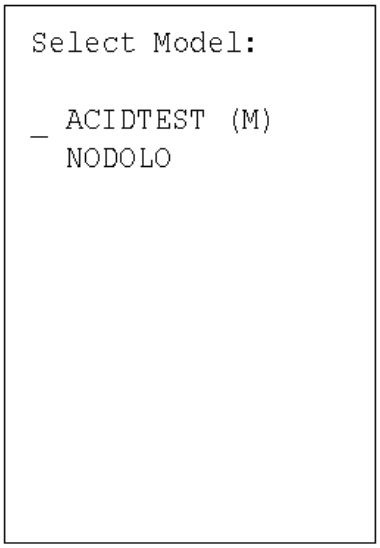
Press the ENTER key to continue. Continue the model generation as you have before.

Step 2: Add a sub-model to a process block

Return to Process Build and select the "Neutralizer" block.

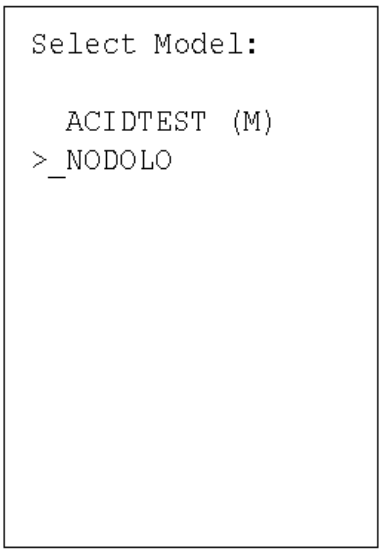


Select **Model** in the action line.



The current model for this process block is highlighted. The designation "M" indicates that the model ACIDTEST is the master model. Only those sub-models that are valid are displayed (that is they contain a subset of species in the master model).

Position the cursor on the model NODOLO and press the SPACEBAR.



Save the block and re-run the process.

The new results are presented below:

Stream	Formation	Acid Injection	To Wellhead	Base Feed	To Discharge
Phase	Mixed	Aqueous	Mixed	Aqueous	Mixed
Temperature, C	40	25	39.1787	25	69.1035
Pressure, atm	1.5	1	1	1	1
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	98.23009	90.24517	188.4756	63.26812	251.378
CO2	1.64E-04		3.539312		0.365239
CAO	8.22E-05		1.769656		2.65E-05
MGO	8.22E-05		1.769656		4.78E-05
ORDDOL	1.769576				
HCL		9.754827	9.754808		9.754829
NA2O				5.228082	5.228079
CACO3					1.30149
CAMG3CO34					0.468149
MGOH2					0.365165
Total mol/hr	100	100	205.309	68.4962	268.861
Total g/hr	2095.98	1981.47	4077.45	1463.83	5541.28
Volume, m3/hr	0.0018977	0.00182583	0.0987188	0.00113076	0.00505866
Enthalpy, cal/hr	-7.67E+06	-6.54E+06	-1.42E+07	-5.10E+06	-1.93E+07
Vapor fraction			0.01815921		
Solid fraction	0.0176958				0.007940162
Organic fraction					

The results are considerably different. The streams “Formation”, “Acid Injection”, “To Wellhead”, and “Base Feed” all use the master model while the stream “To Discharge” (which is calculated by the neutralizer block) uses the sub-model.

In the first case presented, we had ORDDOL as a species in the stream “To Discharge”. That species does not appear since it was not in the sub-model.

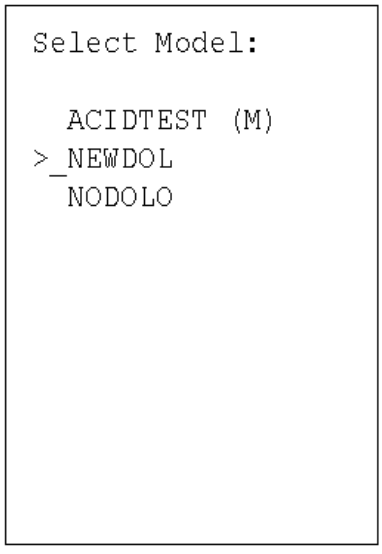
Case 3: Hiding the Master Model

The inflow stream “Formation” contains ORDDOL which is incorrect. The actual species is Dolomite. We now need you to create yet a new sub-model with the following attributes:

Name:	NEWDOL
Inflow Species:	H2O
	DOLOMITE
	HCL
	NACL
Database:	GEOCHEM
Remove Solids:	CAMG3CO34, DISDOLPPT, ORDDOLPPT

In the first block MIX, use the MODEL action and select this new model.

The Model Selection screen looks like this:



Save the model and re-run the process. You will now notice that we are not using the master model in part of the process.

Stream	Formation	Acid Injection	To Wellhead	Base Feed	To Discharge
Phase	Mixed	Aqueous	Mixed	Aqueous	Mixed
Temperature, C	40	25	39.1777	25	69.1028
Pressure, atm	1.5	1	1	1	1
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	98.23009	90.24517	188.4756	63.26784	251.378
CO2	1.64E-04		3.539312		0.36522
DOLOMITE	1.769576				
CAO	8.22E-05		1.769656		2.65E-05
MGO	8.22E-05		1.769656		4.78E-05
HCL		9.754827	9.754808		9.754831
NA2O				5.228055	5.228061
CACO3					1.30148
CAMG3CO34					0.4681561
MGOH2					0.365146
Total mol/hr	100	100	205.309	68.4959	268.861
Total g/hr	2095.98	1981.47	4077.45	1463.82	5541.27
Volume, m3/hr	0.00189774	0.00182583	0.0987181	0.00113075	0.00505866
Enthalpy, cal/hr	-7.67E+06	-6.54E+06	-1.42E+07	-5.10E+06	-1.93E+07
Vapor fraction			0.01815917		
Solid fraction	0.0176958				0.007940088
Organic fraction					

You can now see that dolomite appears in the feed stream.

Case 4: Using a sub-model in a stream.

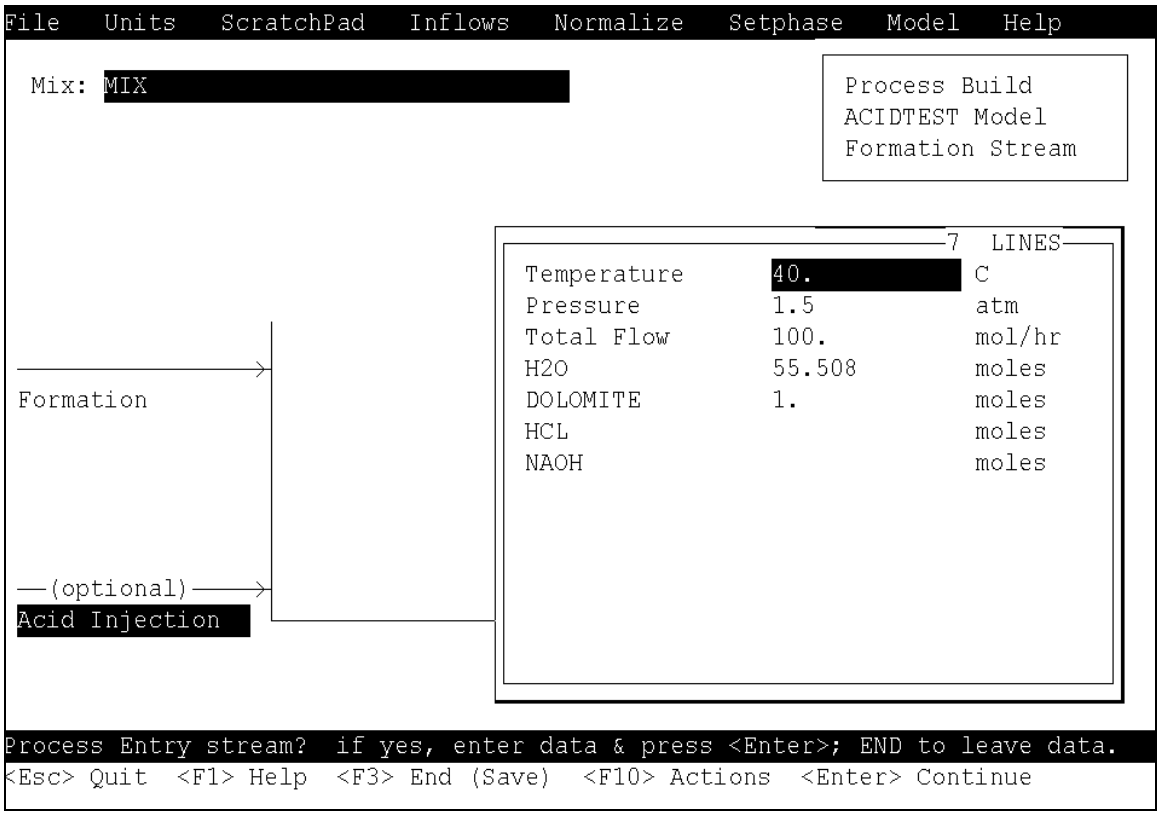
Finally, we can further modify the process. Perhaps we need a model that contains no solids as a feed. We will now create a new model and use it in the stream "Formation".

Name: NOSOLID
Inflow Species: H2O
DOLOMITE
HCL
NACL

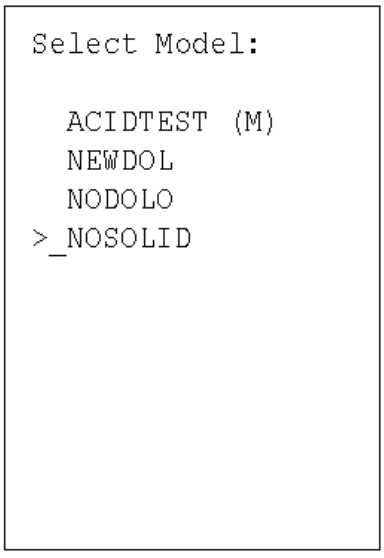
Database: GEOCHEM
Remove Solids: Exclude All Solids

Return to Process Build and select the first block MIX.

Select the stream "Formation"



Select **Model** from the action line.



Select the model NOSOLID

Save the block and re-run the process.

The results are below:

Stream	Formation	Acid Injection	To Wellhead	Base Feed	To Discharge
Phase	Aqueous	Aqueous	Mixed	Aqueous	Mixed
Temperature, C	40	25	37.7575	25	68.015
Pressure, atm	1.5	1	1	1	1
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	98.23067	90.24517	188.4756	62.95259	251.0899
CACO3	1.769667				1.292519
MGCO3	1.769667				
HCL		9.754827	9.754808		9.754824
CO2			3.539312		0.3383408
CAO			1.769656		2.74E-05
MGO			1.769656		5.09E-05
NA2O				5.202009	5.202007
CAMG3CO34					0.4771157
MGOH2					0.3382628
Total mol/hr	101.77	100	205.309	68.1546	268.493
Total g/hr	2095.98	1981.47	4077.45	1456.53	5533.98
Volume, m3/hr	0.00173984	0.00182583	0.0977682	0.00112512	0.00504979
Enthalpy, cal/hr	-7.67E+06	-6.54E+06	-1.42E+07	-5.07E+06	-1.93E+07
Vapor fraction			0.01806092		
Solid fraction					0.007850856
Organic fraction					

The solid dolomite is no longer in the feed stream.