

第 98 期：Builder2021-CCS 过程向导

Builder/GEM/Results 2021.10

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碳埋存的数值模拟用户一直苦于机理较多不知从何下手，Builder2021 版本新增 CCS 过程向导，恰好解决了这一难题。

CCS 向导帮助工程师轻松搭建 CO₂ 封存模型，包括各种封存机理。在该向导的第 2 步中，用户可以选择例如滞后模拟的束缚气封存，CO₂ 溶于水模拟的溶解封存，离子溶解或地球化学模拟矿化捕集等。

使用地球化学模拟时，同时选择水蒸发模拟，可以考虑盐析导致的注入能力降低。Step 3 中提供三大化学反应数据库，工程师可以选择水相或矿物质反应。同时为基础研究的用户提供了三个便捷的缺省选项：1) 缺省使用最小组分数的 CCS 建模；2) 缺省使用碎屑岩进行 CCS 建模；3) 缺省使用碳酸盐进行 CCS 建模。（注：碳酸盐岩主要由方解石 (CaCO₃) 和白云石 (CaMg[CO₃]₂) 两种碳酸盐矿物组成，碎屑岩由碎屑成分和填隙物成分（包括杂质和胶结物）组成）

如果选择滞后作用模拟束缚空间封存，在选择相对渗透率曲线后会出现滞后对话框，选择各种不同的捕集选项，并在图形中展示相对渗透率曲线滞后捕集效果。

本讲义使用 2D 机理模型，通过两个完整的练习，演示 Builder2021-CCS 向导流程，并对计算结果进行必要解读。

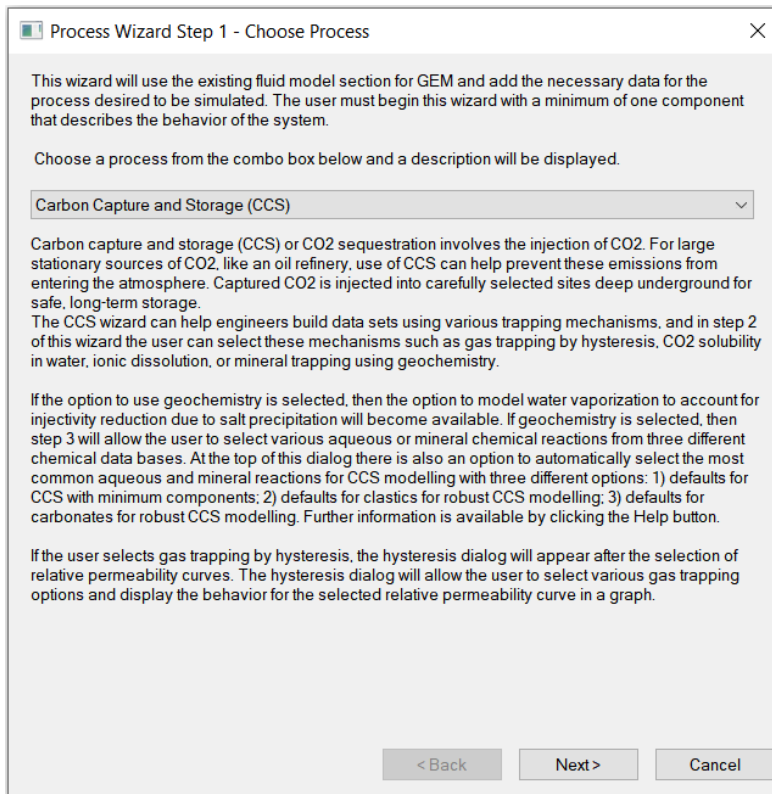
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练习一、溶解封存和束缚空间封存

本节的目的是在基础模型的构造封存基础上,添加溶解封存和束缚空间封存模拟。溶解封存利用 CO₂ 在一定压力/温度下溶于水相来达到封存的目的。溶解封存很大程度上取决于压力、温度和与水体接触的表面积。束缚空间封存利用相对渗透率曲线从驱替转向吸入的效应来圈闭非润湿相(本例中为气)。

1. 将 **EXERCISE_1_BASECASE.dat** 拖入 Builder 图标, 在 I/O Control 部分 → **Titles and Case ID**, 设置 **Title: CASE_1: CO₂ 2D BASE CASE+HYS+SOL**。
2. 在左边树视图中选择 **Components → Process Wizard**。
3. 通过下拉菜单选择 **Carbon Capture and Storage (CCS)**。



4. 点击 **Next**。CO₂ 溶解模拟 (Solubility) 和滞后模拟 (Hysteresis) 功能已经激活, 其他机理在稍后的练习中添加。

Step 2 - Input Specific Data For Carbon Capture and Storage (CCS) ×

Select CCS trapping mechanisms	
CO2 Solubility in water (always selected)	<input checked="" type="checkbox"/>
Model rock dissolution and mineral trapping with geochemistry	<input type="checkbox"/>
Model CO2 trapping by relative permeability hysteresis	<input checked="" type="checkbox"/>
Select CCS Options	
Model temperature effects with the GEM THERMAL option	<input type="checkbox"/>

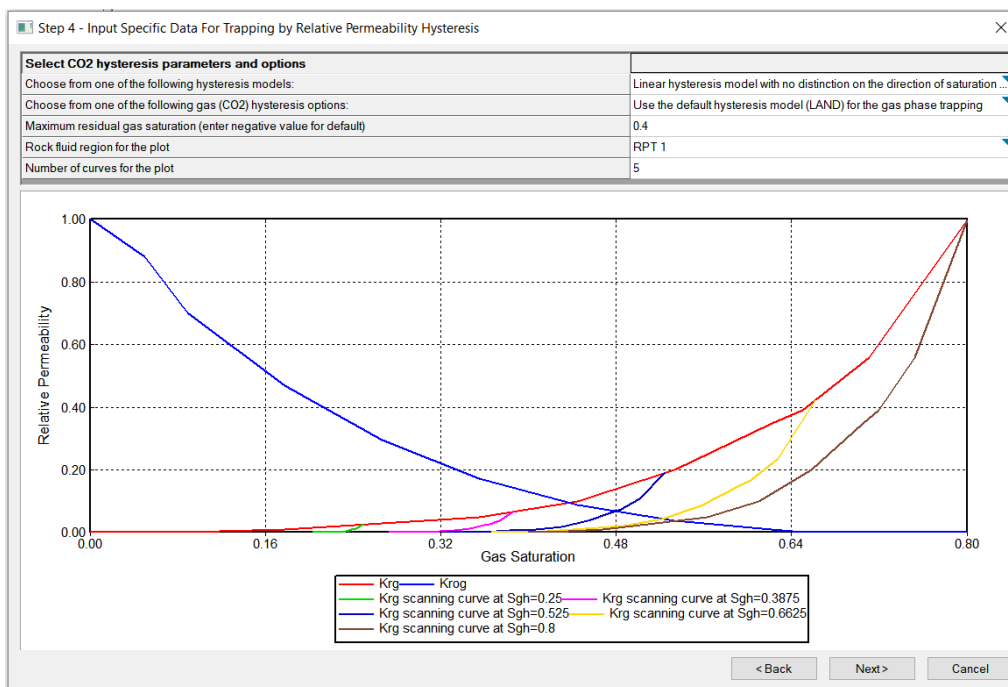
5. 点击**Next**跳转到**Step 3**。点击**Rock Fluid Region Number 1**，表明对该曲线使用滞后模拟。

Step 3 - Set Rock Fluid Regions ×

Select rock fluid regions to use for hysteresis trapping. If any of the selected regions already contain more than one set, then these sets will be deleted

Rock Fluid Region Number 1

6. 在Step 4:
- 1) 双击顶部的第一行，选择滞后模拟方法，这里选择**Linear**线性滞后；
 - 2) 第二行选择具体线性滞后模型，在本例中是**Land**模型；
 - 3) 第三行，选择最大残余气体饱和度（Maximum residual gas saturation）。默认情况下，Sgmax为Sgcrit和1-Swcon的中点。或者自定义Sgmax值，这里将设置**0.4**；
 - 4) 这里还展示了GEM在模拟过程中使用的吸入曲线和边界吸入曲线。默认显示的曲线数量是5条，但您可以根据需要修改这个数字以显示不同数量的曲线；
 - 5) 完成后单击**Next**。



7. 最后一步，选择 **Well Name** 注入井名，点击 **Finish**，在弹出的对话框中点击 **OK** 退出。

Step 5 - Choose Wells, Dates, and Set Injection Composition

Oil Components for gas/solvent Injectors	
CO2 injection (gas mole fraction)	100

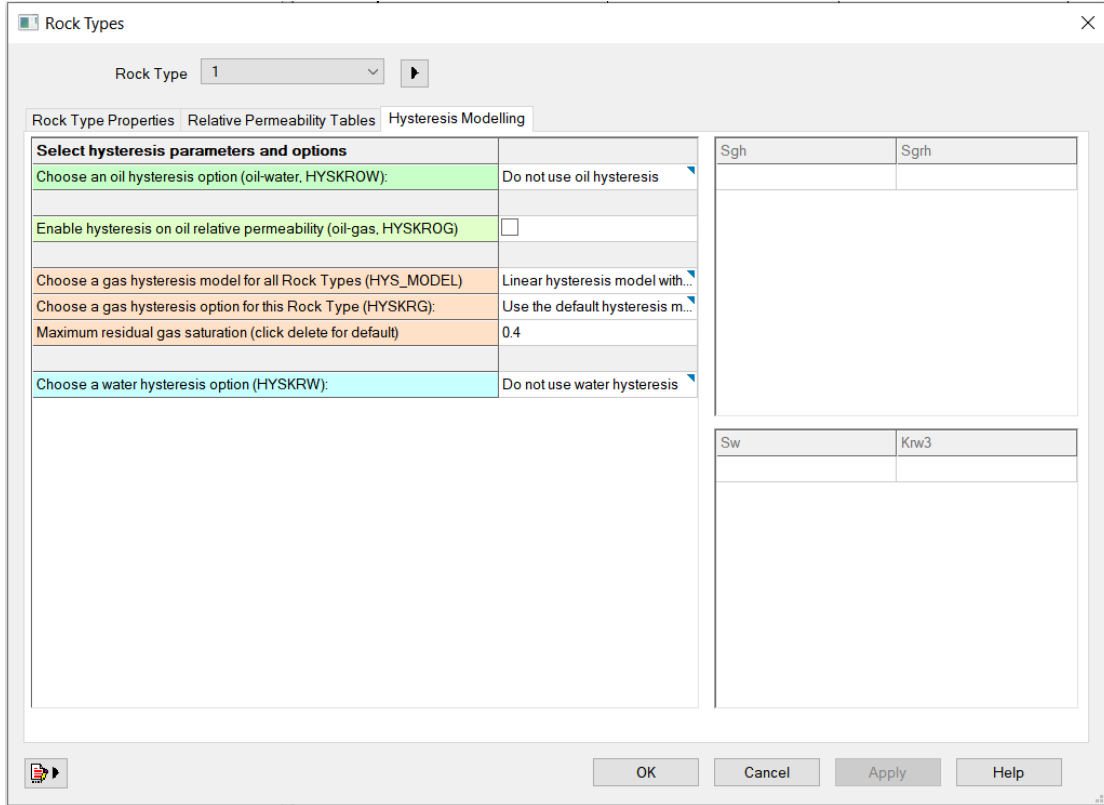
Well Name	Date
<input checked="" type="checkbox"/> CO2_INJECTOR	2030-01-01 0:00:00

Sort Well/Date Display:
 Auto Select Wells:

 All
 Producers
 Injectors
 Highlighted
 Match name / wildcard

Buttons:

8. Builder 顶部菜单栏 **File** → **Save As** , 保存文件名为 **EXERCISE_2A_SOLUBILITY_HYSTERESIS.dat**
9. 左侧树视图, **Rock-Fluid**→**Create/Edit Rock Types**, 第三个选项卡**Hysteresis Modelling**, 可以看到向导生成的有关滞后模拟的设置。



10. 在CCS向导中, 流体模型部分的AQUEOUS-VISCOSITY KESTIN被删除。该关键字用于计算水相粘度的相关式, 且与温度、压力和矿化度相关, 如未定义, 则水相粘度为Visw(恒定值)。该关键字对计算结果略有影响(可忽略), 在流体模型中添加水相粘度计算关键字。

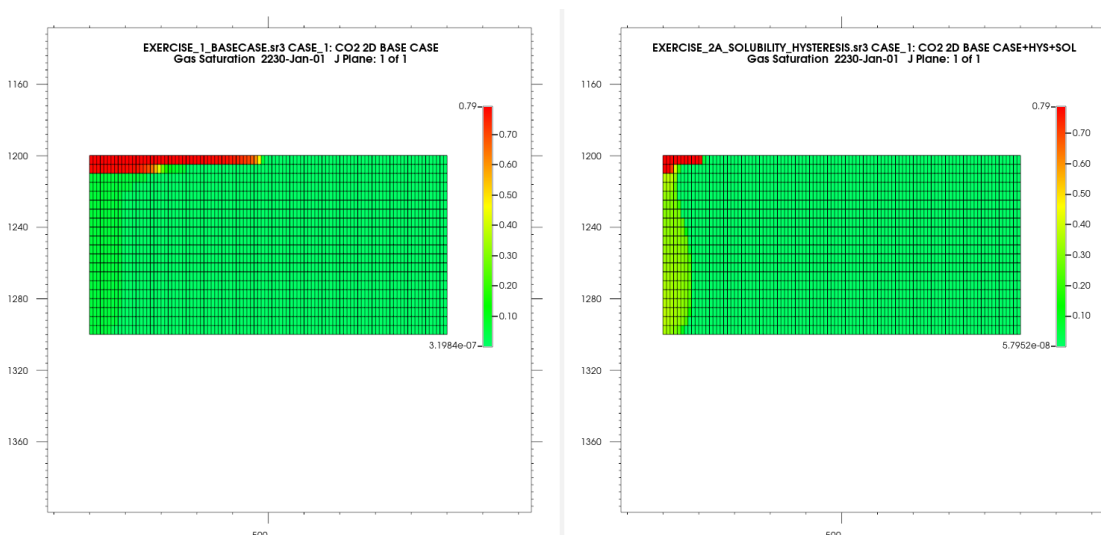
AQUEOUS-VISCOSITY KESTIN

11. 在cEDIT中打开, 可以查看到通过Process Wizard添加的关键字。下面是这些关键字的一个简单释义。

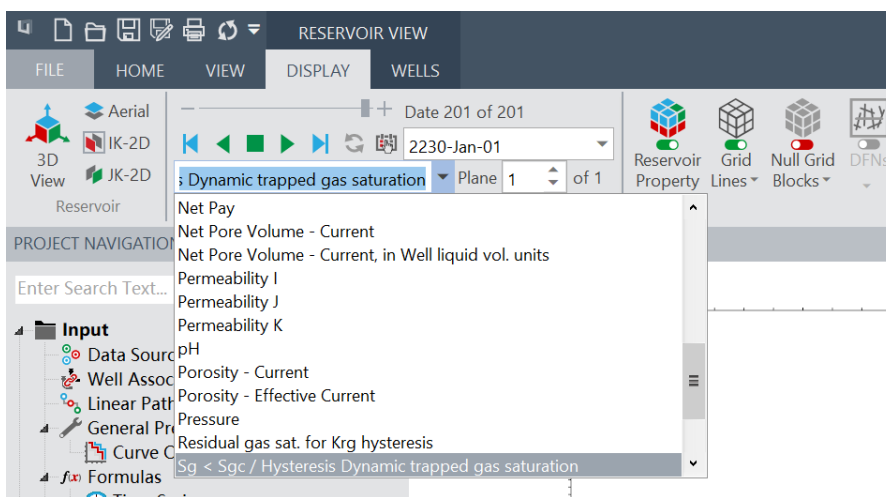
GEM关键字	功能
SOLUBILITY HENRY	基于Henry亨利定律的气体组分在水中的溶解
HENRY-MOD1-CO2	Henry常数相关式的改进版本, 适用于温度150° C和压力110MPa的溶解模拟

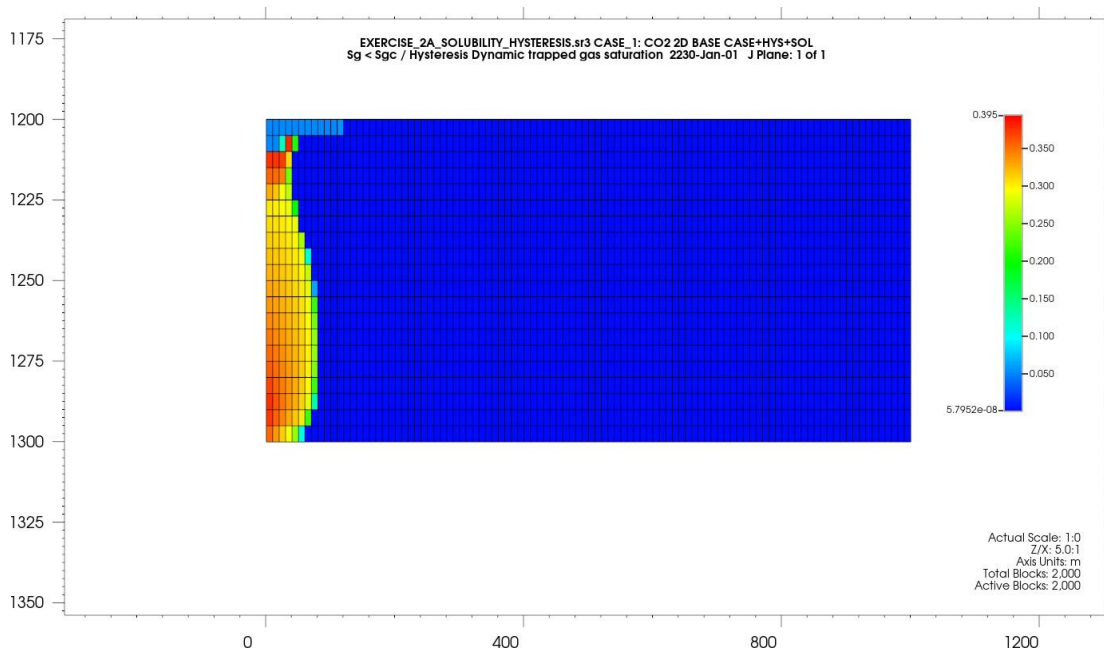
BIN-TDEP-CO2	在模拟开始时, 将根据储层平均温度计算CO2-H2O或H2S-H2O的二元相互作用系数。
HYS_MODEL LINEAR	激活缺省的线性滞后模型
HYSKRG	Land滞后模型的最大残余气饱和度

12. 将模型拖至GEM模拟器计算。
13. 将该结果与EX 1的结果进行比较。将对应的sr3文件拖至Results图标, 左侧树视图Reservoir→EXERCISE_2A_SOLUBILITY_HYSTERESIS.sr3→IK 2D View, 可以查看和对比剖面图。由于束缚空间封存和溶解封存的共同作用, 更多的天然气被封存在咸水层中。在EX 2中, 天然气运移到构造顶部的量较少。

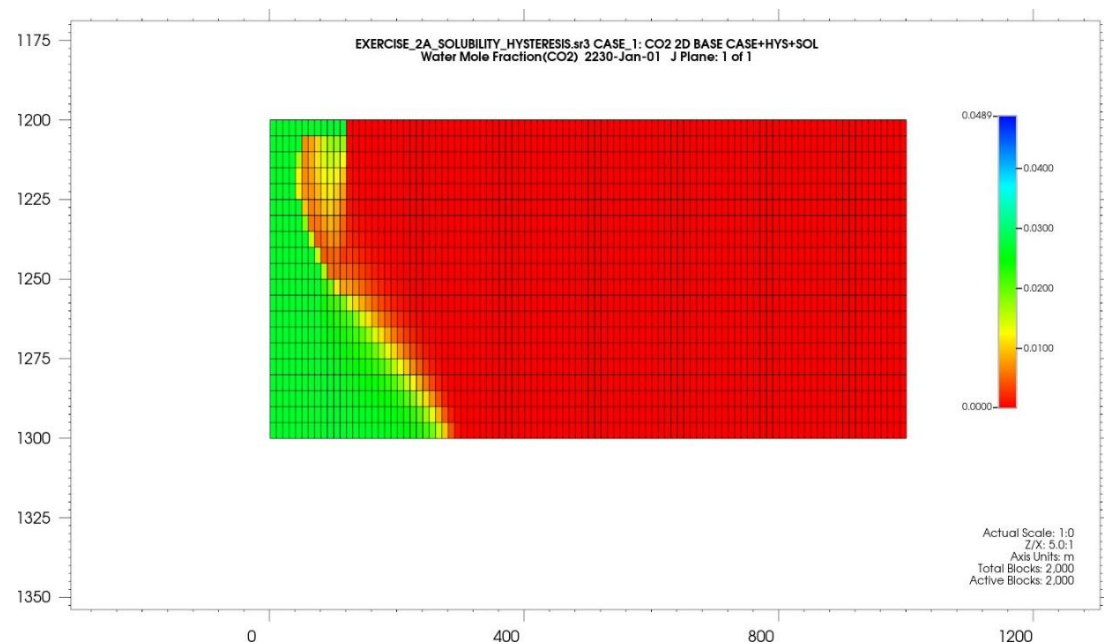


14. 点击菜单栏Display, 选取最后一个时间点, 属性选择Sg < Sgc / Hysteresis Dynamic Trapped Gas Saturation属性图, 看查看封存气含量分布。





15. 同样方法, 分析水中CO₂的摩尔分数如何随时间变化, 还可以查看由于CO₂在水中的溶解而引起的水相密度的变化。



16. EXERCISE_2A_SOLUBILITY_HYSTERESIS.out文件的最后, CO₂ Storage Summary 中可读取不同封存形式的CO₂量, 也可以与注入的CO₂总量进行比较。



Comp	Cum Inj gmole	Cum Prod gmole	Accum gmole	Acc/(Inj-Pro)	Recovery %	Error mol in place, %
CO2	1.27748E+08	0.00000E+00	1.27758E+08	1.00008E+00	0.00000E+00	7.83753E-03
CH4	0.00000E+00	0.00000E+00	2.84220E-03	1.00000E+00	0.00000E+00	2.97685E-04
CO2_T	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	2.74118E+05	1.00000E+00	0.00000E+00	2.76100E-03

Total Cum Inj, mol = 1.27748E+08 Ave. Acc/(Inj-Pro) = 1.00002E+00
 Total Cum Prod, mol = 0.00000E+00 Ave. Error, % mol in place = 2.72405E-03
 Total Accum, mol = 1.28032E+08

CO2 Storage Amounts in Reservoir	Moles	kg
Gaseous Phase	= 0.00000E+00	0.00000E+00
Liquid Phase	= 0.00000E+00	0.00000E+00
Supercritical Phase	= 9.75969E+07	4.29524E+06
Trapped Sg < Sgc / Hysteresis	= 7.68295E+07	3.38127E+06
Dissolved in Water	= 3.04256E+07	1.33903E+06

Mole Percent Hydrocarbon Recovered: Total-HC-Prod/Total-HC-Originally-In-Place = 0.0000

17. 如果未添加AQUEOUS-VISCOSITY KESTIN，计算结果如下。

Cumulative Field Total at Reservoir Conditions for Components.....

Comp	Cum Inj gmole	Cum Prod gmole	Accum gmole	Acc/(Inj-Pro) %	Recovery mol in place, %	Error
CO2	1.27746E+08	0.00000E+00	1.27755E+08	1.00007E+00	0.00000E+00	7.45908E-03
CH4	0.00000E+00	0.00000E+00	2.15203E-03	1.00000E+00	0.00000E+00	2.25399E-04
CO2_T	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00	3.26960E+05	1.00000E+00	0.00000E+00	3.29323E-03

Total Cum Inj, mol = 1.27746E+08 Ave. Acc/(Inj-Pro) = 1.00002E+00
 Total Cum Prod, mol = 0.00000E+00 Ave. Error, % mol in place = 2.74443E-03
 Total Accum, mol = 1.28082E+08

CO2 Storage Amounts in Reservoir	Moles	kg
Gaseous Phase	= 0.00000E+00	0.00000E+00
Liquid Phase	= 0.00000E+00	0.00000E+00
Supercritical Phase	= 9.75121E+07	4.29151E+06
Trapped Sg < Sgc / Hysteresis	= 7.67638E+07	3.37837E+06
Dissolved in Water	= 3.05077E+07	1.34264E+06

Mole Percent Hydrocarbon Recovered: Total-HC-Prod/Total-HC-Originally-In-Place = 0.0000

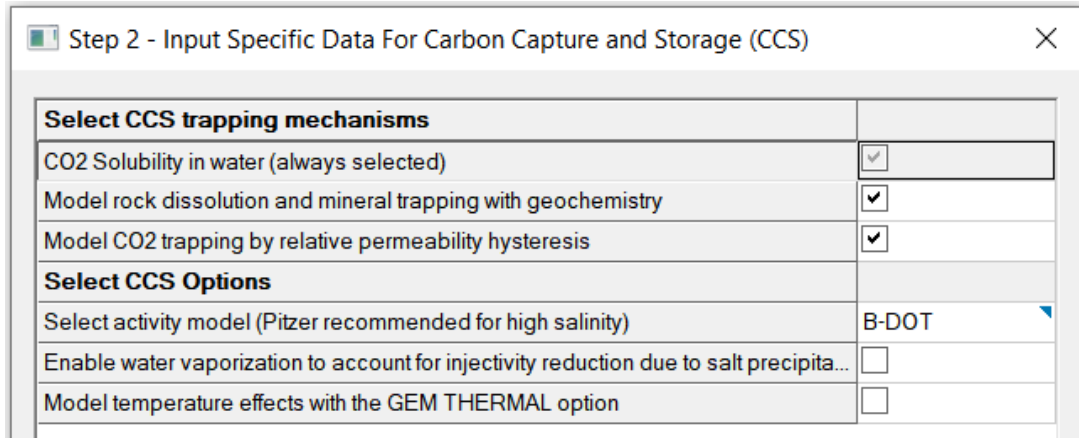
练习二、矿化封存

本节是在练习一（束缚空间封存和溶解封存）模型基础上，加入矿化封存模拟。矿化封存 CO2 是最安全的埋存形式，在四种机制中需要的时间也是最长的，其中一个原因是 CO2 在以矿化形式沉淀之前必须先溶于水相。

1. 在Builder2021中打开**EXERCISE_2A_SOLUBILITY_HYSTERESIS.dat**。
2. I/O Control → Titles and Case ID，填写标题 **CASE_2: CO2 2D BASE**

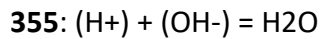
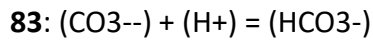
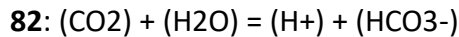
CASE+HYS+SOL+MIN。

3. 点击 **Components** → **Process Wizard**, 选择 **CCS**, **NEXT** 后跳转到 **Step 2**。
4. 勾选 **Model rock dissolution and mineral trapping with geochemistry**, 其他不需设置。

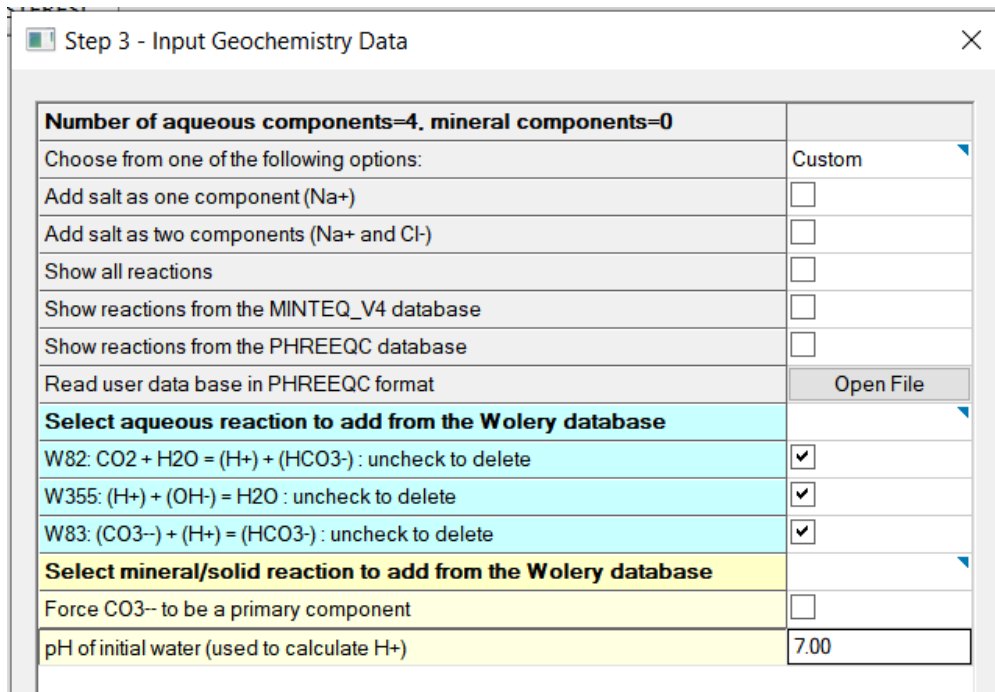


Select CCS trapping mechanisms	
CO2 Solubility in water (always selected)	<input checked="" type="checkbox"/>
Model rock dissolution and mineral trapping with geochemistry	<input checked="" type="checkbox"/>
Model CO2 trapping by relative permeability hysteresis	<input checked="" type="checkbox"/>
Select CCS Options	
Select activity model (Pitzer recommended for high salinity)	B-DOT
Enable water vaporization to account for injectivity reduction due to salt precipita...	<input type="checkbox"/>
Model temperature effects with the GEM THERMAL option	<input type="checkbox"/>

5. Step 3 添加地球化学反应相关数据。
6. 在蓝色的下拉列表下, 选择如下的 **Aqueous Reactions**:

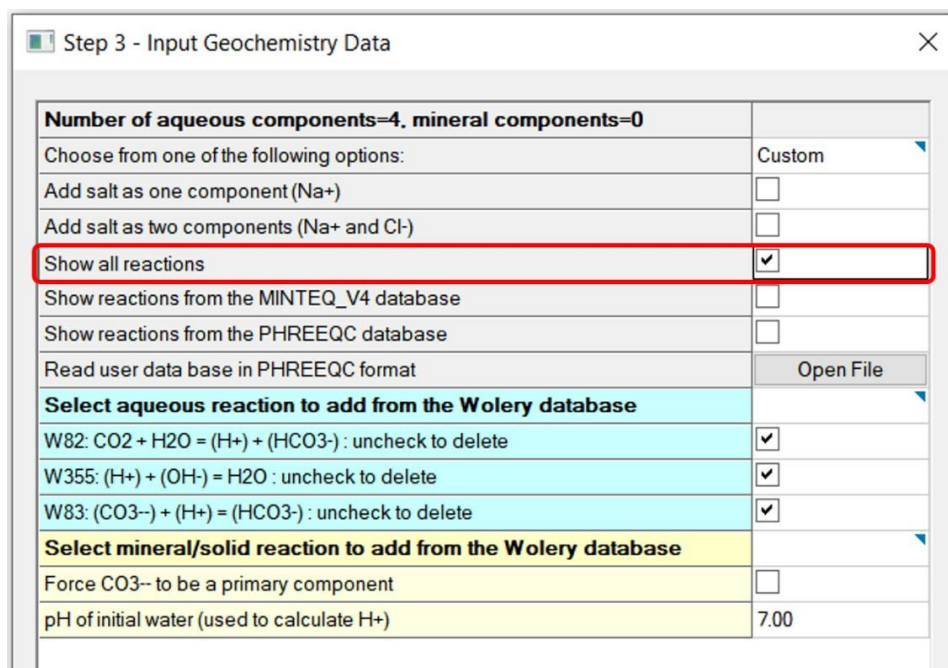


同时, 输入 **pH=7**。



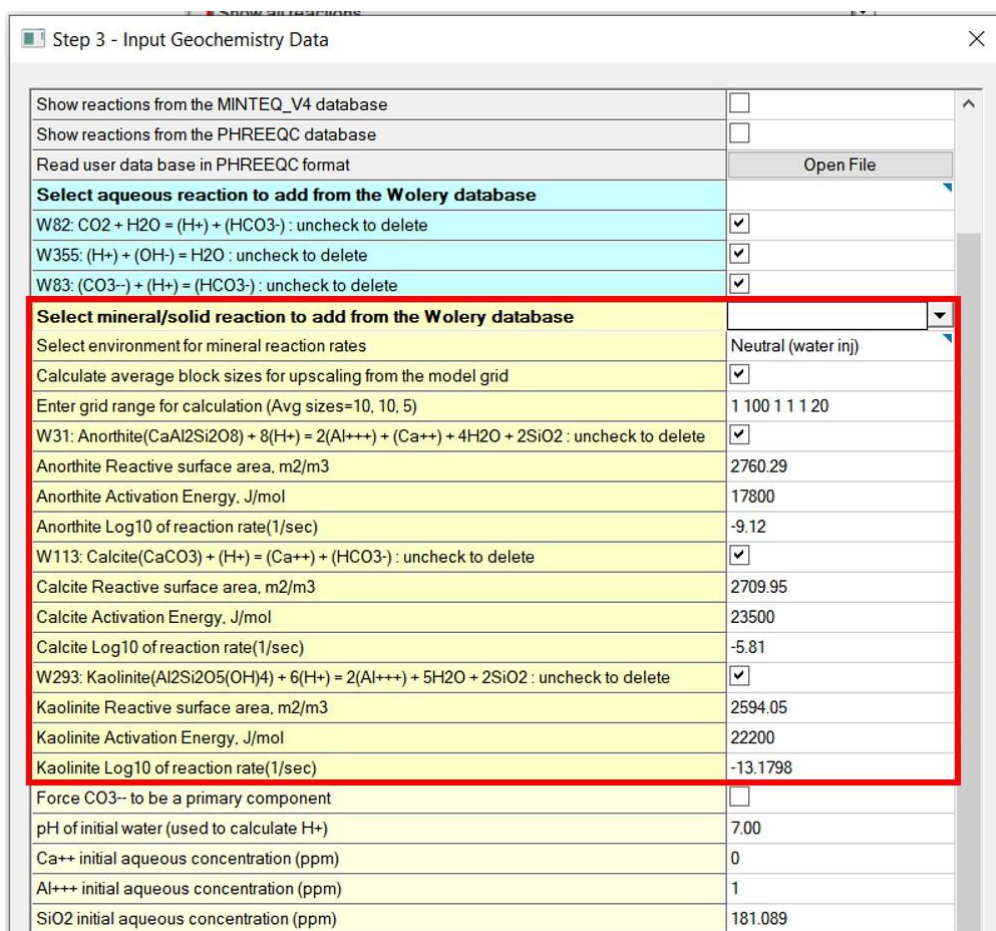
Number of aqueous components=4, mineral components=0	
Choose from one of the following options:	Custom
Add salt as one component (Na+)	<input type="checkbox"/>
Add salt as two components (Na+ and Cl-)	<input type="checkbox"/>
Show all reactions	<input type="checkbox"/>
Show reactions from the MINTEQ_V4 database	<input type="checkbox"/>
Show reactions from the PHREEQC database	<input type="checkbox"/>
Read user data base in PHREEQC format	Open File
Select aqueous reaction to add from the Wolery database	
W82: $\text{CO}_2 + \text{H}_2\text{O} = (\text{H}^+) + (\text{HCO}_3^-)$: uncheck to delete	<input checked="" type="checkbox"/>
W355: $(\text{H}^+) + (\text{OH}^-) = \text{H}_2\text{O}$: uncheck to delete	<input checked="" type="checkbox"/>
W83: $(\text{CO}_3^{--}) + (\text{H}^+) = (\text{HCO}_3^-)$: uncheck to delete	<input checked="" type="checkbox"/>
Select mineral/solid reaction to add from the Wolery database	
Force CO_3^{--} to be a primary component	<input type="checkbox"/>
pH of initial water (used to calculate H^+)	7.00

7. 黄色区域为 **Mineral Reactions**。缺省条件下, 向导提供了所有可用反应的一部分, 这里, 我们需要所有的反应, 勾选 **Show all reactions**。

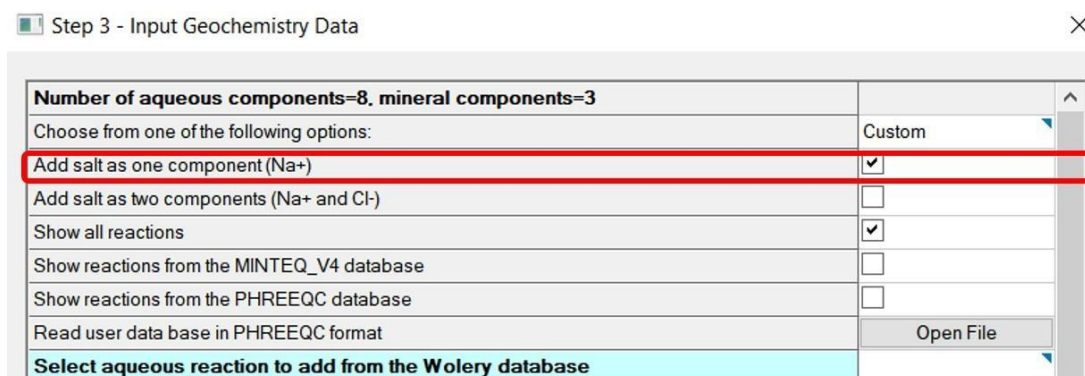


Number of aqueous components=4, mineral components=0	
Choose from one of the following options:	Custom
Add salt as one component (Na+)	<input type="checkbox"/>
Add salt as two components (Na+ and Cl-)	<input type="checkbox"/>
Show all reactions	<input checked="" type="checkbox"/>
Show reactions from the MINTEQ_V4 database	<input type="checkbox"/>
Show reactions from the PHREEQC database	<input type="checkbox"/>
Read user data base in PHREEQC format	Open File
Select aqueous reaction to add from the Wolery database	
W82: $\text{CO}_2 + \text{H}_2\text{O} = (\text{H}^+) + (\text{HCO}_3^-)$: uncheck to delete	<input checked="" type="checkbox"/>
W355: $(\text{H}^+) + (\text{OH}^-) = \text{H}_2\text{O}$: uncheck to delete	<input checked="" type="checkbox"/>
W83: $(\text{CO}_3^{--}) + (\text{H}^+) = (\text{HCO}_3^-)$: uncheck to delete	<input checked="" type="checkbox"/>
Select mineral/solid reaction to add from the Wolery database	
Force CO_3^{--} to be a primary component	<input type="checkbox"/>
pH of initial water (used to calculate H^+)	7.00

8. 在黄色区域的下拉菜单中, 选择如下反应: 钙长石 **Anorthite (no. 31)**, 方解石 **Calcite (no. 113)**, 高岭石 **Kaolinite (no. 293)**。



9. 指定一个组分用于定义矿化度，使用Na⁺离子。选中窗口顶部的**Add salt as one component (Na⁺)**。



10. 现在定义初始浓度。滑动到Process Wizard窗口的下方，并输入以下数据。
Al⁺⁺⁺和SiO₂浓度根据典型的水层数据缺省输入。

Force CO3-- to be a primary component	<input type="checkbox"/>
pH of initial water (used to calculate H+)	7.00
Ca++ initial aqueous concentration (ppm)	500
Na+ initial aqueous concentration (ppm)	30000
Al+++ initial aqueous concentration (ppm)	1
SiO2 initial aqueous concentration (ppm)	181.089
Set constant initial mineral volume fractions	<input checked="" type="checkbox"/>
Anorthite initial volume fraction	0.0088
Calcite initial volume fraction	0.0088
Kaolinite initial volume fraction	0.0176

11. Next, 点击**Rock Fluid Region Number 1** 模拟滞后, Next跳转到Step 5。

Step 4 - Set Rock Fluid Regions ×

Select rock fluid regions to use for hysteresis trapping. If any of the selected regions already contain more than one set, then these sets will be deleted

Rock Fluid Region Number 1

12. Step 5, 滞后模拟设置无需更改。

13. Step 6, 选择注入井名, 点击**Finish**, 在弹出的对话框中点击OK。

Step 6 - Choose Wells, Dates, and Set Injection Composition

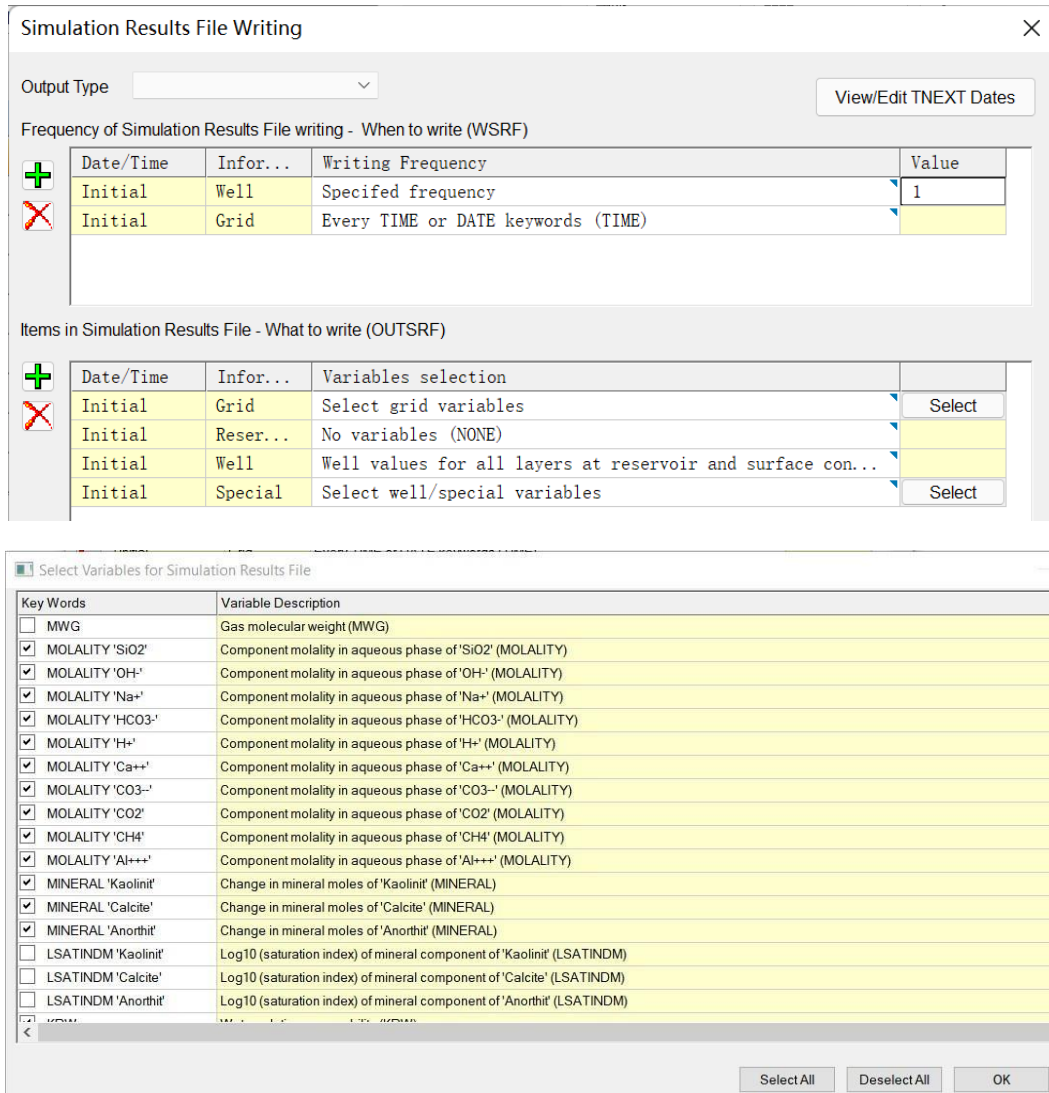
Aqueous Components for Water Injectors	
H+ injection composition (ppm)	0.000101
Ca++ injection composition (ppm)	1e-08
Na+ injection composition (ppm)	1e-08
Al+++ injection composition (ppm)	1e-08
SiO2 injection composition (ppm)	1e-08
HCO3- injection composition (ppm)	0.0
OH- injection composition (ppm)	0.0
CO3-- injection composition (ppm)	0.0

Well Name	Date
<input checked="" type="checkbox"/> CO2_INJECTOR	2030-01-01 0:00:00

Sort Well/Date Display:
 Auto Select Wells:

 All
 Producers
 Injectors
 Highlighted
 Match name / wildcard

14. **I/O Control**→**Simulation Results Output**, 点击**OUTSRF-Grid**后的**Select**, 选择如下参数, 计算后在**Results**中可以查看矿物和水相相关的输出。



The image shows two screenshots from the software interface. The top screenshot is the 'Simulation Results File Writing' dialog box. It has an 'Output Type' dropdown and a 'View/Edit TNEXT Dates' button. Below is a table for 'Frequency of Simulation Results File writing - When to write (WSRF)'. The bottom section is 'Items in Simulation Results File - What to write (OUTSRF)', which is currently expanded to show a list of variables to be written.

Date/Time	Infor...	Writing Frequency	Value
Initial	Well	Specified frequency	1
Initial	Grid	Every TIME or DATE keywords (TIME)	

Date/Time	Infor...	Variables selection	Select
Initial	Grid	Select grid variables	Select
Initial	Reser...	No variables (NONE)	
Initial	Well	Well values for all layers at reservoir and surface con...	
Initial	Special	Select well/special variables	Select

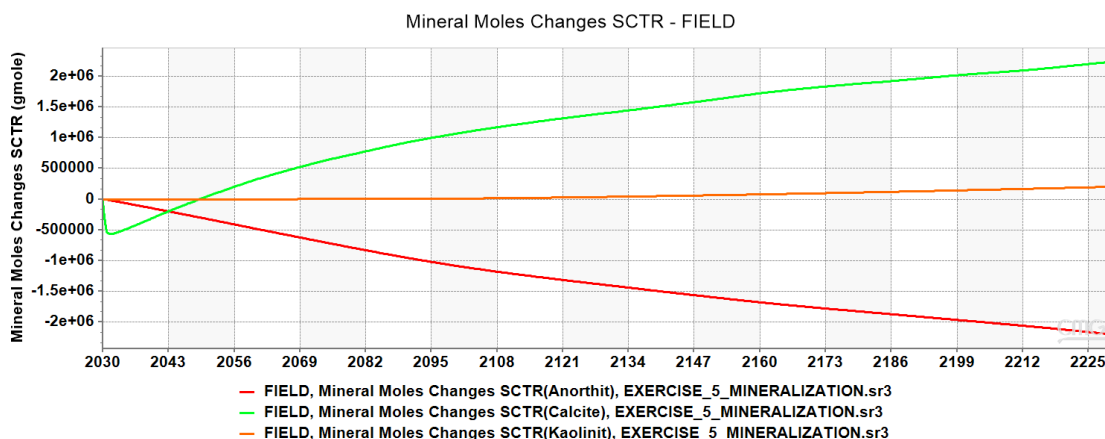
The bottom screenshot is the 'Select Variables for Simulation Results File' dialog box. It contains a list of key words and their descriptions, with checkboxes for selection.

Key Words	Variable Description
<input type="checkbox"/> MWG	Gas molecular weight (MWG)
<input checked="" type="checkbox"/> MOLALITY 'SiO2'	Component molality in aqueous phase of 'SiO2' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'OH'	Component molality in aqueous phase of 'OH' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'Na'	Component molality in aqueous phase of 'Na' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'HCO3'	Component molality in aqueous phase of 'HCO3' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'H'	Component molality in aqueous phase of 'H' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'Ca++'	Component molality in aqueous phase of 'Ca++' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'CO3--'	Component molality in aqueous phase of 'CO3--' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'CO2'	Component molality in aqueous phase of 'CO2' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'CH4'	Component molality in aqueous phase of 'CH4' (MOLALITY)
<input checked="" type="checkbox"/> MOLALITY 'Al+++'	Component molality in aqueous phase of 'Al+++' (MOLALITY)
<input checked="" type="checkbox"/> MINERAL 'Kaolinit'	Change in mineral moles of 'Kaolinit' (MINERAL)
<input checked="" type="checkbox"/> MINERAL 'Calcite'	Change in mineral moles of 'Calcite' (MINERAL)
<input checked="" type="checkbox"/> MINERAL 'Anorthit'	Change in mineral moles of 'Anorthit' (MINERAL)
<input type="checkbox"/> LSATINDM 'Kaolinit'	Log10 (saturation index) of mineral component of 'Kaolinit' (LSATINDM)
<input type="checkbox"/> LSATINDM 'Calcite'	Log10 (saturation index) of mineral component of 'Calcite' (LSATINDM)
<input type="checkbox"/> LSATINDM 'Anorthit'	Log10 (saturation index) of mineral component of 'Anorthit' (LSATINDM)

15. 保存为**EXERCISE_3_MINERALIZATION.dat**。
16. Builder 2021.10版本的CCS向导中, 矿物质体积分数关键字无法写入, 需要在文本添加。在cEDIT中打开模型, 找到初始条件部分, 写入:
- VOLUMEFRACTION-MINERAL**
- 0.0088 0.0088 0.0088
17. 同练习一, 在流体模型的最后加入水相粘度计算关键字。
- AQUEOUS-VISCOSITY KESTIN**
18. 将**EXERCISE_3_MINERALIZATION.dat**文件拖至**GEM**中运行。

19. 通过绘制Sector中的Anorthite钙长石、Calcite方解石和Kaolinite高岭石的 Mineral Moles Changes矿物质物质的量的变化，分析地层中矿物质的改变情况。操作步骤：将对应的sr3文件拖至Results图标，左侧树视图Plots→Time Series，根据下图选择输出，Add To New Plot。在整个模拟过程中Anorthite钙长石逐渐溶解，而Kaolinite高岭石逐渐沉淀，方解石Calcite最初溶解，然后沉淀。

CURVE SELECTOR				
DATA TYPE	DATA SOURCES	DATA	PARAMETER	COMPONENT
Enter Search Text...	Enter Search Text...	Enter Search Text...	mineral	Enter Search Text...
Wells Layers Groups Sectors Special History Block Properties	EXERCISE_5_MINERALIZATION.sr3	FIELD	Mineral Moles Changes SCTR(SC) Mineral Moles SCTR(SC)	Anorthite Calcite Kaolinite



小结

GEM 模拟 CCS，除了向导外，自带算例的 GHG (GREENHOUSE GAS) 文件夹（位置：模板目录 CMG Templates\GEM\2021.10\TPL）有 50 余个 CO2 封存案例，供学习和参考。

相关讲义和链接如下：

[第 88 期: 水溶气数值模拟操作流程 - Learn CMG](#)

[公开课第 35 课: 全新 Results 后处理模块应用技巧-高级篇 \(★50\) - Learn CMG](#)

[公开课第 33 课: 全新 Results 后处理模块应用技巧-油藏篇 \(★50\) - Learn CMG](#)

[公开课第 31 课: 全新 Results 后处理模块应用技巧-曲线篇 \(★50\) - Learn CMG](#)