Value Through Technology

OLI Tips #12
Using ESP Private databases..

You should know how to use a private database in the OLI software. In this example, we will add the species dolomite ($CaMg(CO_3)_2$) which does not exist in the PUBLIC database but does exist in the GeoChem database[1].

1. Start ESP and begin to create a chemistry model
2. Create an ESP/Process or OLI/Toolkit stream (your choice).
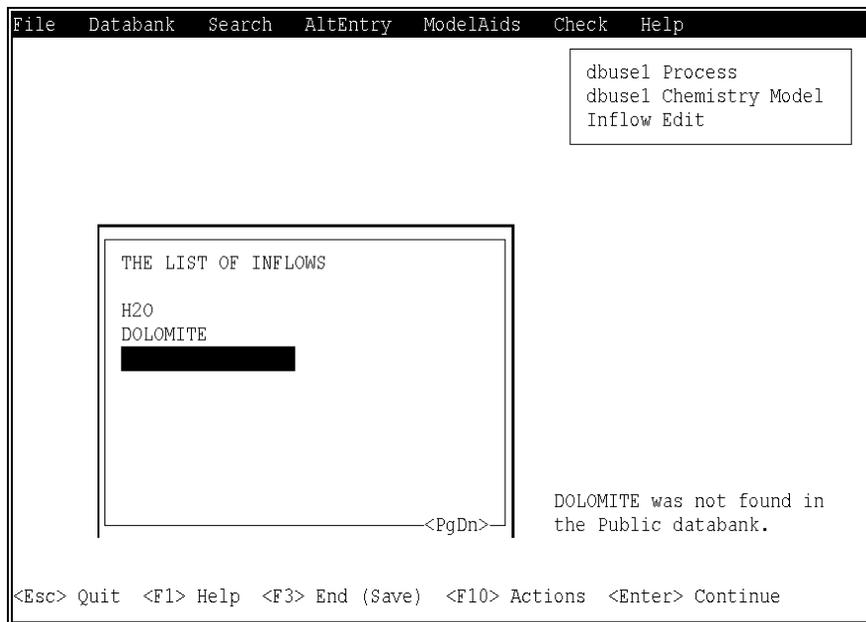3. Create a chemistry model name
4. Enter the species Dolomite

```
File    Databank    Search    AltEntry    ModelAids    Check    Help

                                           dbuse1 Process
                                           dbuse1 Chemistry Model
                                           Inflow Edit



        ┌─────────────────────────────────────┐
        │ THE LIST OF INFLOWS                  │
        │                                      │
        │ H2O                                  │
        │ DOLOMITE                             │
        │ ███████████████████                  │
        │                                      │
        │                                      │
        │                                      │
        │                              DOLOMITE was not found in
        │                  ─<PgDn>─    the Public databank.
        └─────────────────────────────────────┘

<Esc> Quit  <F1> Help  <F3> End (Save)  <F10> Actions  <Enter> Continue
```

Figure 1 Model definition inflow list. Note the warning message

Assuming the dolomite is spelled correctly, you will receive a message that *Dolomite was not found in the Public databank.* This is true. Dolomite is located in the GeoChem database.

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[1] Although the GeoChem database is provided by OLI Systems, it is still considered a private database. The user must perform these actions to access the data in the program.

5.   Use the <Action> key and select **Databank** from the Action Line.
6.   Enter the name **GEOCHEM** to the list. Up to ten names can be entered.

```
Using Which Databanks?

Databank Names:
GEOCHEM
```
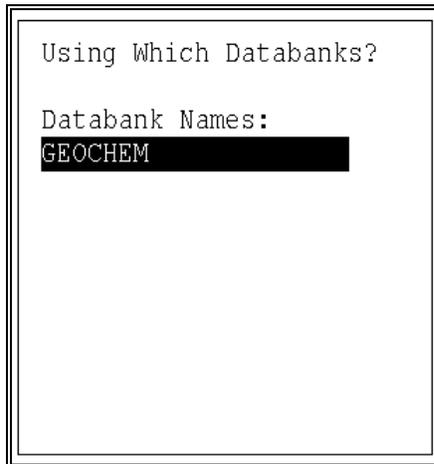
Figure 2 Adding a private database

Each database is entered in the order of importance with the PUBLIC database have the lowest priority. Obviously if a species is not in the PUBLIC database then it will be looked for in GEOCHEM (for this example).

If a species appears in both GEOCHEM and PUBLIC, then the species from GEOCHEM is used. Once a species is located in a database (with the PUBLIC being searched last), then the look up stops.

The following figure shows that GEOCHEM was used during the database search and occurred before the PUBLIC databank.
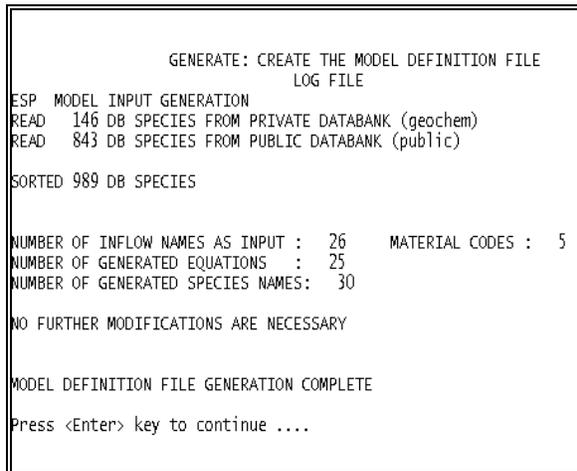
```
                GENERATE: CREATE THE MODEL DEFINITION FILE
                              LOG FILE
ESP  MODEL INPUT GENERATION
READ   146 DB SPECIES FROM PRIVATE DATABANK (geochem)
READ   843 DB SPECIES FROM PUBLIC DATABANK (public)

SORTED 989 DB SPECIES


NUMBER OF INFLOW NAMES AS INPUT :   26     MATERIAL CODES :   5
NUMBER OF GENERATED EQUATIONS    :   25
NUMBER OF GENERATED SPECIES NAMES:   30

NO FURTHER MODIFICATIONS ARE NECESSARY


MODEL DEFINITION FILE GENERATION COMPLETE

Press <Enter> key to continue ....
```

Figure 3 AutoGen results

7.   Finish the model generation as you wish or press the <Esc> to exit. There is one final point. The specification of the database will not be retained in either Process or the Toolkit until you begin to actually fill out the Process or the Stream.