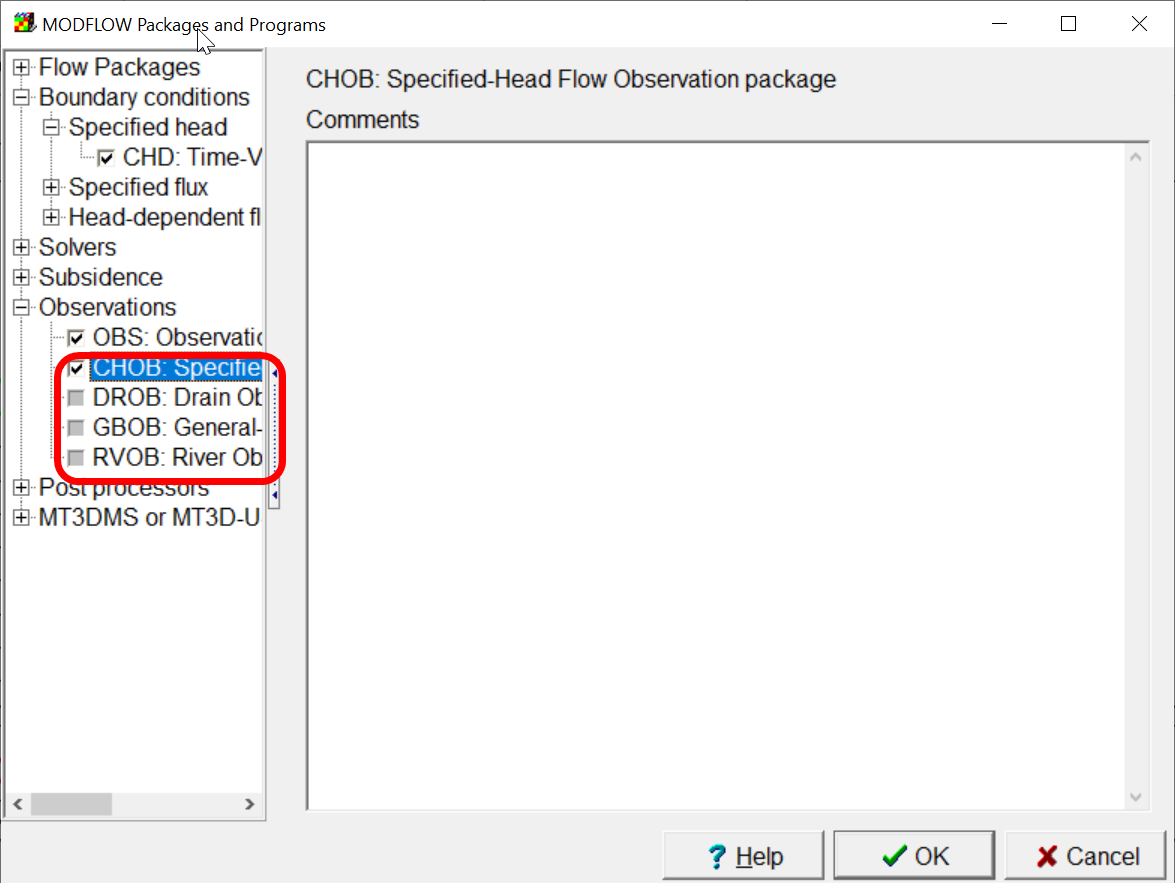
Defining Observations for PEST in ModelMuse Beta 1.

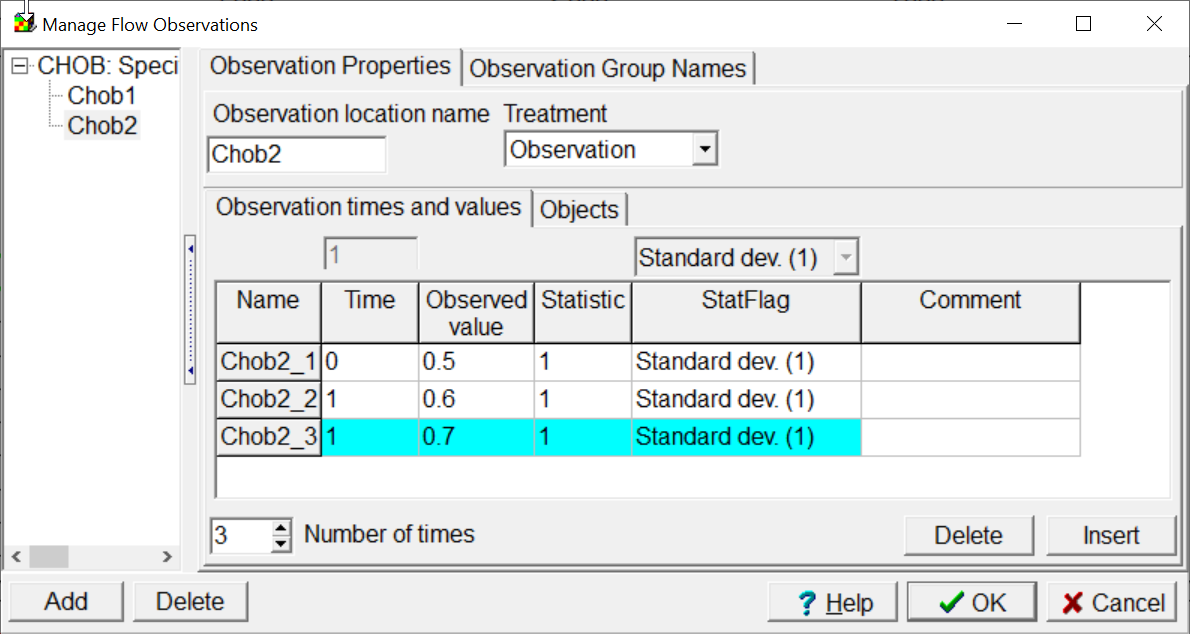
The current beta version of ModelMuse allows the modeler to define observations in ModelMuse. When this is done, ModelMuse will export one or more script files that can be used with utility programs to both extract observations from the model input files and to generate and instruction file for PEST. There are three different utility programs for this purpose and they are distributed along with this beta version of ModelMuse. Documentation for the utility programs is also included. The observations can all be defined in similar ways within ModelMuse but a different utility program is required depending on whether the model is a MODFLOW-2005 (or related), MODFLOW 6, or SUTRA model. Examples of ModelMuse model files are include with the beta release to illustrate how the various observation types can be defined.

# MODFLOW 6

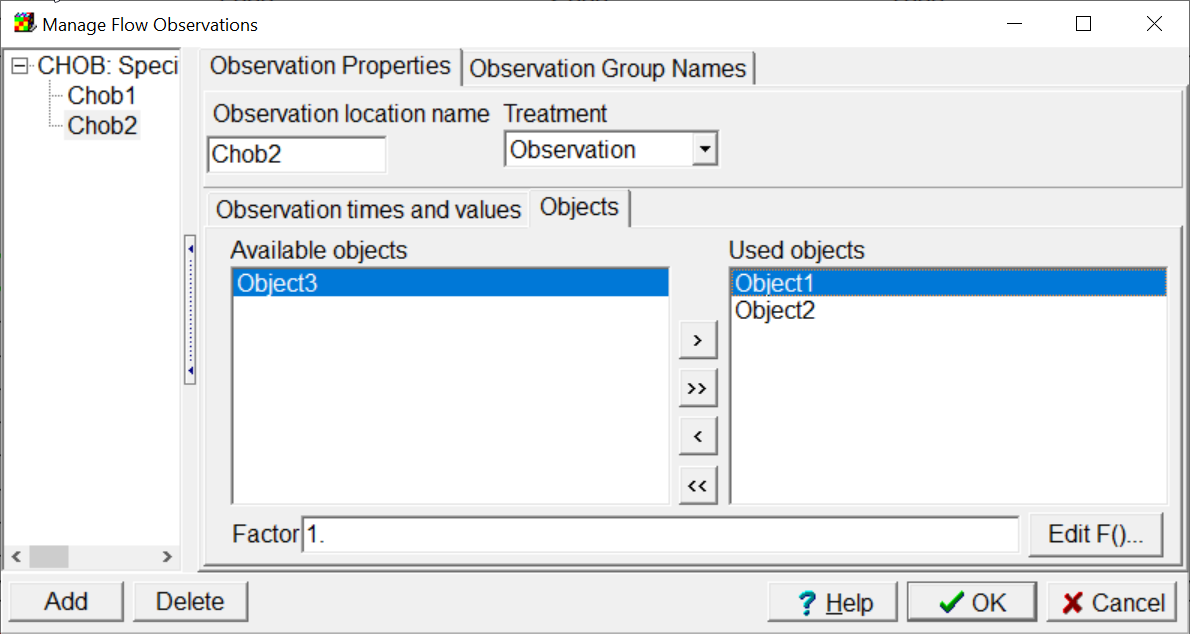
The first change to ModelMuse is in the MODFLOW Packages and Programs dialog box. In the beta version, the checkboxes for the CHOB, DROB, GBOB, RVOB packages are present whereas in the released version of ModelMuse, they are only present in MODFLOW-2005 and related models such as MODFLOW-NWT. The CHOB, DROB, GBOB, RVOB packages are not part of MODFLOW 6 but ModelMuse now allows the modeler to define observations for PEST for the CHD, DRN, GHB, and RIV packages in (nearly) the same way as was done with MODFLOW-2005. The big difference is that behind the scenes, ModelMuse will take care of aggregating flow data from different boundary cells using a separate utility program rather than relying on MODFLOW to do the aggradation.



If any of the checkboxes for the CHOB, DROB, GBOB, RVOB packages is checked, another dialog box will be displayed, the Manage Flow Observations checkbox. It will be displayed either when the MODFLOW Packages and Programs dialog box is closed or when the user selects “Model|Manage Flow Observations”. This dialog box has been part of ModelMuse for a number of years so you can read about it in the ModelMuse help. In brief, the modeler defines observation groups by clicking the Add button. Each observation group can be used to define one or more observations. All the observations in an observation group will involve the same boundary cells but each observation will have a different observation time. In the example below, two observation groups have been defined named Chob1 and Chob2. In the Chob2 group, there are three observations named Chob\_1, Chob\_2, NS Chob\_3. Each of these observations have a separate observation time.

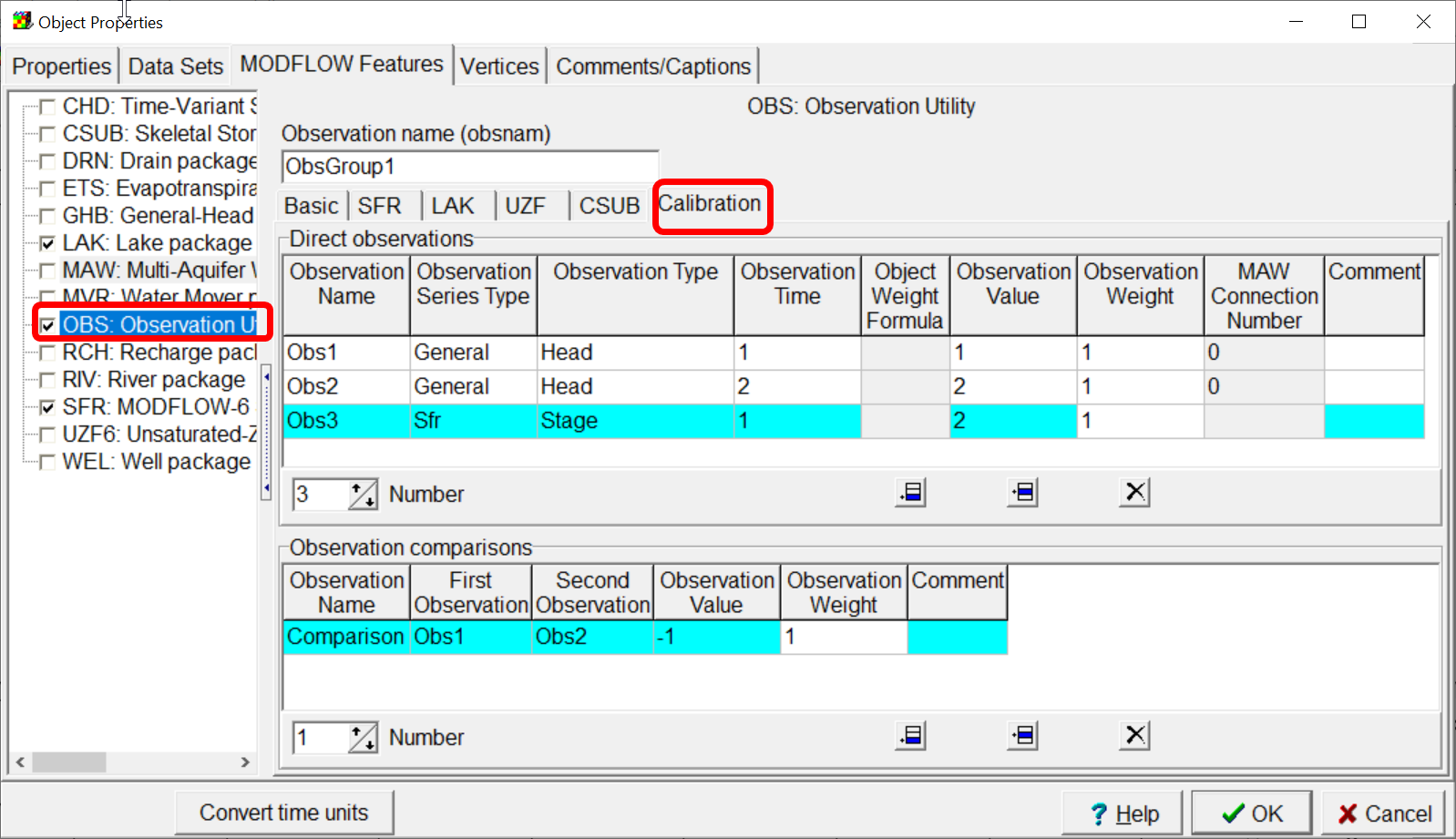


Each flow observation must have one or more boundary cell associated with it. In the case illustrated below, there are three specified head boundaries defined by objects names Object1, Object2, and Object3. The flows through the specified head boundaries defined by Object1 and Object2 are part of the observation while the flow through the specified head boundaries defined by Object3 are not part of the observation. In MODFLOW-2005, there is a “Factor” formula associated with each object. The formula would be evaluated at each boundary cell associated with the object. The formula should evaluate to a number between 0 and 1. MODFLOW-2005 would multiply flow the boundary cell by the factor and sum of all the products would be the simulated value for the observation. This allowed the user to include only part of some flows through a boundary cell in the observation. In practice, however, modelers nearly always left the factor at the default value of 1 so that all of the boundaries defined by an object will be fully included in the simulated value. Because of this and because it was simpler for me, **the Factor formula is not used with flow observations in MODFLOW 6**.



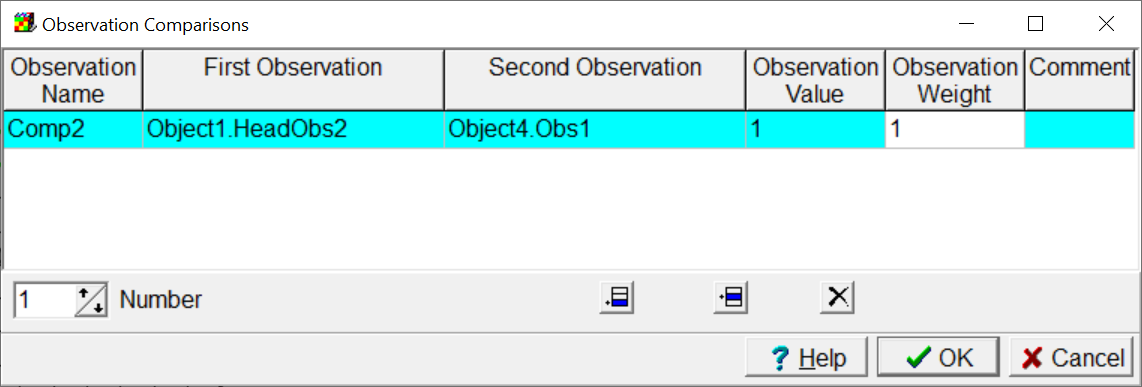
The Observation Utility in MODFLOW 6, allows you to specify observations of various types. These observation types are documented in the file mf6io.pdf distributed with MODFLOW 6. For all these observation types, MODFLOW 6 will produce a time-series of values for cells or groups of cells. Typically, the simulation times will not correspond exactly with the observation time. For some observation types, such as head observations, it may also be desirable to interpolate between the cell centers of the cells around the observation location to the location of the observation. ModelMuse, in conjunction with a utility program will interpolate in time and space to the time and location of the observation. For spatial interpolation, a finite-element basis function will be used to interpolate to the observation location.

For each observation used for PEST parameter estimation, you must create and object. Most often, it will need to be a point object because most observation types are defined at a single point. If it is possible to define an observation for calibration purposes with an object, an extra tab named Calibration will be present on the OBS pane of the Object Properties dialog box. For each observation, you must define the observation name, observation type, observation time, value and weight. You can ignore the “Object Weight Formula”. I plan to eliminate it. In the lower half of the pane, you can define observation comparisons as observations. The observed value for an observation comparison should be the difference between the observed value of two observations defined in the upper half of the Calibration tab. In this case, the value of the comparison is -1 which is the value of the value of Obs1 minus the value of Obs2. At present, ModelMuse does not actually use the observation value or observation weight. They will be used in the future. If an observation is used in an observation comparison, however, it would normally be appropriate to set the weight of that observation to zero. (That isn’t done in the illustration below.



Observation comparisons defined in the lower half of the Calibration tab would normally be between observations of the same type at different times. However, ModelMuse does not restrict you from defining comparisons between any of the calibration observations defined by the object.

It is also possible to define observation comparisons between observations defined by different objects. This is done in the “Model|Edit Object Comparisons” dialog box as illustrated below. ModelMuse does not restrict such observation comparisons to observations of the same type or observations made at the same time. A typical use of such a comparison observation would be when the user has observed a gradient in head between two locations and has measured the difference in elevations of the well heads but has not surveyed in the elevations of the well head from a known survey marker. Because the true elevations of the well heads are not known, the weights assigned to the heads at those wells would need to be low. However, the difference in the elevation of the well heads is known and hence the weight that could be assigned to the difference in head between the wells would be considerably higher.



ModelMuse uses the observations defined in the model to create to input files for the utility program Mf6ObsExtractor. One of the input files is used to extract simulated values at specific times and locations from the MODFLOW 6 output files. The other input file is used to create an instruction file for PEST. A simplified version of the sequence operations when performing automated parameter calibration is as follows.

1. Run the uncalibrated model once.
2. Generate an instruction file with Mf6ObsExtractor.
3. Start automated parameter calibration.
4. PEST runs MODFLOW 6.
5. PEST runs Mf6ObsExtractor to extract simulated values.
6. PEST reads the simulated values using the instruction file from step 2.
7. If the PEST stopping criteria have not been met go to step 4.

Mf6ObsExtractor is documented in a separate file. Mf6ObsExtractor has the potential to be used independently of ModelMuse. Mf6ObsExtractor can be compiled to run on Windows, Linux, and MacIntosh operating systems using the open source Free Pascal compiler.

# MODFLOW-2005

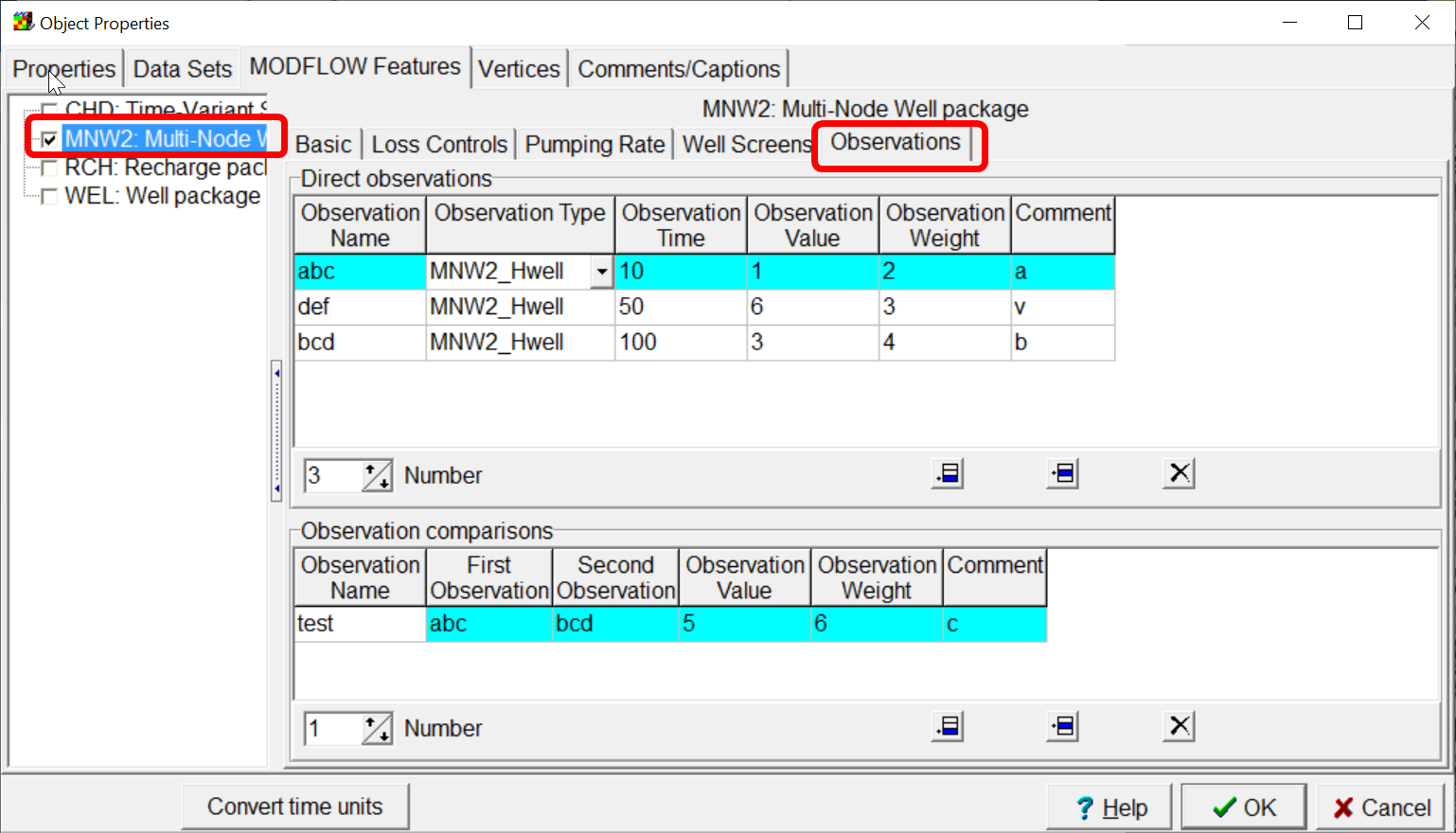
Methods for defining observations of head and flow through some boundary conditions are built into MODFLOW-2005 and other versions of MODFLOW based directly on it such as MODFLOW-NWT. This is done in the MODFLOW-2005 Observation Process. The output from the Observation Process packages consist of files that list the observation name, corresponding simulated values and a few other pieces of data for each simulated value. These are easily read by parameter calibration programs such as PEST.

However, there are several packages in MODFLOW-2005 that produce output that could potential be compared with observed values for the purposes of calibrating a model, but which do not produce the simple files generated in the Observation Process. These include the GAGE, MNWI, SUB, SWT, and SWI packages.

This beta version of ModelMuse allows the user to define observations at specific locations and times with those packages similarly to how observations are defined in ModelMuse with MODFLOW 6. The utility program ObsSeriesExtractor is used to extract values at particular locations and times from the MODFLOW output files.

## MNWI Package with the MNW2 Package

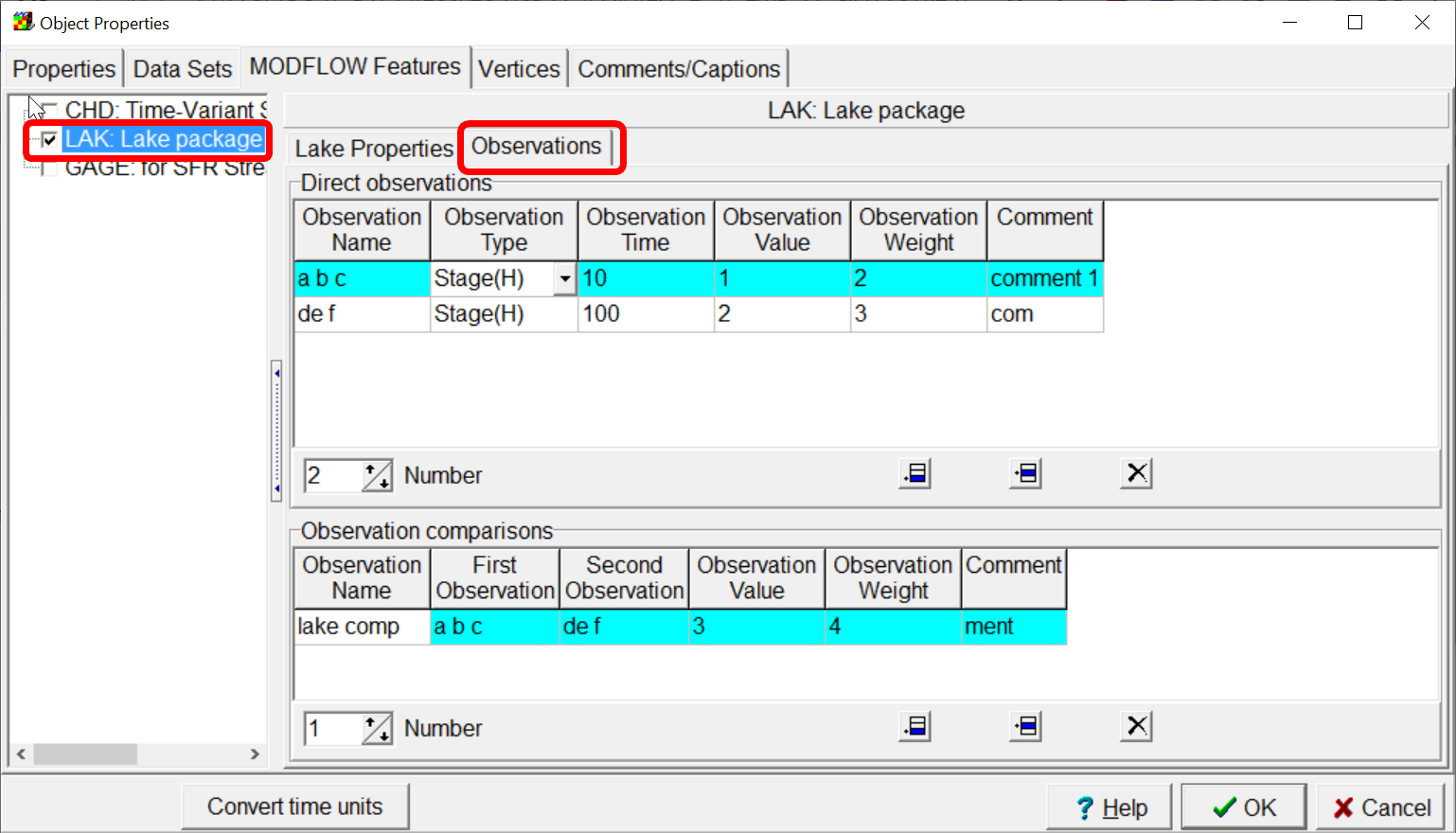
The MNWI package produces time-series data related to the MNW2 package. To define a calibration observation the MNWI package, the user edits an object that defines a well in the MNW2 package and switches to the Observations tab of the MNW2 pane on the Object Properties dialog box. As with observations in MODFLOW 6, the user defines observation names, types, times values and weights. The modeler can also define comparisons between two observations defined for the same MNW2 well. The allowed observation types are the ones that apply to an entire well namely, (1) the flow into the well, (2) the flow out of the well, (3) the net flow to or from the well, (4) the cumulative flow to or from the well and (5) the head in the well.



## GAGE Package with Lakes

The GAGE package produces time-series data for both the LAK and SFR packages. When defining an observation for calibration with the LAK package, the user edits an object that defines a lake and switches to the Observations tab of the Lake package pane. Just as before, the user defines observations names, types, times, values, and weights and can also define comparisons between to observations defined for the same lake. The following types of observations can be defined for lakes.

* Stage
* Lake volume
* Precipitation
* Evaporation
* Runoff
* Groundwater inflow
* Groundwater outflow
* Surface water inflow
* Surface water outflow
* Withdrawals
* Lake inflow
* Total lake conductance
* Change in head in a time step
* Change in lake volume in a time step
* Cumulative change in head
* Cumulative change in lake volume



## GAGE Package with SFR Streams

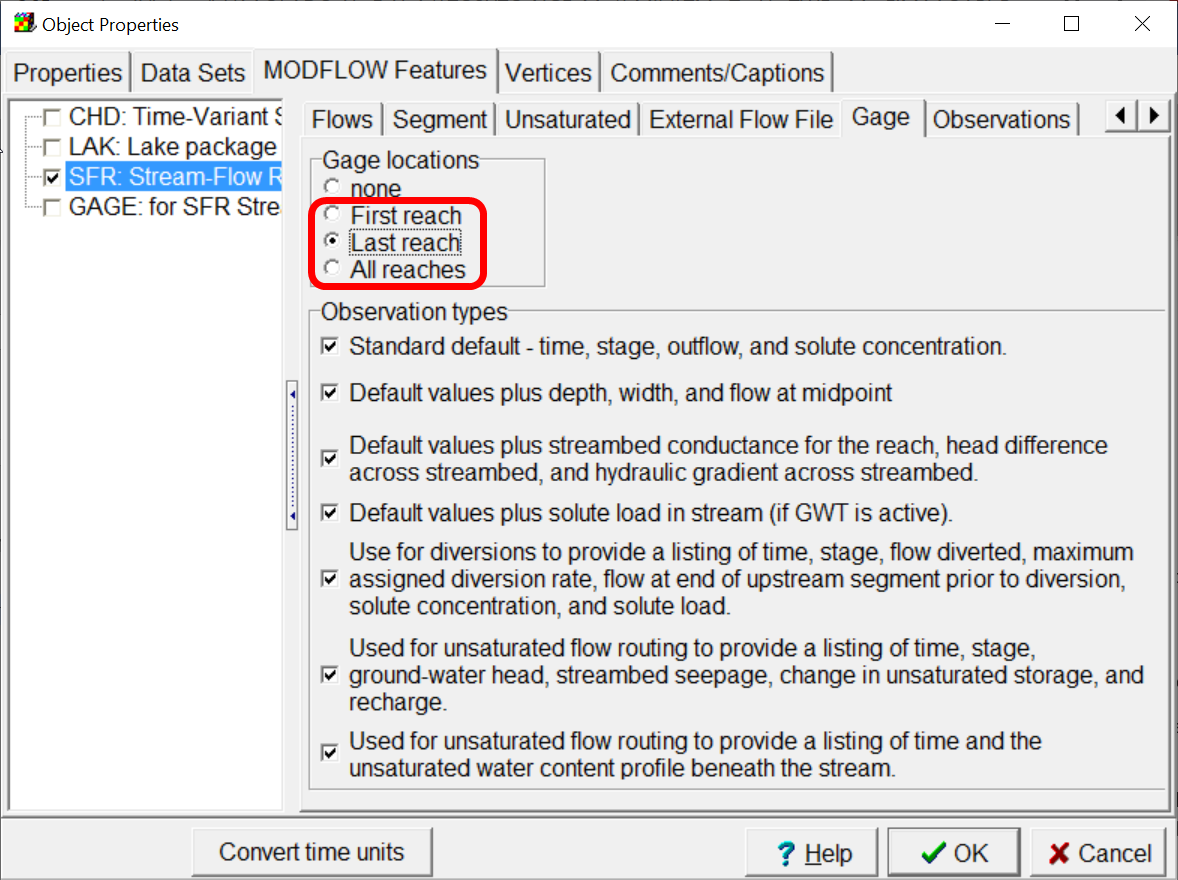
The gage package produces a variety of output for individual stream reaches. When used for calibration purposes, the following observation types can be used.

* Stage
* Stream flow
* Depth
* Width
* Midpoint flow
* Precipitation
* Evapotranspiration
* Runoff
* Conductance
* The difference in head between the stream and its connected groundwater model cell
* The hydraulic gradient across the streambed
* Groundwater flow

Of these, only groundwater flow makes sense when applied to all the reaches in a segment.

When defining an observation for a stream the user can either edit an object that defines a stream or use a point object in the same cell as a stream reach.

To define an observation for calibration with an object that defines a stream segment, the user edits the object in the Object Properties dialog box and selects either First reach, Last reach, or All reaches on the Gage tab of the SFR pane. Doing so will cause the Observations tab to appear.



On the observation tab, the user defines observations and observation comparisons in the same way as before. If All reaches was selected on the Gage tab, only Groundwater flow will be available as an observation type and the computed value of groundwater flow will be the sum of the groundwater flow through all the reaches in the segment. If first reach or last reach is selected, all the observation types will be available but they will only apply to the first or last reach in the segment. To specify a calibration observation for a single reach that is neither the first not last reach in a segment, create a point object in the same cell as the reach of interest and define them on the Observations tab of the Gage pane on the Object Properties dialog box.

