Tony's Notes … updated: 4th December 2023

Note from Neil on 1st December

The files which SAGIS uses are: GIS1.csv and Di .csv. Peter will be testing these with SAGIS.

Tony added: The Di files for 161 include extra columns for the contributions to mean load and mean concentration. They are based on contributions to all the Monte Carlo shots of river water quality. Contributions to percentiles can also be added to these files.

The Ei.CSV files are drafts that give the output from Mode 7, 8 and 9 – the simulation of plans to improve river quality.

Tony added: I sent to Neil on 3rd December, the following folders. They contain the latest updates to:

- SIMCAT 148 … FORTRAN source code
- SIMCAT 157 … FORTRAN source code
- SIMCAT 158 … FORTRAN source code
- SIMCAT 161 … FORTRAN source code

The folder SIM160 contains:

- The FORTRAN exe files from the above four sets of source code
- Folders for old versions of the exe files for 148 and 157
- The interface exe – SIM160.exe
- The interface source code for SIM160.exe is in folder WARNBREW. The starter file for using Visual Studio to update SIN160.exe is SIMCAT160.sin.

The FORTRAN code for SIMCAT 161 has 81,738 lines. Though 10,068 of these are comments and about 12,000 are blank lines – spaces between section of code.

Neil's note included:

We really need the 148 and 157 exes only for checking out previous AMP rounds.

We have not used 158, so your latest version would be good to have. Maybe any revisions beyond what you send me could be called 158a etc.

I will send the SIMCAT executables to Peter for SAGIS testing. I will send the Executable system and source code to Pau (Atkins) for installation in the GIT Hub.

We can update later as the codes become revised. I suggest you call the updates 162. What you send me now will be frozen as 161. (We won't be using 161 until after testing – when it will probably be 162. But we need 161 now to see how to store it in the GIT Hub. We can discuss this on Thursday's online meeting.)

Our aim is to have a revised tested version – version 162 – by the end of financial year.

In the long run we should only have to maintain one version with source code, and executables for the older ones archived on the GIT Hub.

Update of Tony's earlier notes:

My SIMCAT interface screen contains:

- Access to versions 161 and 158 (working on the software has led me to prefer labels 161 to 16.1)
- The interface also has access to updates of 157 and 148 that have evolved as a result of work on 158 and 161. This provides more comments in the software code, and removes any minor errors detected. It looks as though you don't need these updates.
- The interface also has a tap-button access to the original versions of 157 and 148 via the old SIMCAT interface. This is so that users can produce and check results from old sets of data.
- 161 uses a read/write system instead of storing data for every reach that will be mixed with another reach at a downstream confluence (or enter a lake). This mean that SIMCAT 161 can run models of 5000 reaches and 30,000 features.
- 161 can also use the contribution of 3000 discharge to each and every one of 5000 Monte Carlo shots of river water quality for each determinand. This provides accurate calculations for apportionment at all points in the modelled river. (We may wish to apply this accurate type of breakdown to individual contributions of bits of diffuse pollution – we already have it for the running total contributions from the different types of diffuse pollution).
- These results for apportionment may be useful to SAGIS.
- 158 provides the method of storing data as arrays. But this has to be limited to 20,000 features and 1700 discharges in order to deal with the new method of apportionment. The output from 158 and 161 are identical except for occasional 1 in 10,000 differences, except where 161 uses the contributions to all shots of river water quality from all upstream discharges.

- 161 (and 158) also includes my draft attempt to deal with fish farms. This may need checking by users familiar with the type data obtained from fish farms. And it has not yet been decided whether the contributions of individual fish farms are to be included in the calculations of apportionment. The total contributions from all upstream fish farms is already included.
- The SIMCAT interface includes buttons to provide on-screen views of all the output files. For a set of data with seven determinands there are 119 of these.
- They include three output files referred to as 004, 005 and 007. These files are helpful to people who are changing the software code. It is a simple matter to write reports to these files when tracking down the cause of glitches.
- There is a button that provides access to the classic Chris Page graphs.
- There is also a button that provide a way of plotting a different graph (ones not as good as those from Chris Page). This could be set up to use other versions that use an EXE file for a graph plotter.
- There is also a button that writes reports in WORD. We could add other reports.
- We could also get SIMCAT to producing a data file for every discharge. Data files that can be used as input to RQP for further calculations for that discharge.
- Software developments are much helped by apps such as EXAMDIFF. Such apps are needed to compare every line and character of source code, and the contents of the output files, for the current and a planned new version of SIMCAT. I have notes that illustrate what is done.
- Any unwanted buttons on the interface can be hidden. Users may prefer a screen with fewer buttons than those needed by people changing the source code. Both could be provided.

Tony Warn
4th December, 2023