Summary

AMBER is a compartment modelling software tool developed by Quintessa Ltd.

This is the Release Note for the AMBER 6.5 software. AMBER 6.5 is a flexible software tool that allows the user to build their own dynamic compartment models to represent the migration and fate of contaminants in a system.

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1 About AMBER

AMBER is a flexible software tool that allows the user to build their own dynamic compartment models to represent the migration and fate of contaminants in a system, for example in the surface and sub-surface environment. Contaminants in solid, liquid and gaseous phases can be considered. AMBER gives the user the flexibility to define:

▲ any number of compartments;
▲ any number of contaminants and associated rates of degradation/decay;
▲ any number of transfers between compartments and the uptake of contaminants by humans and other biota;
▲ non-linear transfer processes (e.g. solubility-limited leaching); and
▲ deterministic, probabilistic, and complex time-varying parameter values.

This flexibility means that the user can implement models specific to their context and tailor generic models to their specific needs.

Key features incorporated into AMBER include:

▲ powerful, user friendly graphical interface;
▲ spatial awareness and 3D visualisation;
▲ fast and accurate Laplace transform and numerical time-step solvers;
▲ time-varying source terms and transfer processes;
▲ unit awareness;
▲ Monte Carlo and Latin Hypercube Sampling options;
▲ built-in graphing of results and Excel export capabilities; and
▲ tailoring of results format.

The primary user documentation for AMBER 6.5 consists of two volumes: the ‘User Guide’ manual and the ‘Reference Manual’. The User Guide introduces AMBER through a series of tutorial exercises and also contains a knowledge base of studies involving AMBER together with guidance on compartment modelling. The Reference Manual provides detailed information on all of the capabilities and functions included in AMBER.
2 Developments included in AMBER 6.5

The main new features included in AMBER 6.5 are described in the sub-sections below, including a summary of minor developments and bug fixes.

2.1 Spatial modelling enhancements

2.1.1 Information overlay

It is possible to choose whether the time of the simulation, and the name of the parameter being rendered, are shown in the 3D view. By right-clicking in the main panel of the 3D View and selecting Rendering results options, a pop-up window appears in which you can toggle these two options on or off (see Show time and Show title in Figure 1).

Figure 1. New 3D display options

2.1.2 Video play through and export of spatially rendered results

AMBER 6.5 introduces the ability to play through, and export, a video of results rendered in AMBER's 3D View. When in the 3D view mode of the spatial model, the video playback and export functionality are accessed via a pair of buttons located with Rendering Results (see Figure 2). It is possible to modify the frame interval of the video via the rendering results options (see Figure 1).
When exporting a video, after the video is generated (see Figure 3), a pop-up window enables the user to select whether to export the video as an animated gif or as a series of images (.png, .bmp, .jpg or .gif), one for each result time of the model (see Figure 4). The user is able to specify the location where those files will be saved. For the animated gif option, the user specifies the file name. For the series of images, the user can specify the name for that series of files, e.g. using "Video_Images.png" as shown in Figure 5. A series of image files (.png, .bmp, .jpg or .gif) are then saved in that location with "Video_Images" as the start of the file name, with ascending numbers for each of the result times in the model (see Figure 6).
Figure 3. Video generation display

Figure 4. Video export options
2.2 Other Developments and Bug Fixes in AMBER 6.5

In addition to the video play through and export described above, AMBER 6.5 includes a series of changes in response to user feedback. Some of these are developments to support the usability of AMBER, and others are issues that have been resolved.

2.2.1 Clarity of parameter import in AMBER GUI

When using import parameters, the .aaf import files can contain a high-level file description and also descriptions associated with the individual parameters (see Figure 7). Such descriptions can be multiline, but must be delimited using quotes (“ “), and cannot contain any quotes in the description itself. However, in previous versions of AMBER, neither of these descriptions as given in the .aaf import file were visible in the GUI.
In AMBER 6.5, both the high-level file description, and the description of the selected import parameter as given in the .aaf file are now displayed when you create the import parameter (see Figure 8). Further, the user is able to add another description to the import parameters at the time of their creation, or by editing the parameter at a later stage. The user description is shown in the Left Panel when the parameter is selected (see Figure 9).

Figure 7. Example import parameter file

Figure 8. New import parameter dialog
2.2.2 Autofit column widths for *Show Values*

When viewing a parameter that has single or double multiplicity as *Show Values*, the values are displayed in a table in the Main Panel. Where those values had many significant figures, the exponent was sometimes hidden with the default column width of that display.

In AMBER 6.5, the column widths in *Show Values* will now automatically size the columns to the best fitting width of the content when that content is wider than the default column width. Values with up to 10 significant figures, and two digits after the E in scientific notation, will now be clearly displayed.

2.2.3 Keyboard shortcuts within the expression editor

The keyboard shortcuts "Ctrl+C" and "Ctrl+V" would not work to copy and paste text when used within the parameter expression editor.

In AMBER 6.5 these keyboard shortcuts now copy and paste text as expected within the parameter expression editor. In addition, other standard keyboard shortcuts, such as "Ctrl+Z" for undo last action, have also been enabled for text editing here.

2.3 Other changes in AMBER 6.5

Below are some of the other developments and bug fixes included in AMBER 6.5.

▲ Information, warnings and error messages associated with calculations carried out in batch mode are now shown in both the .amber and .amberlog files.
The colours used to display values in parameter grids with single or double multiplicity have been toned down, making default values more legible (see Figure 10).

Some case files created with older versions of AMBER contain the legacy option "warn on units errors". In AMBER 6.5, users will receive a warning message if they open such a case file (see Figure 11). Additionally, while this functionality is considered to be a legacy feature, in previous versions of AMBER units errors being treated as warnings would not be reported by check parameters. In AMBER 6.5 they will now correctly appear as warnings.

Removed unimplemented Result time library buttons.

Fixed incorrect result time rendering in 3D view associated with snapshot times or same initial result time as start time.

Fixed issue whereby spatial model points could be created outside of the model bounds.

Fixed issue with integral derived parameters causing application errors when used with constant parameters or spatial parameters in child expressions.

Figure 10. Comparison of the new colours in the parameter grids with the previous colours
Figure 11. Warning message regarding use of legacy "warn on units errors"
3 Issues of relevance to users

Two potential calculation issues have been identified in AMBER, and guidance has been issued to users on how to avoid any potential calculation errors while AMBER developers investigate further:

▲ Guidance regarding the use of sum, largest and smallestPositive functions in expressions (see Section 3.1).

▲ Guidance regarding the use of user units for amounts when using availability schemes (see Section 3.2).

3.1 Use of sum, largest and smallestPositive functions

The sum function finds the sum across the components of a parameter, and can act over all or just a single dimension of the parameter. User feedback has highlighted some unexpected behaviour of this function when used in expressions for parameters with multiplicity, whereby if sum was used in conjunction with binary operators (e.g. +, -, etc.) to evaluate a specific instance of the parameter (rather than the default value) it sometimes evaluates to zero. This issue has been found to affect other contraction nodes (functions that reduce the dimensions of the output as compared to the input), i.e. largest and smallestPositive. This issue is under investigation by AMBER developers. We are therefore issuing the following guidance.

Avoid using the sum, largest and smallestPositive functions in combination with binary operators in expressions for parameters that have multiplicity. Instead create a separate intermediary parameter which contains the sum (or largest or smallestPositive) function only and call upon that intermediary parameter in the original expression.

For example, consider ParamA = ParamB + sum(ParamC*ParamD). Users should avoid writing ParamA in that manner, instead breaking it down to have intermediary parameters as follows:

```
SumOverParam = ParamC*ParamD
SumParam = sum(SumOverParam)
ParamA = ParamB + SumParam
```

3.2 Use of user units with Availability Schemes

Availability schemes in AMBER allow solubility limitation and sorption to be modelled. User feedback has highlighted some incorrect behaviour with availability schemes when using user units (grams, kilograms or Becquerels) for amounts. Specifically, under the following set of circumstances the availability limit will be incorrectly applied:

▲ there are no decays at all in the case file, and

▲ the units for Amount are grams, kilograms or Becquerels, and

▲ an availability limit is given in moles.

In this case the availability limit will be applied with in the wrong units. This will occur for all four availability schemes: Limit, Unavailable Limit, Langmuir, Unavailable Langmuir.
This issue is under investigation by AMBER developers. We are therefore issuing the following guidance. If you have a case with no decays ensure that the units of amount and availability scheme are the same, for example moles and moles, or grams and grams.

If you have any queries about these issues, please contact the AMBER support team (amber@quintessa.org).
4 Videos of AMBER tutorials

Following user requests, we are producing videos of the tutorials that can be found in the AMBER 6.5 User Guide. Videos for the first four tutorials have been published on Quintessa Limited’s YouTube page [https://www.youtube.com/channel/UCzyaK7z5HABWNEDSlAvHmug].
5 Feedback

AMBER is developed in response to user feedback; therefore the AMBER support team encourages users to provide any feedback about the software, especially if you identify a new feature that would enable AMBER to better address your modelling needs, and/or if you have a suggestion to enhance existing AMBER features.

The spatial awareness and 3D visualisation capabilities included in AMBER 6.5 represent key functions that are unique in this calibre of contaminant transport and risk assessment codes. The capabilities provide a basis for further enhancement, we therefore particularly welcome feedback and ideas for how to extend and further enhance these aspects of the software.

The AMBER support team is here to help to address any questions that you have about the use of the software and would be interested to hear if you have any questions. In addition, support agreements entitle existing users to help from AMBER experts if they encounter any problems with developing cases.

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