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Prepared for: Radioactive Waste Management Limited

Your Reference: RWM007409

Our Reference: AMEC/204651/002, Issue 2

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Bibliography

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Abstract

This user guide is provided for a modelling tool (SMOOG) for assessing potential gas generation during the long-term management of the UK's radioactive waste. The original version of the tool addressed gas generation for intermediate-level (ILW) and certain low-level (LLW) waste in vented packages. The present version (version 7.0) also provides capabilities to assess post-closure gas generation from unvented spent fuel (SF) and high-level waste (HLW) packages, and to assess loss of waste package integrity. The modelling tool is intended to address gas generation from these wastes during their transport and underground storage and after their possible eventual isolation in a closed geological disposal facility (GDF). The tool is intended to be applied in a consistent fashion across these phases in the life of the wastes. To maintain this consistency, the model focuses on gas generation on a waste package or, equivalently, a waste stream basis. GDF or vault scale gas production is obtained by summing over representative waste streams present. The main gas generating processes represented are corrosion of metals, radiolysis, microbial degradation of organic molecules, and radioactive decay. Production of bulk gases (hydrogen, carbon dioxide and methane), the release of radioactive gases (gaseous species containing $^3$H and $^{14}$C and $^{222}$Rn, $^{81}$Kr, $^{85}$Kr, $^{39}$Ar and $^{42}$Ar) and the evolution of the volume of the wasteform due to corrosion (for assessing waste package integrity) are modelled.
Executive Summary

This user guide is provided for a modelling tool (SMOGG) for assessing potential gas generation during the long-term management of the UK’s radioactive waste. The original version of the program addressed gas generation for intermediate-level (ILW) and certain low-level (LLW) waste in vented packages. The present version (version 7.0) also provides capabilities to assess post-closure gas generation from unvented spent fuel (SF) and high-level waste (HLW) packages, and to assess loss of waste package integrity. The modelling tool is intended to address gas generation from these wastes during their transport and underground storage and after their possible eventual isolation in a closed geological disposal facility (GDF). The original scope of the model had been agreed with Nirex on the basis of earlier work and through discussion, and the tool is intended to be applied in a consistent fashion across the phases indicated in the life of the wastes. Subsequently a number of enhancements have been implemented. This version of the user guide includes revisions to describe the use of these enhancements.

The model specified focuses on gas generation on a waste package or, equivalently, a waste stream basis. This maintains the required consistency of approach for different circumstances (even after closure, containers are expected to retain their integrity for the time during which most gas is generated). GDF or vault scale gas production is obtained by summing over representative sets of characteristic packages that are present. The model represents the following gas generation processes:

a) Corrosion of stainless steel, carbon steel, Zircaloy, uranium, Magnox and aluminium to produce hydrogen;

b) Release of radionuclides $^3$H, $^{14}$C, $^{81}$Kr, $^{85}$Kr, $^{39}$Ar, $^{42}$Ar in gaseous form (i.e. incorporated into gaseous molecules in the case of $^3$H and $^{14}$C) from stainless steel, carbon steel, Zircaloy, uranium, Magnox and aluminium due to corrosion and diffusion;

c) Degradation of cellulose to produce glucose or ISA, and subsequently microbial degradation of glucose or ISA to produce carbon dioxide and methane;

d) Release of $^{14}$C containing gases from microbial degradation of glucose or ISA;

e) Radon production from radioactive decay of $^{226}$Ra and its parents;

f) Production of gas by radiolysis of cementitious materials containing water, cellulose and a number of polymeric materials;

g) Release of $^{14}$C-containing gases by radiolysis of small molecules;

h) Release in gaseous molecules of “trapped” $^3$H and $^{14}$C from graphite;

i) Reaction between carbon dioxide and hydrogen generated by other processes to produce methane.

Corrosion also causes volume expansion of the wasteform. This can lead to loss of wasteform and container integrity due to cracking. The corrosion model is therefore also used to calculate wasteform volume changes for use in the assessment of the times at which wasteform and container integrity are lost.

A separate “driver” tool has also been developed to automate calculations within the main model for a large number of waste streams or scenarios (e.g. with parameter values being random samples from defined distributions). The driver allows large numbers of calculations to be performed without having to set up each calculation manually, which would be impractical. The current version of the driver stores only the calculated times at which wasteform and container integrity are lost, so is only suitable for performing waste package integrity calculations.
To aid the interpretation of the large amount of output data generated by a calculation, functionality to generate plots of any of the results is provided within the main modelling tool. A further stand-alone tool has also been developed that provides the same functionality, but also allows results from different calculations to be plotted together.
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1 Introduction

As part of its aims to provide the UK with safe, environmentally sound, and publicly acceptable options for the management of radioactive materials, Radioactive Waste Management Limited (RWM) (previously the Nuclear Decommissioning Authority Radioactive Waste Management Directorate (NDA RWMD) and United Kingdom Nirex Limited (Nirex)) undertakes assessments of gas generation from packaged wastes in the UK radioactive waste inventory. RWM also assesses the times for which wasteforms and containers retain their integrity. These assessments are carried out for the following purposes:

a) Providing packaging advice to waste producers, including advice on the transport of waste through the public domain;

b) Modelling the operational period of a geological disposal facility (GDF) for intermediate-level waste (ILW) and certain low-level waste (LLW). (In this report, this phase is deemed to include underground “storage” between emplacement in the GDF vaults and final closure. This period, which is also referred to as a care and maintenance period, may be several hundred years if a deferred GDF closure strategy is adopted;)

c) Modelling the post-closure period of such a GDF (that is, gas generation from the wastes following GDF closure). For this phase of the GDF life, there is also the need to consider gas generation from spent fuel (SF) and high-level waste (HLW) that may be emplaced in the GDF, for example, in the context of co-disposal with ILW and LLW.

RWM wishes to ensure that the approaches taken to the treatment of gas generation in the above three areas are consistent, by adopting a standardised approach to the assessment of gas generation across these activities. To meet this aim a modelling tool for assessing gas generation in these three areas has been produced. The original model specification was based on the report [1] commissioned by Nirex to review its current approaches to gas generation in the above areas, and provide advice, as necessary, about where a more co-ordinated approach to the assessment of gas generation might be required and where the approaches adopted might require development. During the year following the initial release of the computational implementation of the model, a need for additional facilities in the model was identified. This included a need to be able to model gas generation from SF and HLW packages as well as from the ILW and LLW packages considered initially.

Wasteforms and containers could lose their integrity because of cracking arising from expansion of the wasteform associated with corrosion. RWM wishes to ensure that a consistent approach to modelling corrosion is used in assessing gas generation and loss of wasteform and container integrity. The requirements of the gas generation model were therefore extended to provide for modelling of waste package integrity.

It is anticipated that assessment of the times at which wasteforms and containers lose their integrity will require performing calculations either for a large number of waste streams, or alternatively for a large range of scenarios for typical waste streams to allow the effect of uncertainties in model parameters to be assessed. A multi-run driver tool has therefore been developed to provide an automated interface to the main modelling tool for performing large numbers of calculations and collating the times of loss of wasteform and container integrity that are output from each of the calculations.

As the amount of output data generated by a calculation is large, it is expected that results will need to be displayed graphically. To aid this, functionality to generate plots of any of the results is provided within the main modelling tool. A further spreadsheet tool has also been developed that

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1 Surface storage of wastes prior to acceptance for disposal in a GDF is here termed “interim storage”.

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provides the same functionality, but also allows results from different calculations to be plotted together.

This revised user guide describes the operation and data requirements of the RWM gas generation model including the newly implemented enhancements. The corresponding computer implementation has been named SMOGG (Simple Model of Gas Generation). A detailed specification of the representation of the processes relevant to gas generation and waste package integrity within the model can be found in the companion report [2]. This document refers to SMOGG Version 7.0. It is anticipated that future enhancements to SMOGG will lead to a reissuing of this document to take account of the changes.

An overview of the components of SMOGG and general installation and set-up instructions are given in Section 2. Operation of the main SMOGG model is described in Section 3. Operation of the SMOGG multi-run driver is described in Section 4. Operation of the separate graph plotting tool is described in Section 5. Finally, Section 6 discusses the verification performed for each of the components of SMOGG.

This report was prepared by AMEC under contract to RWM between July 2014 and July 2015, in association with the implementation of the enhancements included in SMOGG Version 7.0. The report is based upon, and solely refers to, information available at that time. The information contained in this report has been verified under arrangements established by AMEC, which comply with ISO 9001. The views expressed and conclusions reached are those of the authors and do not necessarily represent those of RWM.
2 SMOGG Components and Set-up

2.1 Overview of the Components of SMOGG

The main SMOGG model consists of three components:

- A customised Excel spreadsheet that provides the user interface for input of data, viewing results output and generation of graphs;
- A C++ application that performs the calculations;
- An Excel add-in that contains Visual Basic macros that control the data input, interface with the C++ application and process the output.

The add-in writes input data to temporary files that are subsequently read by the C++ application. The C++ application is launched by the add-in, and results, written to temporary files by the C++ application, are loaded back into the spreadsheet by the add-in. The temporary files are deleted on the successful completion of a calculation. The operation of the main SMOGG model is described in Section 3.

Two further components of SMOGG are:

- A ‘driver’ Excel spreadsheet that provides an automated interface to the main spreadsheet for sequentially performing large numbers of calculations;
- An Excel add-in that contains Visual Basic macros that control the data input to the driver spreadsheet, interface with the main SMOGG spreadsheet and process the output from the main SMOGG spreadsheet.

Use of these components is not required for performing individual calculations (i.e. they can be performed using only the main model). The operation of this multi-run driver spreadsheet is described in Section 4.

The final components of SMOGG are:

- A Excel spreadsheet that provides the user interface to aid in the plotting of graphs of the results of SMOGG calculations;
- An Excel add-in that contains Visual Basic macros that control the extraction of results from the main SMOGG spreadsheet and the plotting of graphs, based on the input selections made in the spreadsheet.

This component is also not required to perform SMOGG calculations, but is provided to assist with post-processing results, if required, once calculations have been completed. The operation of this graphing tool is described in Section 5.

2.2 Computer Environment

SMOGG v7.0 has been developed for use with Excel 2007 and Excel 2010. It has been tested with these versions of Excel running on Windows 7 (both 32 bit and 64 bit). It is recommended that one of these environments is used to operate SMOGG v7.0.

It should be noted that SMOGG v7.0 has not been designed to operate with 64 bit versions of Excel.
2.3 Installation of SMOGG

An installation directory “C:\Program Files\Smogg\v7.0\” should be created manually. The C++ application “SmoggApplication.dll” should be placed in it. Each of the Excel add-ins “SmoggAddIn.xlam”, “SmoggDriverAddIn.xlam” and “SmoggPlotAddIn.xlam” should also be placed in it.

To use the main SMOGG model, the Excel spreadsheet “SmoggSpreadsheet.xlsm”, which provides the main user interface for a SMOGG calculation, can be placed in any directory from which it can access the installation directory by referencing its absolute path. The user may rename copies of this spreadsheet as required. The intermediate temporary files “InputData.txt”, “CumulativeGas.txt”, “GasRates.txt” and “OtherResults.txt” will be written to the directory containing the copy of the spreadsheet from which the calculation is being run.

To use the SMOGG multi-run driver, the spreadsheet “SmoggMultirunDriver.xlsm”, which provides the user interface for sequentially performing large numbers of calculations, can be placed in any directory from which it can access the installation directory by referencing its absolute path. The user may rename copies of this spreadsheet as required. To enable use of the main SMOGG spreadsheet (“SmoggSpreadsheet.xlsm”) by the multi-run driver, the main spreadsheet should be placed in the directory containing the copy of the multi-run driver spreadsheet. The intermediate temporary files “InputData.txt”, “CumulativeGas.txt”, “GasRates.txt” and “OtherResults.txt” will also be written to the directory containing the copy of the SMOGG multi-run driver spreadsheet.

To use the SMOGG graphing tool first requires that calculations have been set up and the results calculated in one or more copies of the main SMOGG spreadsheet, to provide the data for plotting. The Excel spreadsheet “SmoggPlot.xlsm” can then be placed in any directory from which it can access the installation directory by referencing its absolute path and the directories containing the results in the copies of the main SMOGG spreadsheet by referencing their relative paths. The user may rename copies of the graphing spreadsheet as required.
3 Operation of the Model

3.1 Introduction

This section describes the main SMOGG model and its operation. As indicated in subsection 2.1, the main SMOGG model consists of three parts. The first is a user interface consisting of an Excel spreadsheet (SmoggSpreadsheet.xlsm), the second is a pre-compiled C++ program (SmoggApplication.dll) that performs the calculations and the third is an Excel add-in (SmoggAddIn.xlam) containing Visual Basic macros that control the use of the spreadsheet and provide the link to the C++ program. Inventory, run-scenario and calculation parameters are entered into the spreadsheet. The add-in controls the creation and deletion of waste package data sheets, the execution of the C++ program, the final processing and printing of the results and, optionally, the generation of graphs to display the results. The C++ program performs the algebraic and numerical calculations of gas generation rates, cumulative amounts of gas generation, amounts of materials remaining in the packages, and wasteform volume changes.

The calculations of gas generation, material consumption and wasteform volume change can be divided into three time periods. The first is a period of waste storage and GDF operation under aerobic conditions. In this period it is assumed that there is a limited supply of water. The second time period is from GDF closure to GDF resaturation. Water is added at a constant rate due to resaturation. However, if the water is not replenished at a faster rate than the gas generation processes consume it, the rates of the processes are reduced accordingly. The third time period is after GDF resaturation when there is assumed to be an unlimited supply of water. The conditions after closure are initially aerobic but become anaerobic as gas generation processes consume the oxygen in the closed GDF.

The models for gas generation are:

- Corrosion of stainless steel, carbon steel, Zircaloy, uranium, Magnox and aluminium to produce hydrogen;
- Release of radionuclides ($^3$H, $^{14}$C, $^{81}$Kr, $^{85}$Kr, $^{39}$Ar, $^{42}$Ar) in gaseous form (i.e. incorporated into gaseous molecules in the case of $^3$H and $^{14}$C) from stainless steel, carbon steel, Zircaloy, uranium, Magnox and aluminium due to corrosion and diffusion;
- Degradation of cellulose to produce glucose or ISA, and subsequently microbial degradation of glucose or ISA to produce carbon dioxide and methane;
- Release of $^{14}$C containing gases from microbial degradation of glucose or ISA;
- Radon production from radioactive decay of $^{226}$Ra and its parents;
- Production of gas by radiolysis of cementitious materials containing water, cellulose and a number of polymeric materials;
- Release of $^{14}$C-containing gases by radiolysis of small molecules;
- Release in gaseous molecules of “trapped” $^3$H and $^{14}$C from graphite;
- Reaction between carbon dioxide and hydrogen generated by other processes to produce methane.

A schematic view of the gas production processes and their dependencies is given in Appendix A.

Additionally, to model waste package integrity, the corrosion model is extended to include calculations of net volume change due to the consumption of metal and the production of metal oxide / hydroxide. These volume changes are used to calculate wasteform strain. The times at which wasteform and container integrity are lost are then the times at which the strain reaches critical values.
3.2 Structure of the Main Spreadsheet User Interface

3.2.1 Overview

When the main SMOGG spreadsheet is initially opened it contains seven visible worksheets. These worksheets contain cells for entering data (coloured light blue, when required), cells containing calculated data (uncoloured) and buttons that run Excel Visual Basic macros (blue text on grey backgrounds).

Before a calculation can be run with the model there are two stages to complete. Firstly, a number of run parameters are specified on a worksheet for general data. Secondly, a worksheet is completed for each group of waste packages that have the same (i.e. sufficiently similar) inventory and conditions. As noted above, the cells into which data should be entered on these worksheets are coloured light blue. However, this colouring is controlled by conditional formatting, so that only data that are required to complete the dataset given the data already entered are indicated by the colouring. This means that only a small number of cells are coloured initially (as, for example, no corrosion parameters are required if there is no metal inventory), but as certain data (typically inventory data) are entered additional cells will become coloured, indicating additional data that are required. When each data value is entered simple validation is carried out to check that the value is appropriate (e.g. inventory values must be non-negative), and where relevant that it is consistent with other related values that have been entered.

The next stage is the calculation. This is controlled by an Excel Visual Basic macro. The calculation stage can be broken down into three steps:

- First, the macro causes the data entered in the worksheets to be written to a file (InputData.txt);
- Secondly, it launches the program (SmoggApplication.dll) that reads the data, performs the calculations and writes the results for each waste package to three files (CumulativeGas.txt, GasRates.txt and OtherResults.txt);
- Finally, it reads the results into the spreadsheet, displays the package results and the totals of all the package results on separate worksheets and restores the plots of results on any graphs that have been set up previously.

After the macro is run, the data and results worksheets and the results on any graph worksheets in the spreadsheet are protected. This preserves the relationship between the data entered into the worksheets and the results. If additional package worksheets or changes to the data are required, then a macro to unprotect the worksheets must be run. This macro will delete all previous result worksheets and results on graph worksheets. This will also occur on re-running the calculation. Note that when results are deleted the set up of any graphs generated using the graphing facility will be preserved; results will be automatically re-plotted on these graphs once they have been recalculated.

Each of the worksheets is described in the rest of subsection 3.2, followed by a description of a typical calculation in subsection 3.3. If invalid or inconsistent data are placed in any of the worksheets then an error message is displayed in a message box. If this occurs during data entry the user must enter permissible or consistent data or no data in the cell being edited before continuing. If this occurs on attempting to run the calculation the calculation is not performed; the user is required to enter permissible or consistent data before the calculation will run.
3.2.2 Description of the General Data Worksheet

The worksheet “General Data” contains input data applicable to the calculation as a whole. A screen-shot of a typical “General Data” worksheet is given in Figure 1.

Cells “B4” and “B6” allow the user to add a unique name to the workbook and a description of the calculation. These cells do not affect the calculation and are not propagated into the results.

A macro calculates the number of package worksheets (see below) included in the calculation and writes this to Cell “B8”. Package worksheets are added by the user but can be optionally excluded from the calculation. Cell “B8” should not be edited.

The other two sets of cells on “General Data” specify the time-points for which the calculation outputs results and the choice of units for the non-radioactive gas results. All the times entered should be non-negative.

Cells “B10” and “B11” specify the start and end times for the calculation. The end time must be greater than the start time. Cell “B13” specifies the time of GDF closure. Cells “B14” and “B15” specify the rate of water inflow after closure and the time of GDF resaturation; one of these values must only be specified. The closure time must be less than the resaturation time (if specified). The closure time and resaturation time can be outside the limits of the start and end times. A calculation can therefore be run, for example, entirely before closure, entirely after resaturation or entirely between closure and resaturation. Clearly, to perform a calculation beginning or ending at the time of resaturation, this time must be specified in preference to the water inflow rate. Cells running from “B17” to “B28” and beyond can be used to obtain the results of calculations at additional output times.

Cell “G9” contains a drop-down list to specify whether the results for the non-radioactive gases are output using moles or m$^3$. There is a choice of “mole” or “m$^3$”. If “m$^3$” is chosen, cells “G13” and “G14” appear for the user to enter the temperature and pressure needed in order to convert output from the gas generation calculation from moles of gas to m$^3$ of gas. Default values of 273.15 K and 1.0x$10^5$ Pa (one atmosphere) appear in cell “G13” and cell “G14” respectively. The user can overwrite these default values. In cell “E13” the user can also choose the units in which to specify the temperature (Kelvin or degrees Celsius) by selecting from a list.

On worksheet “General Data” there are seven buttons that launch macros. At cell “A1” there are four buttons to alter the package data worksheets:

- Button “New sheet” makes a copy of default data worksheet “DefaultPackageData” and prompts the user to name the new data worksheet with a unique name. All package data worksheets start with the prefix “Data-” and the user need only fill in the remaining part of the name. A default name “Package#” is supplied to add to the prefix, where # is the lowest number that makes the data worksheet unique. It is intended that the worksheet “DefaultPackageData” can be used to set up default rate data so that when used as a basis for constructing a new package data worksheet it saves having to enter data that are expected to be the same each time. The user is required to enter new inventory data and can also edit the rate data if appropriate (or if not set up on “DefaultPackageData”);
- Button “Copy sheet” makes a copy of an existing data worksheet. The user is prompted for the name of an existing data worksheet and the name to assign to the copy. The prefix “Data-” is assumed and the user need only fill in the remaining part of the name. A default name

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2 Screenshots of parts of SMOGG Excel sheets are provided in this document to help users to identify those parts of the worksheets to which reference is being made. These are not, however, meant to replace direct reference to the main SMOGG Excel workbook itself, which will provide a more readable and complete identification of the features being described.
“Package#” is supplied to add to the prefix for the copy, where # is the lowest number that makes the data worksheet unique. The copy can be edited with new inventory and rate data;

- Button “Rename sheet” renames existing data worksheets. The user is prompted for the name of an existing data worksheet and a new unique name (the prefix “Data-” is assumed and the user need only fill in the remaining part of the name). Any selected results on graph worksheets that refer to the waste stream corresponding to the renamed data worksheet are also updated to reflect the new name;

- Button “Delete sheet” deletes a data worksheet. The user is prompted for an existing data worksheet, which is deleted permanently from the spreadsheet (the prefix “Data-” is assumed and the user need only fill in the remaining part of the name). Any selected results on graph worksheets that refer to the waste stream corresponding to the deleted data worksheet are also deleted.

At cells “C1” to “D1” is one button labelled “Unprotect data and results for editing”. After a calculation has been performed and the results have been generated the worksheets are protected. This is to preserve consistency between results and data. If the user wishes to alter the data in the worksheets this button must be used to remove the previous results and unprotect the worksheets.

At cell “F1” there is one button labelled “Calculate” to perform the calculation based on the data worksheets. This button causes the data entered in the data worksheets to be written to a file “InputData.txt”, the C++ program “SmoggApplication.dll” to be launched, and, on exit from the program, the results to be read back into the results worksheets (and copied to any graph worksheets as appropriate). The program reads the data from “InputData.txt”, performs the calculations and writes the results for each waste package to three files, “CumulativeGas.txt”, “GasRates.txt” and “OtherResults.txt”, from which the results are read back into the spreadsheet.

Pressing “Calculate” will remove any previous results from the spreadsheet. The package results that are read in and the totals are displayed on separate worksheets. The results worksheets have the prefix “CumulativeGas-” for cumulative amounts of gas generated, the prefix “GasRates-” for gas generation rates and the prefix “OtherResults-” for non-gas results such as amounts of materials remaining in the packages and volume change of waste materials. After the results have been generated, the data and results worksheets and the results on any graph worksheets in the spreadsheet are protected. This preserves the relationship between the data entered into the worksheets and the results of the calculation.

At cell “H1” is one button labelled “New blank graph sheet”, which generates a worksheet containing a template graph and a table in which any of the results generated by the calculation can be selected for plotting on the graph. Pressing the button prompts the user to name the new graph worksheet with a unique name. All graph worksheets start with the prefix “GraphSheet-” and the user need only fill in the remaining part of the name. Further information on the use of this worksheet is provided in subsection 3.2.7.

### 3.2.3 Description of the Constants Worksheet

The worksheet “Constants” contains fixed input data that are used for all calculations. It is not intended that these data are edited by the user, but they are displayed on this worksheet so that all the parameter values used in the calculations are provided to the user.

The worksheet is divided into several sections. The first section is called “General constants” and contains a number of constants used in a number of places throughout the calculations. The constants used to convert between different units, either where there are alternative units available for some input parameters, or where the units used differ between the input data and the calculations or between the calculations and the output results required, are specified in this section.
The “Metal properties” section defines the molar mass of each of the metals modelled and the molar density of each of the corrosion products that are used in the corrosion reaction calculations.

The “Corrosion reaction stoichiometries” section defines the number of moles of each of the materials involved in the corrosion reactions that are consumed per mole of the metal consumed, as given by the corrosion reactions detailed in [2]. Either water or oxygen is consumed in each reaction as indicated by positive values. The relevant corrosion product and hydrogen are products of the reactions, so the values for these are negative. The data in cells “C26” to “F31” provide the data for the corrosion reactions that occur under aerobic conditions, and the data in cells “G26” to “J31” provide the data for the corrosion reactions that occur under anaerobic conditions.

The “Other material properties” section defines the molar masses of cellulose and glucose / ISA that are used in the organic degradation calculations. It also defines the molar mass and density for water that are used in a number of calculations in the model.

The “Radionuclide decay data” section defines the data used in the radiolysis model. For each radionuclide modelled this includes its decay constant, the α, β and γ energy released by each decay (this also includes contributions from decay of any short-lived daughters that are not explicitly included in the model, i.e. have half-lives of less than 10 days), any daughter radionuclides (that are included in the model) generated by the decay and the fraction of the decays that generate them. The latter data, known as the branching data, define the radioactive decay chains that allow the decay and ingrowth calculations to be performed.

The “Radionuclide decay data for 222Rn generation” section defines the data used in the model for radon generation from radioactive decay. As for the radiolysis model, this requires the calculation of decay and ingrowth of radionuclides, but only for those that are in the decay chain that produces 222Rn. Therefore this section provides decay constants and branching data for the relevant radionuclides. This data is presented separately from the data for radiolysis since, although most of the values are the same, 222Rn is not included in the radiolysis model (because its half-life is less than 10 days) and the data for 226Ra are different due to the inclusion of 222Rn in this case.

3.2.4 Description of the DefaultPackageData Worksheet

The worksheet “DefaultPackageData” is provided to allow default rate data to be set up, so that when used as a basis for constructing a new data worksheet it saves having to enter data that are expected to be the same each time. It is used in conjunction with the button “New sheet”, which appears both on worksheet “General Data” and on existing data worksheets, to provide a partially complete data worksheet for editing by the user, provided that data have first been set up on this worksheet, otherwise it will provide an empty data worksheet for editing. The structure of all data worksheets is consequently the same as the structure of worksheet “DefaultPackageData”. Data worksheets are described below.

3.2.5 Description of the Data-##############3 Worksheets

A data worksheet contains inventory and rate data for a specific type of waste package or waste stream. A screen-shot of a typical data worksheet is given in Figure 2 (parts 1-8). Waste packages that can be treated identically form a waste stream. For each waste stream there is a separate data worksheet. The calculations are performed for a single representative waste package in each waste stream for each emplacement time (emplacement times are discussed below). (An exception to this is that if waste package integrity calculations are included the input is

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3 The string “##############” is used in this document to indicate a string of between 1 and 12 characters chosen by the user to uniquely identify an input data sheet for a package or waste stream within the workbook. The string is subsequently used to form the names of the corresponding output worksheets, “CumulativeGas ##############”, “GasRates-##############” and “OtherResults-##############”.
restricted to allow only one package per waste stream.) The results (gas generation rates, cumulative amounts of gas generated, amounts of materials remaining in the packages and volume changes of waste materials) for each representative waste package are then multiplied by the number of waste packages in the waste stream emplaced at the same time and summed. This forms the output for each data worksheet.

The names of data worksheets are all prefixed by “Data-” and can have between 1 and 12 additional characters or numbers. The data worksheets are created using the buttons “New sheet” or “Copy sheet”. The name entered using the macros that are run from these buttons is copied to cell “B8”. This cell should not be edited. (Note that all Excel worksheets require unique names.)

The buttons “Rename sheet”, “New sheet”, “Copy sheet”, “Delete sheet”, “Unprotect data and results for editing”, “Calculate” and “New blank graph sheet” at cells “A1” to “H1” are duplicates of the buttons appearing on worksheet “General Data” described above.

Cell “B4” allows the user to omit this data worksheet from the calculation. Inclusion requires the value to be set to “no”.

The rest of the data worksheets are divided into several sections. The first section is called “General data” (not to be confused with the “General Data” worksheet) and contains package data relevant to all gas generation processes considered in the gas generation model.

Cell “B9” allows the user to provide a description of the waste packages in the waste stream. This description is not propagated by the calculation into the results worksheets.

Cells “B11” to “B23” contain a number of single data items:

- The total mass of waste (and any other materials) in the package. This must be greater than zero;
- The initial mass of water in the package. This can be zero but must be less than the total mass of waste (since this mass must be included in the value for the total mass of waste);
- The activity of tritium initially in the waste and the rate of diffusion of water into the package before closure. These must be non-negative;
- The time of package grouting. This can be left blank if the package is already grouted at the start time of the calculation. (It is assumed that all packages will be grouted before the GDF is closed.) If a time is set it must be between the start time of the calculation and the time of GDF closure;
- The mass of water added to the package when it is grouted. This can be left blank if the time of package grouting is not set. If a mass is set it must be greater than zero;
- The mass of encapsulation grout (excluding any water) in package. This must be non-negative;
- The mass of water in the backfill at closure. This must be non-negative;
- The available oxygen in the package at closure. This must be greater than zero. Note that a value of zero for the oxygen content is used by the program to identify anaerobic conditions. This means that if a user wishes to run a calculation with an aerobic phase prior to GDF closure but becoming anaerobic “immediately” at closure, this value should be set to a small but non-zero number. The amount of oxygen may be specified in either moles or m³ at STP (i.e. standard temperature and pressure, as defined by the data on the “Constants” worksheet) by selecting the appropriate unit from the list in cell “C19” adjacent to the data input cell;
- The void volume in the package and in the backfill. These should include pore space within the solid materials and any additional spaces not filled by solid materials. When multiplied by the water density (the value of which is specified on the “Constants” worksheet), the void volume in the package must be greater than or equal to the sum of the initial mass of water in the package and the mass of water added to the package when grouted (if any), and the void
volume in the backfill must be greater than or equal to the mass of water in the backfill at closure;

- The fraction of carbon dioxide generated that reacts with cements. This must be between zero and one. The amount of carbon dioxide generated by organic degradation and the amount of $^{14}\text{CO}_2$ generated by each of the processes modelled are reduced by this fraction;

- An indicator of whether carbon dioxide and hydrogen react to form methane. If this reaction is required “yes” should be input, otherwise “no” should be input. $^{14}\text{CO}_2$ is also converted to $^{14}\text{CH}_4$ in proportion to the amount of bulk carbon dioxide converted to methane. The reaction is assumed to be instantaneous on a time step basis. If it occurs, the reaction of carbon dioxide with cement is assumed to occur preferentially to this reaction.

The corrosion of metals (and hence the generation of hydrogen and release of radioactive gases) can depend on temperature. To incorporate temperature dependence, each waste stream can have a profile of temperature against time and each metal can have a profile of a rate-factor against temperature. If any temperature / time pairs are set in the rows starting at cells “C24” and “C25” (and continuing for as many consecutive columns as required), the model will use the rate-factor / temperature pairs, if also set, for each metal in the section “Corrosion rates” (see below). The times for any temperature / time pairs set must be in ascending order. The temperature can be specified in either Kelvin or degrees Celsius by selecting the appropriate unit from the list in cell “B25”.

The assignment of a corrosion rate is made in two steps. Firstly, a temperature is calculated for the time when the corrosion rate is required. If the time lies between the values supplied in the temperature / time profile, linear interpolation is used to deduce a temperature value. If the time lies outside of the range of the profile, the first or last temperature value is used. Secondly, the temperature is used to calculate a rate-factor. If the temperature lies between the values supplied in the rate-factor / temperature profile, linear interpolation is used to deduce a rate-factor value. If the temperature lies outside of the range of the profile, the first or last rate-factor value is used. The corrosion rate at the time required is the product of the input corrosion rate constant and the rate-factor.

The packages in each waste stream can be placed in the GDF at different times. The spreadsheet allows for the total number of waste packages in the waste stream to be divided into subgroups that are placed in the GDF at a discrete number of times before GDF closure. The default is to enter one emplacement time in cell “C26” and one associated number of packages (the total for the waste stream) in cell “C27”. If more pairs of emplacement times and numbers of packages are required, they are entered in the cells to the right of “C26” and “C27” (continuing for as many consecutive columns as required).

The “Unvented container data” section specifies data specific to this type of waste. In particular this section is relevant to containers of HLW or SF, as these will be sealed. For sealed containers it is assumed that no processes leading to gas generation or volume changes of materials can occur within them until they are breached, therefore the timing of container failure is required. To allow for containers becoming breached over a period of time two times are specified, the time of initial container failure and the time of complete container failure in cells “B32” and “B33” respectively. The most important gas generating process for wastes in sealed containers is expected to be corrosion. Therefore, the gas generated by corrosion is scaled from zero at the first time to its full value at the second time. For other processes, the simpler approach of initiating the gas generation at the first time is considered sufficient. Most other waste containers will be vented, so calculations for these wastes require only that cell “B31” is set to “no”.

The next section, “Spent fuel data”, specifies the data required in the case of a Magnox spent fuel waste stream. For other types of waste the only input required is to set cell “B37” to “no”. Magnox spent fuel wastes comprise a uranium rod encased in Magnox. Therefore, some of the Magnox must corrode to expose the uranium before corrosion of the uranium can commence. This is
modelled by requiring a fixed fraction of the Magnox to corrode before uranium corrosion is initiated. This parameter is set in cell “B38”.

The “Physical containment data” section specifies data for calculating the times at which the wasteform and container lose their integrity because of cracking caused by expansion of the wasteform associated with corrosion. These calculations are optional. If the calculations are not required no data need be entered in this section of the data worksheet. If these calculations are required all four data items must be set. The available void volume (that materials produced can fill without straining the wasteform) must be non-negative. The remaining items (the wasteform volume and critical linear strains) must all be greater than zero. In addition, the waste stream must contain only one waste package (i.e. cell “C27” must be set to one and no other data entered on this row).

The next section, “Metal inventory”, is relevant to the corrosion and diffusive radionuclide release models. Data is input in cells “B49” to “G53” and “B54” to “C55”. The corrosion model for each metal has separate contributions for waste in sphere and plate geometries and for container walls as plate. The data required are:

- The metal densities (which are copied into the data worksheet when generated from worksheet “DefaultPackageData” if set up beforehand);
- The masses and initial sphere radii for the sphere components of the metal waste;
- The masses and initial plate thicknesses for the plate components of the metal waste;
- The masses and initial wall thicknesses for the metal container components. The container components are restricted to stainless and carbon steels.

In the section “Corrosion rates”, parameters are entered in order to calculate the corrosion rates for each metal at each time step. For each set of conditions for which a metal has a different corrosion rate, two corrosion rate parameters and two characteristic times are required by the corrosion model. Optionally, temperature dependence can be incorporated into the corrosion rate by multiplicative factors determined from a profile based on user supplied pairs of temperatures and factors. Default corrosion rate data can be copied into the data worksheet when generated from worksheet “DefaultPackageData” if set up beforehand.

The first set of corrosion rate data is for stainless steel. There are separate data required for the four time periods “atmospheric”, “aerobic”, “anaerobic before resaturation” and “anaerobic after resaturation”. In the first of these periods a corrosion rate parameter and characteristic time are supplied in cells “B60” and “C60” for acute corrosion. Acute corrosion corresponds to the rapid initial corrosion that occurs when fresh metal is exposed or when the metal is placed in a corrosive environment from which it has no initial protective layer. In cells “B63” and “C63” a corrosion rate parameter and characteristic time are supplied for chronic corrosion. Chronic corrosion corresponds to the slower long-term corrosion of metal that has accumulated a significant protective layer. The chronic corrosion rate decreases less rapidly as the growth of the protective layer decelerates.

The corrosion rates can also be made temperature dependent. If one or more rate-factor/temperature pairs are entered in cells starting at “E60” and “E61” (and continuing for as many consecutive columns as required in order of ascending temperature), a temperature dependent rate-factor can be calculated and used to multiply the acute corrosion rate. The temperature data can be specified in either Kelvin or degrees Celsius by selecting the appropriate unit from the list in cell “D60” (this unit will apply to all the temperature data associated with stainless steel corrosion). The temperature supplied from the waste stream temperature/time profile is used in the calculation of the rate-factor. If the temperature corresponds to a temperature entered in the profile, the corresponding rate-factor value is used. If the temperature lies between the values supplied in the rate-factor/temperature profile, linear interpolation is used to deduce a rate-factor value. If the temperature lies outside of the range of the profile the first or last rate-factor value is used. Similarly, a rate-factor can be calculated for chronic corrosion by entering one or more rate-
factor / temperature pairs in cells starting at “E63” and “E64” (and continuing for as many consecutive columns as required in order of ascending temperature).

The corrosion parameters can be similarly set for the “aerobic”, “anaerobic before resaturation” and “anaerobic after resaturation” time periods for the stainless steel metal. If required, parameters can also be set for carbon steel, Zircaloy, uranium, Magnox and aluminium. Each metal has corrosion parameters for specific time periods when rates could be substantially different.

Magnox and aluminium have corrosion rates for atmospheric conditions, for before resaturation of the GDF with groundwater (under high pH, aerobic or anaerobic conditions), and for after resaturation (when it is assumed conditions will be anaerobic). Stainless steel, carbon steel and uranium have rates for atmospheric conditions, for high pH, aerobic conditions, for anaerobic conditions before resaturation, and for anaerobic conditions after resaturation. Zircaloy is assumed not to corrode under any aerobic conditions. Zircaloy therefore has rates for anaerobic conditions before resaturation and for anaerobic conditions after resaturation.

The corrosion rates for atmospheric conditions apply to waste metal before packages are grouted and to external surfaces of stainless steel and carbon steel containers until GDF closure. (Internal surfaces of steel containers are assumed to corrode at the same rate as the equivalent steel waste.)

For any metal, the corrosion rate used during any time step during resaturation (under anaerobic conditions) is calculated by linear interpolation between the rate for before resaturation and the rate for after resaturation. The contribution of each rate is determined from the ratio of the amount of water remaining that derived from that present at closure and the amount present due to groundwater inflow. The characteristic times entered for before resaturation are used for after resaturation to retain continuity in the calculation.

In the section “Radionuclides present in metals”, data can be entered to initialise the model to calculate the release of radioactive gases as a result of corrosion and also diffusion of radioactive gases from metals. There is a separate subsection, each having the same format, to enter the data for each metal.

Within a subsection, for each of the radionuclides modelled, an inventory can be specified for the radionuclide in the portion of the metal modelled as spheres. However, a positive inventory can be specified only if the mass of the metal as spheres, set in the section “Metal inventory”, is positive. The radionuclides can also be given non-uniform distributions within the metal by specifying values for two parameters. The parameters that describe the distribution of the radionuclides are called $\alpha$ (which must have values between zero and one) and $\gamma$ (which must have values greater than or equal to zero). These are defined in reference [2]. If radioactive inventories are entered but no $\alpha$ or $\gamma$ parameters are entered, default values of one and zero are assumed, giving a uniform distribution. Data can be specified in the same way for the portion of the metal modelled as plates (provided that a portion of the metal exists as plates). Parameters that describe solid-state diffusion can also be entered for each radionuclide (except $^{14}$C, as it is assumed not to diffuse through any of the metals). If a diffusion parameter is specified, a uniform distribution for that radionuclide must be specified (by setting $\alpha$ and $\gamma$ appropriately). Finally, since $^{14}$C can be released in two forms, as CO$_2$ and as other gases (assumed to be CH$_4$), the fraction (between zero and one) released as CO$_2$ can be specified. By default it is assumed that none of the $^{14}$C is released as CO$_2$ (i.e. the fraction is zero).

The data for gas generation from the degradation of cellulose are entered in two sections. In the section “Cellulose degradation”, a value is entered to specify one of two models for cellulose degradation.

The first model is chosen by selecting “1” from the list in cell “B249”. This model, which has glucose as an intermediate to gas generation, is initialised by entering non-zero values for either or
both of the bulk and soluble cellulose masses in cells “B252” and “C252”. If either of these values is entered, the dissolution and hydrolysis rates in cells “D252” and “E252” must be positive.

The second model is chosen by selecting “2” from the list in cell “B249”. This model, which has ISA as an intermediate to gas generation, is initialised by entering non-zero values for one or more of the amorphous and crystalline reactive and stopped cellulose masses in cells “B255” to “C256”. If any of these values are entered, the hydrolysis and degradation rates must be positive and the mid-chain scission rates must be greater than or equal to zero in cells “D255” to “F256”.

The section “Gas production from glucose / ISA” provides the remainder of the data required to calculate gas generation from the glucose or ISA intermediates produced by the degradation of cellulose.

An initial mass of glucose / ISA in addition to that which will be produced from cellulose degradation can be added by entering a non-zero value in cell “B260”. The cellulose degradation model treats this as a mass of the intermediate corresponding to the model selected in cell “B249”. The rate of gas production from the glucose or ISA is dependent on the pH and the presence of oxygen, nitrate and sulphate. The pH is determined by whether the package has been grouted, which is specified by the time of package grouting in the “General data” section. A pH appropriate for atmospheric conditions is assumed before grouting and a high pH after grouting. Since it is assumed that all packages will be grouted before GDF closure, it is assumed that the pH will be high after this time (and in particular for all times when conditions are anaerobic). The mass of oxygen is also specified in the “General data” section. Initial masses of nitrate and / or sulphate can be set by entering positive values in cells “C260” and / or “D260”. If the initial amount of glucose or ISA is non-zero, an initial activity of $^{14}$C in the glucose or ISA can be set by entering a positive value in cell “E260”. This will allow production of carbon dioxide and methane that contain $^{14}$C.

Non-zero values can be entered in cells “B263” to “B267” for the rate constants, under each of the conditions, for processes in the second phase of cellulose degradation during which glucose or ISA degrades to carbon dioxide and methane. If any of these rate constants are zero, the corresponding process is assumed not to occur. For the atmospheric degradation, aerobic degradation, nitrate reduction and sulphate reduction processes, the number of moles of carbon dioxide produced per mole of glucose or ISA must be entered in cells “C263” to “C266”. For the anaerobic degradation process without nitrate or sulphate, the number of moles of carbon dioxide and methane produced per mole of glucose or ISA must be entered in cells “C267” and “D267”. The total number of moles of gas produced per mole of glucose or ISA for each of the processes must be between zero and six.

If there is oxygen available, the glucose or ISA degradation processes will initially be atmospheric or high pH aerobic, for ungrouted or grouted packages respectively. When ungrouted packages are subsequently grouted the conditions will then become high pH aerobic. On consumption of all the oxygen anaerobic degradation will begin. While nitrate remains present in the waste the anaerobic degradation process for the glucose or ISA will be nitrate reduction. Nitrate reduction will continue until all the nitrate is consumed. In the absence of nitrate, while sulphate remains present in the waste the anaerobic degradation process for the glucose or ISA will be sulphate reduction. Sulphate reduction will continue until all the sulphate is consumed. In the absence of both nitrate and sulphate the anaerobic degradation process for the glucose or ISA will be anaerobic degradation without nitrate and sulphate (methanogenesis).

The section “Radiolysis” provides the data for the radiolysis model. The model can perform calculations of gas generation (which is treated as hydrogen) from radiolysis of one or more of the following: cementitious materials containing water (within waste containers and in the associated backfill after GDF closure), cellulose, halogenated plastics, condensation polymers, other non-halogenated plastics, halogenated rubbers, non-halogenated rubbers, organic ion exchange resins and polymer encapsulants. The model also calculates the release of $^{3}$H from water and $^{14}$C as $^{14}$CO$_2$ and as $^{14}$CH$_4$ from small molecules (i.e. from the $^{14}$C-containing glucose or ISA specified...
in the “Gas production from glucose / ISA” section). For radiolysis to occur, radiolytic energy releases from the decay of radionuclides are required. These energy releases can be calculated from a radionuclide inventory given the decay energies of the radionuclides (which are specified on the “Constants” worksheet). The gas generation from a substance by radiolysis depends on the product of the fraction of the radiolytic energy released that is absorbed by the substance and a G-value.

To initialise the radiolysis model for any substance, a positive inventory for one or more of a comprehensive fixed set of 112 radionuclides must be entered in cells “C271” to “C382”. To initialise the radiolysis model for a particular substance, the mass of that substance must be non-zero and at least one of the corresponding G-values must also be non-zero. The masses of water and encapsulation grout are entered in the “General data” section, the masses of cellulose in its various forms are entered in the “Cellulose degradation” section, and the inventory of $^{14}$C in small molecules is entered in the “Gas production from glucose / ISA” section. The masses of other materials for which radiolysis can be modelled are not required in other models so are entered in cells “B385” to “B391”. The G-values are entered in cells “B394” to “D402” and cells “B405” to “G405”. Separate G-values are required for each type of decay ($\alpha$, $\beta$ and $\gamma$) and for each gas produced. The G-values can be specified in either moles per Joule or molecules per 100 eV by selecting the appropriate units from the list in cell “A393”.

In addition, for $\gamma$-radiation, since some of the energy may be absorbed outside the waste containers, the fraction (between zero and one) absorbed within the containers must be entered in cell “B407”. Finally, for the radiolysis of water (within cementitious materials), the consumption of water can be modelled by entering a value greater than or equal to one for the water consumed per unit of hydrogen production in cell “B408” (a value of one converts all the water to hydrogen). Alternatively, a value of zero can be entered to neglect the water consumption, if desired. (The consumption of organic materials are not modelled, as the fractions consumed by radiolysis are not expected to be significant.)

In the section “Radon from radioactive decay”, a model to calculate the radon generated from the radioactive decay of radium and its parents is added to the gas generation calculation by entering the initial inventory of $^{226}$Ra, $^{232}$Th, $^{234}$U, $^{238}$U, $^{239}$Pu, $^{241}$Pu, $^{242}$Am, $^{244}$Cm, $^{246}$Cm and $^{250}$Cf in cells “C413” to “C423”. The hold-up factor (also called emanation coefficient) entered in cell “B425” is the ratio of radon escaping from the waste container to that produced by decay of radium. The hold-up factor should have a value between zero and one. The radon remaining in the waste container is assumed to decay in the container and not contribute to overall active gas generation.

In the section “Radionuclide release from graphite”, the model to calculate active gas release from graphite is initialised by entering an initial inventory for either or both of $^{14}$C and $^3$H in graphite in cells “B429” and “C429”. The model accounts for rapid release of a fraction of each inventory and slower release of a further fraction of each inventory, with any remaining fraction not released. For each inventory added, these fractions must be entered in cells “B430” to “C431”.

The rate of release of each releasable fraction of $^{14}$C and $^3$H is specified by a rate constant. The rate is dependent on the pH and the presence of oxygen. The pH is determined by whether the package has been grouted, which is specified by the time of package grouting in the “General data” section. A pH appropriate for atmospheric conditions is assumed before grouting and a high pH after grouting. Since it is assumed that all packages will be grouted before GDF closure, it is assumed that the pH will be high after this time (and in particular for all times when conditions are anaerobic). The mass of oxygen is also specified in the “General data” section.

For each inventory added, non-zero values for the release rate constants under each of the conditions can be entered in cells “B434” to “D437”. Finally, since $^{14}$C can be released in three forms, as CO$_2$, as CO and as other gases (assumed to be CH$_4$), the fractions (between zero and one) released as CH$_4$ and CO for each set of conditions can be entered in cells “B438” to “D439”. By default it is assumed that all of the $^{14}$C is released as CO$_2$ (i.e. the fractions are all zero).
3.2.6 Description of the GasRates-############, CumulativeGas-############ and OtherResults-############ Worksheets

Pressing the button “Calculate” on worksheet “General Data” or on any “Data-############” worksheet runs a calculation and generates a set of results for each data worksheet on three results worksheets.

Results worksheets named with a prefix “GasRates-” contain gas generation rates for each non-active and active gas from each process (far right), for the total for all processes for each non-active and active gas, and for the sum of the totals of all processes for all non-active gases and for all active gases (far left). Results worksheets named with a prefix “CumulativeGas-” contain cumulative amounts of gas generated for the categories described above. The values of rates and cumulative amounts are output at the calculation start time, the calculation end time, and each time entered by the user in worksheet “General Data” (including the closure time and resaturation time) that lies between these times. These values are also output for any additional times at which packages are added to the GDF (specified in cells to the right of “B26” in each data worksheet). The rates and cumulative amounts from each waste stream are each added and written to worksheets “GasRates-AllPackages” and “CumulativeGas-AllPackages”. A screen-shot of part of a typical “GasRates-############” worksheet is given in Figure 3.

Results worksheets named with a prefix “OtherResults-” contain amounts of materials (e.g. oxygen, water, metals, organic materials, radionuclides) remaining in the waste packages for each source of each material, temperature, volumes of solid corrosion product (oxide / hydroxide) produced for each metal in each geometry, volume change of waste materials due to corrosion of each metal in each geometry and linear strain of the wasteform due to the volume changes. These results are output at the same times as the gas generation rates and cumulative amounts of gas generated. In contrast to the gas generation results, the other results for each waste stream are not added to produce results for all waste streams (in fact this is not appropriate for some of the results). However, for each waste stream, the times of exhaustion of materials in the waste packages are calculated (by extrapolation from the results for the amounts of the materials remaining at the two output times before exhaustion), and, if suitable data has been specified on the data worksheet under the section “Physical containment data”, the times at which wasteform and container integrity are lost due to cracking are calculated (by interpolation of the results for linear strain). These times for each waste stream are written to worksheet “OtherResults-AllPackages”. A screen-shot of part of a typical “OtherResults-############” worksheet is given in Figure 4.

3.2.7 Description of the GraphSheet-############### Worksheets

Pressing the button “New blank graph sheet” on worksheet “General Data” or on any “Data-############” worksheet generates a graph worksheet that provides a simple method for plotting a graph of any of the results on any of the results worksheets. A number of graphs can be plotted by generating further graph worksheets (either by pressing the button “New blank graph sheet” again or by pressing the button “Copy This Graph Sheet” on any existing graph worksheet).

The graph worksheets generated mirror the graph worksheets in the graphing tool, and provide the same functionality, except that only results from within the current spreadsheet can be plotted, so the option to select results from different SMOGG calculations (in cells “B8” to “B27”) is not available (these cells are automatically filled in). (This also means that the additional “Dataset Selection” worksheet that is part of the graphing tool is not mirrored.) The description of these worksheets is given as part of the description of the worksheets in the SMOGG graphing tool in subsection 5.2.3, so is not repeated here.

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4 The string “###############” is used in this document to indicate a string of between 1 and 19 characters chosen by the user to uniquely identify a graph sheet within the workbook.
It is also possible for the user to create additional graphs manually from the data in the worksheets prefixed with “GasRates-”, “CumulativeGas-” and “OtherResults-”.

3.3 Running a Typical Calculation

SMOGG v7.0 has been developed to be used with 32 bit versions of either Excel 2007 or Excel 2010, and has been tested for these versions of Excel running on Windows 7. Therefore one of these environments should be used to run SMOGG v7.0.

The following describes the steps in a typical calculation:

1. In worksheet “General Data”, optionally provide a name and description for the workbook.

2. In worksheet “General Data”, enter start, finish and closure times, and either a water inflow rate after repository closure or a resaturation time. Optionally enter further times at which results are required.

3. In worksheet “General Data”, choose the amount unit (“m³” or “mol”) for the non-active gas results.

4. If there are no existing data worksheets (prefixed by “Data-”), use button “New Sheet” on worksheet “General Data” to obtain a new data worksheet. The user will be prompted for a unique name for the data worksheet. The new data worksheet should be edited to obtain the required inventory and rate values for the waste stream to be modelled. The process can be repeated for further waste streams or Step 5 applied.

5. If there are existing data worksheets (prefixed by “Data-”), use button “Copy Sheet” on worksheet “General Data” to obtain a copy that can be edited to obtain the required inventory and rate values for the waste stream to be modelled. The user will be prompted for the name of the worksheet to be copied and a unique name for the copy. The process can be repeated for further waste streams.

6. Once the set of data worksheets have been compiled, the calculation can be run (note that at this stage data worksheets can be omitted by setting their cell “B4” to “yes”). Press button “Calculate” on worksheet “General Data” or any of the data worksheets.

   If there are pre-existing results worksheets when the “Calculate” button is pressed then these will be deleted. If there are pre-existing graph worksheets when the “Calculate” button is pressed then the results on these will be deleted. The results will be calculated by the C++ application, displayed on results worksheets and copied to any graph worksheets as appropriate.

   Three results worksheets will be generated for each data worksheet, one for the gas generation rates, one for the cumulative amount of gas generated and one for the other results (amounts of materials remaining in packages, temperature, volume change of materials and linear strain of wasteform). For a data worksheet named “Data-<name>” the results worksheets will be called “GasRates-<name>”, “CumulativeGas-<name>” and “OtherResults-<name>”. There are also three special results worksheets: “GasRates-AllPackages” and “CumulativeGas-AllPackages” containing the sum of the individual waste stream gas generation results; and “OtherResults-AllPackages” containing the times of exhaustion of materials and the times at which wasteform and container integrity are lost for each waste stream. Once the “Calculate” macro has finished a message box with text “Calculation completed” will appear. Press “OK” to remove the message box.

7. To generate graphs of the results, the steps are the same as Steps 3 to 5 given in subsection 5.3 for the generation of graphs in the SMOGG graphing tool, except that to obtain a new graph worksheet the button “New blank graph sheet” on worksheet “General Data” or any of the data worksheets must be used, and selection of a dataset should be skipped.

8. The previous seven steps represent a complete modelling cycle. If revisions or additions to the data worksheets are now required a further cycle can be started. Once the “Calculate”
button has been pressed on worksheet “General Data” or any of the data worksheets the data worksheets are protected. To make revisions of the data worksheets the button “Unprotect data and results for editing” must be used. This button will delete all results worksheets (the “GasRates-AllPackages”, “CumulativeGas-AllPackages” and “OtherResults-AllPackages” worksheets will be cleared of data) and all results on any graph worksheets.
4 Operation of the Multi-run Driver

4.1 Introduction

This section describes the SMOGG multi-run driver spreadsheet interface and its operation. As indicated in subsection 2.1, the SMOGG multi-run driver is an Excel spreadsheet (and an associated Excel add-in) in which large numbers of SMOGG calculations can be set up, and then can be run automatically (in a sequential manner) using the main SMOGG model. The main SMOGG model (the Excel spreadsheet and the C++ executable) is used by the driver in the same way as for individual calculations (as described in Section 3), except that the driver automates the input of data and the running of calculations that otherwise would be performed by the user.

4.2 Structure of the Driver Spreadsheet User Interface

4.2.1 Overview

The SMOGG multi-run driver spreadsheet contains five worksheets. Just as for the main SMOGG spreadsheet, these worksheets contain cells for entering data (coloured light blue), cells containing calculated data (uncoloured) and buttons that run Excel Visual Basic macros (blue text on grey backgrounds).

To enable the driver to provide the data to the main SMOGG spreadsheet, two of the worksheets mirror worksheets in the main SMOGG spreadsheet. The remaining three worksheets are then used to specify additional data, to provide controls for using the driver and to display results extracted from the main SMOGG spreadsheet.

Before a set of calculations can be run with the driver, data must be input. There are three data input steps to complete. Firstly, a number of general run parameters that are the same for all the calculations are specified on a worksheet. Secondly, parameters defining the waste package inventory and conditions that are the same for all the calculations are specified on another worksheet. Finally, a worksheet is completed defining all the general and package parameters that vary between calculations and so were not specified on the previous two worksheets.

Once data have been input, calculations can be performed using one of a number of Excel Visual Basic macros. The calculations can be broken down into four steps.

- Firstly, the macro determines the range of calculations to be run, either automatically or through user input, depending on the run option selected.
- Secondly, the macro opens the main SMOGG spreadsheet and copies the data entered in the driver worksheets that are the same for all the calculations to the appropriate cells in the data worksheets of the main spreadsheet.
- Thirdly, for each calculation, the macro:
  - copies the data entered in the driver worksheets that vary between calculations to the appropriate cells in the data worksheets of the main spreadsheet,
  - runs the calculation macro associated with the main spreadsheet,
  - copies the results from the main spreadsheet to its results worksheet,
  - saves a copy of the main spreadsheet (if required).
- Finally, the macro closes the main SMOGG spreadsheet.

After a calculation macro is run, the worksheets in the spreadsheet are protected. This preserves the relationship between the data entered into the worksheets and the results. If changes to the
data are required, then one of two macros to unprotect the worksheets must be run. One of these macros will delete all previous results. If the results are not deleted, subsequently editing the unprotected data worksheets will automatically delete results as required to preserve the relationship between the data and the results. Re-running calculations will also delete previous results for the calculations that are re-run.

If invalid or inconsistent data are placed in any of the worksheets then an error message is displayed in a message box. If this occurs during data entry the user must enter permissible or consistent data or no data in the cell being edited before continuing. If the error is detected during the processing of a calculation by the macros the calculations are aborted. If this occurs in the macros associated with the main SMOGG spreadsheet (rather than the macros associated with the driver spreadsheet), the user will also be required to close the main spreadsheet (without saving it) before further calculations can be run.

Each of the worksheets in the SMOGG multi-run driver spreadsheet is described in the rest of subsection 4.2, followed by a description of a typical set of calculations in subsection 4.3.

4.2.2 Description of the Calculation Control Worksheet

The worksheet “Calculation Control” contains a number of buttons that launch macros. The nine buttons at cells between “B11” and “I25” launch macros that run and / or save calculations. After calculations have been performed the data is protected; the two remaining buttons at cells between “C5” and “H7” launch macros to unprotect the data so that it can be further edited.

The first calculation button, “Run All Calculations”, performs the following steps:

- It opens the main SMOGG spreadsheet and initialises the main spreadsheet by:
  - setting up a blank package data worksheet in the main spreadsheet,
  - copying the data from the “General Data” worksheet to the “General Data” worksheet in the main spreadsheet,
  - copying the data from the “Package Data” worksheet to the blank package data worksheet created in the main spreadsheet.
- It then loops over each of the calculations on the “Parameters” worksheet. For each calculation it:
  - copies the data on the corresponding row of the “Parameters” worksheet to the specified cells of the specified data worksheets in the main SMOGG spreadsheet,
  - launches the macro associated with the main spreadsheet that performs the calculation,
  - copies results from the “OtherResults-AllPackages” worksheet of the main spreadsheet to a row in the “Results” worksheet, labelling the row in the “Results” worksheet with the calculation reference on the “Parameters” worksheet.
- Once all calculations have been completed, it closes the main SMOGG spreadsheet.

The calculation button “Run and Save All Calculations” performs the same steps as the “Run All Calculations” button, but in addition also saves a copy of the main SMOGG spreadsheet for each calculation after copying the results. The calculation button “Save All Calculations” also performs the same steps, except that it saves a copy of the main SMOGG spreadsheet and does not copy the results.

The calculation buttons ending “…Single Calculation” perform the same steps as the corresponding “…All Calculations” buttons, but for only one of the calculations specified on the “Parameters” worksheet. The user is prompted to select the calculation to be performed by specifying the calculation reference. Similarly, the calculation buttons ending “…Range of Calculations” perform the steps for every calculation between two calculations on the “Parameters” worksheet. The user
is prompted to select the first and last calculations defining the range by specifying the calculation references.

After calculations have been performed and results have been copied into the “Results” worksheet, the data and results worksheets are protected. This is to preserve consistency between the data and the results. Subsequently, if the user wishes to alter the data, the data must first be unprotected. There are two options for unprotecting data:

- The button labelled “Unprotect Data for Editing” unprotects the data but the results are retained initially. Changes to the data are monitored and individual results are deleted as necessary to maintain consistency between the data and results. This option is useful if data on the “Parameters” worksheet for only one or a few calculations is to be edited, as the results for only these calculations will be deleted, and therefore only these calculations (rather than all the calculations) will need to be re-run to obtain a complete set of results.
- The button labelled “Unprotect Data and Remove Results” unprotects the data and removes all the results immediately.

### 4.2.3 Description of the General Data Worksheet

The worksheet “General Data” contains general input data that are the same for all the calculations (any general data that varies between calculations should be entered in the “Parameters” worksheet described below). This worksheet mirrors the “General Data” worksheet of the main SMOGG spreadsheet. The description of this worksheet is therefore given as part of the description of the worksheets in the main SMOGG spreadsheet in subsection 3.2.2.

### 4.2.4 Description of the Package Data Worksheet

The worksheet “Package Data” contains data defining the waste package inventory and conditions that are the same for all the calculations (any package data that vary between calculations should be entered in the “Parameters” worksheet described below). This worksheet mirrors the “Data-#####” worksheets of the main SMOGG spreadsheet. The description of this worksheet is therefore given as part of the description of the worksheets in the main SMOGG spreadsheet in subsection 3.2.5.

### 4.2.5 Description of the Parameters Worksheet

The worksheet “Parameters” contains both general input and package data that vary between calculations. The data specified in this worksheet must be data that would be specified on either the “General Data” worksheet or a “Data-#####” worksheet in the main SMOGG spreadsheet if the calculation was performed as a single calculation. These data, in combination with the data specified on the “General Data” and “Package Data” worksheets, must form a complete and valid SMOGG dataset. Data items that are specified on the “Parameters” worksheet should not be given values on the “General Data” or “Package Data” worksheet, as these latter values would be overwritten with the values specified on the “Parameters” worksheet for all calculations.

There are three blocks of data in the “Parameters” worksheet: the parameter references, the calculation references, and the parameter values. A screen-shot of part of a typical “Parameters” worksheet is given in Figure 5.

Cells “C2” to “C4” and cells to the right of these contain the references for each parameter that varies between calculations. The cells in row 2 are optional, and allow the user to label each parameter. The cells in rows 3 and 4 define the worksheet and cell respectively that each parameter would be entered in if it did not vary between calculations. The worksheet should therefore be specified as either “General Data” or “Package Data”. The cell should be referenced in the standard Excel format of column letter(s) followed by row number (e.g. “B12”). These cells
are used by the macros to determine the number of variable parameters in the calculations, so no blank columns should be left between parameters.

The data on each row from row 7 down refers to a particular calculation. Cell “A7” and cells below this contain the reference (e.g. a waste stream name, variant name or realisation number) for each calculation. These cells are used by the macros to determine the number of calculations in the set, so no blank rows should be left between calculations. In principle, data can be specified for more than a million calculations (given the size of a worksheet in Excel). However, to avoid the size of the spreadsheet file becoming too large it is recommended that a somewhat smaller number of calculations are kept in one copy of the spreadsheet. Further copies can easily be made to contain further calculations as necessary.

Cell “C7” and cells to the right and/or below this contain the values for each parameter for each calculation. The values should be entered so that they appear in the appropriate row for the calculation, and in the column in which the reference for that parameter is defined. Each value entered should be valid data for the cell referenced, as if it had been entered in that cell (as described for the “General Data” and “Data-Number” worksheets in subsection 3.2).

### 4.2.6 Description of the Results Worksheet

Once a set of calculations has been run, the worksheet “Results” contains the times at which wasteform and container integrity are lost due to cracking (if determined) for each calculation that has been performed. These results for each calculation are copied from the worksheet “OtherResults-AllPackages” of the main SMOGG spreadsheet. The format of the worksheet is straightforward and virtually the same as the part of the worksheet in the main SMOGG spreadsheet from which the results are copied, except that the row labels in the first column refer to the calculations rather than waste packages / streams.

### 4.3 Running a Typical Suite of Calculations

The following describes the stages in performing a typical suite of calculations with the SMOGG multi-run driver spreadsheet:

1. In worksheet “General Data”, optionally provide a description for the suite of calculations. (Note that the name will be supplied automatically for each calculation from the data entered on the “Parameters” worksheet.)

2. In worksheet “General Data”, enter start, finish and closure times, and either a water inflow rate after repository closure or a resaturation time if these are fixed for the suite of calculations. Enter any further times at which results are required for all calculations.

3. In worksheet “Package Data”, enter data for the inventory and rate values that are fixed for the suite of calculations.

4. In worksheet “Parameters”, all data required for a SMOGG calculation that haven’t already been defined on the “General Data” or “Package Data” worksheets must be entered. First, the reference to the worksheet (either “General Data” or “Package Data”) and the cell on the worksheet into which the data will be inserted to complete each dataset must be entered as a column heading for each data item. Optionally, a label for each data item can also be entered as a further part of the column heading. Next, a reference for each calculation (e.g. a waste stream name, variant name or realisation number) must be entered as a row heading. The table of data values for all the data items and calculations must then be filled in, aligned with the corresponding column and row headings.

5. Once the set of data worksheets has been compiled, the calculations can be run. There are nine options for running / saving calculations, accessed by pressing buttons on worksheet “Calculation Control”. The nine options allow either all, one or a subset (range) of the calculations defined on the “Parameters” worksheet to be run, and optionally allow the copy of
the main SMOGG spreadsheet, which is constructed to perform each calculation, to be saved (for completeness, the copies of the main SMOGG spreadsheet can also be saved without actually running the calculations).

If the option to run / save one calculation is selected, a window will appear in which the reference for the calculation (as entered on the “Parameters” worksheet) to be run should be specified. Similarly, for a range of calculations successive windows will appear in which the first and last calculations in the range should be specified. All calculations on rows of the “Parameters” worksheet between the rows of the first and last calculations will be run / saved.

If there are pre-existing results on worksheet “Results” for the calculations specified, then these will be deleted when the calculations are run. Pre-existing results for calculations not being run will not be deleted. For each calculation, the main SMOGG spreadsheet will be populated with the appropriate data and the calculation run (and a copy of the main SMOGG spreadsheet saved if required). After each calculation is run, the times at which wasteform and container integrity are lost will be copied back to the “Results” worksheet of the driver spreadsheet and labelled with the calculation reference. When all calculations have been completed the main SMOGG spreadsheet will be closed, and a message box with text “Calculations completed successfully” will appear. Press “OK” to remove the message box.

Since it is likely to take a considerable time to perform large numbers of calculations, the progress of the calculations is displayed in Excel’s status bar (at the bottom of the Excel window). The display indicates the reference of the current calculation being processed, the count of calculations processed so far (including the current calculation) and the total number to be performed.

6. The previous five steps represent a complete modelling cycle. If revisions or additions to the data worksheets are now required a further cycle can be started. Once one of the run / save buttons has been pressed on worksheet “Calculation Control” the data worksheets are protected. To make revisions to the data worksheets one of the buttons “Unprotect Data for editing” and “Unprotect Data and Remove Results” on the “Calculation Control” worksheet must be used. The latter button will additionally delete all results on the “Results” worksheet. If the former button is used, results will be deleted automatically as required as the data worksheets are edited to maintain consistency between the input data and the results.
5 Operation of the Graphing Tool

5.1 Introduction

This section describes the SMOGG graph plotting tool and its operation. As indicated in subsection 2.1, the SMOGG graph plotting tool is a spreadsheet in which results from one or more SMOGG calculations that are saved in copies of the main SMOGG spreadsheet can be selected and plotted on graphs in a straightforward way. To use the tool requires one or more SMOGG calculations to have been completed and saved in copies of the main SMOGG spreadsheet. The tool then automatically loads results from the calculation spreadsheets as required and plots these on graphs.

The graphing tool can be used to plot any combination of one or more output results against time from one or more SMOGG calculations. It can be used to generate as many different graphs as required. The tool keeps track of the calculations from which the results have been loaded, so the results plotted can be easily updated if calculations are rerun.

The main SMOGG spreadsheet includes a graphing facility based on the graphing tool. Much of the description given below for the graphing tool also applies to the graphing facility within the main SMOGG spreadsheet. The main difference is that the facility within the main spreadsheet only allows results from within that spreadsheet to be plotted.

5.2 Structure of the Graphing Tool User Interface

5.2.1 Overview

When the SMOGG graph plotting tool is initially opened it contains one visible worksheet. This worksheet contains cells for specifying the calculations from which results are required to be plotted (coloured light blue), cells containing imported or calculated data for use by the tool (uncoloured) and buttons that run Excel Visual Basic macros (blue text on grey backgrounds). One of the buttons generates the additional worksheets on which the graphs are plotted. Each additional worksheet contains cells for selecting the results to be plotted and for setting graphing options (coloured light blue), cells containing the imported results and associated calculated data (uncoloured), a template graph and buttons that run Excel Visual Basic macros (blue text on grey backgrounds).

Plotting results from completed SMOGG calculations is performed in three steps:

- First, the calculation spreadsheets must be specified. This allows the tool to check that the calculation spreadsheets are valid SMOGG calculations, and load in information about the packages in each calculation to enable selection of the specific results to be plotted;
- Secondly, each result to be plotted is defined by selecting from lists:
  - the dataset (i.e. SMOGG calculation);
  - the package within the dataset;
  - the result type (i.e. rate of gas generation, cumulative gas generation or other results);
  - the specific parameter from the full list of those applicable to the selected result type;
- Finally, a macro must be run to load the selected results from the main SMOGG spreadsheets to generate each graph. Each time results are updated by running the macro, various checks are also made and the settings for the graph are modified accordingly (e.g. the legend is updated to match the number of lines plotted).
All the worksheets in the tool are set to be protected to prevent inadvertent editing of the unshaded cells. The light blue user input cells and the layout of the graph can be edited at any time. If the selection of results to be plotted is changed, the relevant previously loaded results are removed and an indication is given on the worksheet that the results need to be reloaded by rerunning the macro. This preserves the relationship between the results selected for plotting and the results displayed on the graphs. When results are removed, the formatting of the graphs is preserved, so results can easily be replotted.

It has been assumed that while using the graphing tool all copies of the main SMOGG spreadsheet will be closed. This prevents calculations from being rerun and source results changed while the graphing tool is open, in which case the results in the graphing tool will remain consistent with the source results. To allow for SMOGG calculations being updated (while the graphing tool is closed), on opening the graphing tool, the option to reload all plotted results is automatically provided via a dialogue box (this performs the same actions as the “Update All Data” button described in subsection 5.2.2). It is the responsibility of the user to ensure that consistency between the calculations and the graphing tool is maintained by reloading the results if necessary at this time.

Each of the worksheets in the graphing tool is described in the rest of subsection 5.2, followed by a description of how to generate a typical graph in subsection 5.3.

### 5.2.2 Description of the Dataset Selection Worksheet

The worksheet “Dataset Selection” contains the input filenames of the SMOGG calculations from which results will be plotted, along with some additional information about the structure of the results in each SMOGG calculation that is used by the tool. A screen-shot of the “Dataset Selection” worksheet is given in Figure 6.

Cell “C7” allows the user to add a description of the graphs that are plotted in the workbook. This cell does not have any effect on the graphs plotted.

Cells “C10” to “C29” specify the filenames of the SMOGG calculation spreadsheets from which results will be plotted. For calculation files in the same directory as the copy of the graphing tool, only the filename of the calculation file (which must include the “.xlsm” extension) needs to be specified. For calculation files in other directories, the directory path relative to the directory containing the copy of the graphing tool as well as the filename needs to be specified. Up to 20 datasets (i.e. SMOGG calculations) can be included.

For each dataset given, a description of the dataset, which will be subsequently used to identify it, is also required. By default the description will be set to the input filename excluding any directory path and the “.xlsm” extension. However, an alternative description can be input if convenient, or will be required where the filename is not unique (i.e. if two SMOGG calculation spreadsheets with the same name that are in different directories are specified). Each description is input adjacent to the filename in cells “E10” to “E29”.

A number of other cells on this worksheet are used to store information used by the tool. The number of datasets (i.e. SMOGG calculations) that have been specified is written in cell “D31”. When each filename is input, the tool verifies that the file is a valid SMOGG calculation spreadsheet, and if so determines the number of output time steps in the calculation, the number of packages and their names. This information is stored adjacent to the filename in cells “H10” to “H29” and cells to the right of these.

Along the top of worksheet “Dataset Selection” there are two buttons that launch macros:

- Button “New Blank Graph Sheet” makes a copy of the hidden worksheet “GraphSheet-Template” and prompts the user to name the new graph worksheet with a unique name. All graph worksheets start with the prefix “GraphSheet-“ and the user need only fill in the remaining part of the name. (Note that if no characters are entered, this cancels the action.)
This provides a blank graph worksheet on which results can be selected for plotting and a template graph with standard formatting:

- Button “Update All Data” reloads all the information and results from SMOGG calculation worksheets as specified by the input data. The update process first checks that the input filenames on the “Dataset Selection” worksheet still refer to valid SMOGG calculation spreadsheets. For a filename that does not, the filename, the dataset description and related information for the dataset on the “Dataset selection” worksheet, and all selections and corresponding loaded results on all graph worksheets referring to the dataset are deleted. For a filename that does refer to a valid SMOGG calculation spreadsheet, the time step and package information are reloaded into the “Dataset Selection” worksheet. If this information has changed, all selections and corresponding loaded results on all graph worksheets referring to the dataset are deleted. The update process then reloads the results data (which also updates the graphs) on all the graph worksheets based on each of the results selected for plotting by the user.

5.2.3 Description of the GraphSheet-###################5 Worksheets

Each graph worksheet plots one graph, which can include up to 20 sets of results. Additional graphs can be plotted by generating additional graph worksheets using the buttons on either the existing graph worksheets or on the “Dataset Selection” worksheet. The names of graph worksheets are all prefixed by “GraphSheet-” and can have between 1 and 19 additional characters or numbers. A screen-shot of a typical graph worksheet is given in Figure 7 (parts 1 and 2).

Along the top of each graph worksheet there are five buttons that launch macros:

- Button “New Blank Graph Sheet” generates a new graph worksheet from a hidden template graph worksheet. This is as described for the same button on the “Dataset Selection” worksheet (see subsection 5.2.2);

- Button “Copy This Graph Sheet” is very similar to button “New Blank Graph Sheet”, except that it generates a new graph worksheet by copying the currently displayed graph worksheet rather than the template graph worksheet. This means that any results selections the have been made and any reformatting that has been applied to the graph on the current worksheet will be copied to the new graph worksheet. In this way the user can set up a graph in any format required and produce a number of plots using the same formatting;

- Button “Rename This Graph Sheet” renames the currently displayed graph worksheet. The user is prompted for a new unique name (the prefix “GraphSheet-” is assumed and the user need only fill in the remaining part of the name);

- Button “Update Data” updates the results loaded on the currently displayed graph worksheet. Results are only loaded where a complete selection of the data to be plotted has been made and results for that selection have not already been loaded. This means that results will only be reloading where the data selections have been changed since the results were last loaded (as changing the selection will delete the loaded results). When an update to any of the results is required, the text on the button changes colour to red. As it is assumed that SMOGG calculations will not be rerun while the graphing tool is open, this method of updating is sufficient to keep the loaded results in sync with the calculations while using the graphing tool, providing this is checked initially when the tool is opened (see subsections 5.2.1 and 5.2.2);

- Button “Clear Data” deletes all the selections of data to be plotted and all the loaded results on the currently displayed graph worksheet. Reformatting that has been applied to the graph is retained, except for any formatting of the secondary y-axis and legend, which must be reapplied from the options on the worksheet each time the data is updated (although no lines will be plotted on the graph until new results are loaded);

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5 The string “###################” is used in this document to indicate a string of between 1 and 19 characters chosen by the user to uniquely identify a graph sheet within the workbook.
The rest of each graph worksheet contains a section in which data to be plotted on the graph is selected, a section in which certain graph formatting options must be set, a section displaying the graph and a section into which the results are loaded.

The data selection section consists of a table that allows up to 20 results to be selected for plotting on the graph, one per row in the table. Selections are made in each column in the table as follows:

- In the column headed “Dataset” the SMOGG calculation spreadsheet (i.e. dataset) to which the required result belongs is selected from a list. The list contains the description of each dataset as input on the “Dataset Selection” worksheet;
- In the column headed “Package” the package to which the required result belongs is selected from a list. The list contains the package names relevant to the dataset selected, so the dataset must be selected before the package;
- In the column headed “Results type” the output worksheet within the SMOGG calculation spreadsheet on which the required result exists (i.e. “GasRates”, “CumulativeGas” or “OtherResults”) is selected from a list;
- In the column headed “Parameter” the specific set of results that is required is selected from a list. The list contains the parameters relevant to the results type selected (i.e. a description of all the columns on the relevant output worksheet in the SMOGG calculation spreadsheet), so the results type must be selected before the parameter;
- In the column headed “Legend name” text can be added that will be used to label the result in the graph legend. If these cells are left blank, then default text is added to each once selections are made in each of the first four columns of the data selection table. The default text can be overwitten if required;
- In the column headed “Y-axis” the y-axis on the graph (primary or secondary) against which the result will be plotted can be selected from a list. If these cells are left blank, then each one will default to “Primary” once selections are made in each of the first four columns of the data selection table. At least one result must be plotted against the primary y-axis, so the only option available is “Primary” until this has been selected for at least one result to be plotted.

There are two further columns in the data selection table. The column headed “Comments” allows the user to add any comments relating to each result selected for plotting that may be helpful. These cells do not have any effect on the graphs plotted. The column headed “Status” indicates when the results selected have not yet been loaded. This is indicated by the text “Update Required” in red in the relevant cells. If no text is visible in these cells, this indicates that the results have already been loaded (and are plotted on the graph). These cells are updated automatically as selections are made in the table, and cannot be edited by the user. All the user input cells in the table can be modified at any time. As selections are changed, results are automatically deleted if necessary to ensure consistency between the selections made and the loaded results and the graph is updated as appropriate. However, for efficiency new results are not loaded automatically. The user must initiate the loading of results using the “Update Data” button at the top of the worksheet.

Most of the formatting of the graph that may be required can be applied to the graph directly and will not be changed by the tool. However, as a secondary y-axis is optional and the legend is required to show only those results that have been loaded, these aspects of the graph must be managed by the tool. Because of this there is a graph options section on each graph worksheet that allows the user to set basic features of the secondary y-axis and the legend. The user can set a label for the axis (in cell “C31”), select whether the axis has a linear or logarithmic scale (in cell “C32”), set the minimum and maximum values for the axis scale (in cells “H31” and “H32”), select the position of the legend (in cell “L31”, from the standard set of positions provided by Excel) and select whether the legend has a border (in cell “L32”). Note that the minimum and maximum values for the axis scale are set automatically by Excel if no values are set by the user.
The third section on each graph worksheet is where the graph is displayed. The final section is where the results corresponding to the selections made in the data selection table are loaded. The results are loaded into pairs of columns starting at cell “B66”, providing the output times and corresponding values of the selected parameter. Above the results cells are a number of cells in which additional information is recorded. Cell “B65” and cells to its right provide headings for the loaded data (i.e. for each pair of cells “Time [years]” and the parameter description given in the data selection table). Cell “B63” and alternate cells to its right contain a timestamp indicating when the results were last loaded from the SMOGG calculation spreadsheet. This may be useful for the user to check that the loaded results are in sync with the calculations. Cell “C63” and alternate cells to its right record which y-axis the results are to be plotted against (as specified in the data selection table). Cell “B64” and alternate cells to its right contain information to identify the workbook and worksheet from which the results were loaded. Cell “C64” and alternate cells to its right record the text to be used to label the plot in the graph legend (as specified in the data selection table).

5.3 Generating a Typical Set of Graphs

The following describes the steps in generating a typical set of graphs of results of SMOGG calculations using the SMOGG graph plotting tool:

1. In worksheet “Dataset Selection”, optionally provide a description for the graphs to be generated.

2. In worksheet “Dataset Selection”, enter the filename, including the “.xlsm” extension, (and relative directory path if necessary) of each SMOGG calculation spreadsheet containing results to be plotted. Optionally enter descriptions for these datasets (if the default descriptions do not easily identify the calculations).

3. If there are no existing graph worksheets (prefixed by “GraphSheet-”), use button “New Blank Graph Sheet” on worksheet “Dataset Selection” to obtain a new graph worksheet. The user will be prompted for a unique name for the graph worksheet. The process can be repeated to provide further graph worksheets or Step 4 applied.

4. If there are existing graph worksheets (prefixed by “GraphSheet-”), as an alternative to Step 3, use button “Copy This Graph Sheet” on a graph worksheet to obtain a copy of that worksheet if an additional graph is required. The user will be prompted for a unique name for the new graph worksheet. The process can be repeated to provide further graph worksheets.

5. For each graph worksheet:
   - Select a set of results to be plotted on the graph from the options provided for the dataset, package, results type and parameter, enter a label for the result to be included in the graph legend and select the y-axis against which the result is to be plotted. This can be repeated for up to 20 results.
   - Press button “Update Data” to load the selected results so that they are plotted on the graph.
   - Modify the formatting of the graph as required. This can be done directly on the graph except for changes to the secondary y-axis and the legend. The secondary y-axis label and scale maximum and minimum can be entered in the cells above the graph and options for the secondary y-axis type and legend position and border can be selected in the cells above the graph.

After generating a graph, additional graphs with the same formatting can be generated more easily by applying Step 4 before applying Step 5 for the new graph worksheet.

6. The previous five steps will generate a set of graphs. These steps can be repeated as necessary to modify the results to be plotted or the formatting of the graphs.
6 Verification

Confidence that SMOGG behaves according to its specification, that is that it properly solves the model equations set out in the SMOGG specification [2], (i.e. verification) is derived in two ways:

1. From the application of appropriate QA during the development of the program;
2. From the use of a comprehensive suite of test cases that have been developed to test the model.

AMEC carries out its projects in accordance with the requirements of the ISO 9001:2008 standard. Its Business Management arrangements have been assessed by Lloyd’s Register Quality Assurance (LRQA) against the requirements of this standard and received certification of conformance to it (certificate Number LRQ 0861156/D). In particular, software development is carried out in accordance with the TickIT Guide Issue 5.5.

SMOGG was developed following AMEC’s TickIT compliant procedures. This ensures that:

- The software specification is properly defined and agreed with the customer;
- The appropriate design work is carried out to translate the specification into a computer model. This includes developing and checking the analytical and numerical solution methods needed to implement the model specification, and designing the program architecture;
- The program implementation is managed using proper version control;
- A suite of test cases is defined and reviewed and used to thoroughly test the various models and options provided in the program;
- Proper approval is required before the program can be released to the customer; and
- Continuity of management and quality is ensured throughout the lifetime of the software, including the provision of maintenance.

The comprehensive list of test cases used to verify SMOGG v7.0 is listed in Appendix B. Every effort was made to test the various models implemented in SMOGG against independent calculations. In most cases the independent calculations were carried out in Excel spreadsheets, in a few cases models implemented in Mathematica were used to derive the independent test results, and in one case an independent FORTRAN program was used to calculate the test results. Some tests relate to verifying internal consistency within the program.

In addition to the verification provided by the test cases, verification of the correct behaviour of the various parts of the user interface was provided by informal testing. In particular, example data was used to check that clicking each of the buttons in the main SMOGG spreadsheet, the driver spreadsheet and the graphing tool resulted in the expected action being performed, and editing datasets and selecting options in the graphing tool and main SMOGG spreadsheet was correctly managed.

For SMOGG v7.0, testing has been carried out using 32 bit versions of both Excel 2007 and Excel 2010, running on Windows 7. Therefore one of these environments should be used to run SMOGG v7.0. In particular it should be noted that SMOGG v7.0 is not expected to operate with 64 bit versions of Excel.
7 References


8 Figures

Figure 1  Worksheet “General Data”
Figure 2  Worksheet example “Data-Package1” (part 1)
Figure 2  Worksheet example “Data-Package1” (part 2)
Figure 2  Worksheet example “Data-Package1” (part 3)
### Figure 2  Worksheet example “Data-Package1” (part 4)

#### PACKAGE SPECIFIC DATA

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<th>Radioisotope</th>
<th>Activity in spheres (TBq)</th>
<th>Radon distribution parameter ( a ) in spheres</th>
<th>Radon distribution parameter ( r ) in spheres</th>
<th>Radon distribution parameter ( u ) in plates</th>
<th>Solid-state diffusion coefficient (m/s²)</th>
<th>Fraction released as (^{13}CO_2) (remainder will be (^{12}CO_2))</th>
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<td>Stainless steel</td>
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<td>Carbon steel</td>
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<td>Zircon</td>
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<td>Uranium</td>
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![Worksheet example](image-url)
Figure 2  Worksheet example “Data-Package1” (part 5)
Figure 2  Worksheet example “Data-Package1” (part 6)
Figure 2  Worksheet example “Data-Package1” (part 7)
Figure 2  Worksheet example “Data-Package1” (part 8)
### Figure 3  Worksheet example “GasRates-Package1”
### Table: OtherResults-Package1

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**Figure 4**  Worksheet example “OtherResults-Package1”
Figure 5  Driver spreadsheet worksheet “Parameters”
Figure 6  Graphing tool worksheet “Dataset Selection”
Figure 7  Graphing tool worksheet example “GraphSheet-Graph1” (part 1)
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# Appendices

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<th>Description</th>
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</table>
Appendix A
Schematic of Gas Production Processes in SMOGG
Dotted lines denote that the consumption of the substrate indicated is not modelled. The consumption by the route indicated is assumed insignificant compared with the mass of the substrate present or in comparison with consumption by other processes. The bulk gas generation from radiolysis is designated as hydrogen, but is intended to represent generation of a number of gases. The release from organic degradation of gaseous $^{14}$C is in the form of $^{14}$CH$_4$ and $^{14}$CO$_2$. The nature of the release from other processes might be quite complex and vary with the process; these releases are designated as $^{14}$CH$_4$, $^{14}$CO$_2$ and $^{14}$CO as representing a wider range of possibilities.
Appendix B
Test Cases Used to Verify SMOGG
The test cases in the following table have been used to test the gas generation model SMOGG v7.0.

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Description</th>
<th>Checking</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple 01a</td>
<td>Test of corrosion. Release of hydrogen and radionuclides (including C-14 in two forms) from stainless steel calculated. Includes aerobic and anaerobic periods.</td>
<td>Hydrogen and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_steel.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01b</td>
<td>Test of corrosion. Release of hydrogen and radionuclides from carbon steel calculated. Includes aerobic and anaerobic periods.</td>
<td>Hydrogen and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_steel.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01c</td>
<td>Test of corrosion. Release of hydrogen and radionuclides from Zircaloy calculated. Includes aerobic and anaerobic periods. (Includes corrosion of stainless steel to consume oxygen, giving change in conditions.)</td>
<td>Hydrogen (from Zircaloy) and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_Zircaloy.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01d</td>
<td>Test of corrosion. Release of hydrogen and radionuclides from Magnox calculated. (Includes corrosion of stainless steel to consume oxygen, giving change in conditions.)</td>
<td>Hydrogen (from Magnox) and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_Magnox.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01e</td>
<td>Test of corrosion. Release of hydrogen and radionuclides from uranium calculated. Includes aerobic and anaerobic periods.</td>
<td>Hydrogen and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_U.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01f</td>
<td>Test of corrosion. Release of hydrogen and radionuclides from aluminium calculated. (Includes corrosion of stainless steel to consume oxygen, giving change in conditions.)</td>
<td>Hydrogen (from aluminium) and radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_Al.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------------------------------------</td>
<td>------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>Simple 01g</td>
<td>Test of corrosion. Release of hydrogen from stainless steel containers calculated. Includes aerobic and anaerobic periods.</td>
<td>Amount of metal remaining and hydrogen release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_container.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 01h</td>
<td>Test of corrosion. Release of hydrogen from carbon steel containers calculated. Includes aerobic and anaerobic periods.</td>
<td>Amount of metal remaining and hydrogen release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_container.xls'. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>Simple 02a</td>
<td>Test of diffusion. Release of radionuclides from stainless steel calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 02b</td>
<td>Test of diffusion. Release of radionuclides from carbon steel calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 02c</td>
<td>Test of diffusion. Release of radionuclides from Zircaloy calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 02d</td>
<td>Test of diffusion. Release of radionuclides from Magnox calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 02e</td>
<td>Test of diffusion. Release of radionuclides from uranium calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 02f</td>
<td>Test of diffusion. Release of radionuclides from aluminium calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testdiffusion.xls'.</td>
</tr>
<tr>
<td>Simple 03a</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose under atmospheric conditions.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'glucose-Plot2.nb' (as processed in file 'testglucose.xls').</td>
</tr>
<tr>
<td>Simple 03b</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose aerobic (grouted) conditions.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'glucose-Plot2.nb' (as processed in file 'testglucose.xls').</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
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<tr>
<td>Simple 03c</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose under anaerobic, nitrate-rich conditions.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'glucose-Plot2.nb' (as processed in file 'testglucose.xls').</td>
</tr>
<tr>
<td>Simple 03d</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose under anaerobic, sulphate-rich conditions.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'glucose-Plot2.nb' (as processed in file 'testglucose.xls').</td>
</tr>
<tr>
<td>Simple 03e</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose under anaerobic conditions (with no nitrate or sulphate).</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'glucose-Plot2.nb' (as processed in file 'testglucose.xls').</td>
</tr>
<tr>
<td>Simple 04</td>
<td>Test of organic degradation to ISA and carbon dioxide production from degradation of ISA.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation in file 'ISA-Plot2.nb' (as processed in file 'testISA.xls').</td>
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<tr>
<td>Simple 05</td>
<td>Test of Rn-222 release from decay of Ra-226.</td>
<td>Rn-222 release rate and cumulative release checked against Mathematica calculation in file 'Radon.nb' (as processed in file 'testdecay.xls').</td>
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<tr>
<td>Simple 06</td>
<td>Test of radiolysis of water, cellulose, small organics and a number of other categories of organic materials to produce hydrogen, tritiated hydrogen and C-14-contaminated gas (in two forms). (Includes degradation of organic components, but rate chosen to be insignificant.)</td>
<td>Hydrogen, H-3 and C-14 release rates and cumulative release checked against independent spreadsheet calculation in file 'testradiolysis.xls'.</td>
</tr>
<tr>
<td>Simple 07</td>
<td>Test of release of C-14 (in three forms) and H-3 from graphite.</td>
<td>C-14 and H-3 release rates and cumulative release checked against independent spreadsheet calculation in file 'testgraphite.xls'.</td>
</tr>
<tr>
<td>Simple 08</td>
<td>Test of conversion of carbon dioxide and hydrogen to methane. Carbon dioxide generated from organic degradation as in test case Simple 03e with additional glucose as in test case Simple 11. Hydrogen generated from radiolysis as in test case Simple 06.</td>
<td>Methane, carbon dioxide, hydrogen and C-14 net release rates and net cumulative releases checked against independent spreadsheet calculation in file 'testgas.xls'. (Note: Carbon dioxide, hydrogen and C-14 results from other processes required as input.)</td>
</tr>
<tr>
<td>Simple 09</td>
<td>Test of radionuclide release from corrosion with non-uniform radionuclide distribution in metal. Corrosion as in test case Simple 01a with aerobic period extended to end of calculation.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_RNdist.xls'.</td>
</tr>
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<td>Case ID</td>
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<tr>
<td>Simple 10</td>
<td>Test of H-3 release from tritiated water via corrosion reactions. (Corrosion as in Simple 01d – Magnox only.)</td>
<td>H-3 release rate and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_H3.xls'.</td>
</tr>
<tr>
<td>Simple 11</td>
<td>Test of C-14 release from degradation of ISA. (ISA production as in test case Simple 04.)</td>
<td>C-14 release rates and cumulative release checked against spreadsheet calculation in file 'testISA_C14.xls'.</td>
</tr>
<tr>
<td>Miscell 01</td>
<td>Test of the inclusion of multiple packages within a single waste stream.</td>
<td>Calculation rerun with a single package (see spreadsheet file ‘singlepackage.xlsm’), then all results (except temperature) scaled in spreadsheet file ‘checkmultipackage.xls’ and compared with test case results.</td>
</tr>
<tr>
<td>Miscell 02</td>
<td>Test of the emplacement of a package at a time after the calculation start time. (Only decay occurs within the package until its emplacement.)</td>
<td>Calculation rerun with package emplaced at start time (see spreadsheet file ‘initialemplacement.xlsm’), then active gas and radiolysis results decayed by factor(s) corresponding to test case emplacement time in spreadsheet file ‘checkdecayonly.xls’ and gas release rates and cumulative releases compared with test case results.</td>
</tr>
<tr>
<td>Miscell 03</td>
<td>Test of multiple emplacement times for packages within a single waste stream.</td>
<td>Calculation rerun with each emplacement specified as a separate waste stream (see spreadsheet file ‘singleemplacement.xlsm’), then all results (except temperature) combined in spreadsheet file ‘checkemplacement.xls’ and compared with test case results.</td>
</tr>
<tr>
<td>Miscell 04</td>
<td>Test of radionuclide release from metal by simultaneous corrosion and diffusion.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrdiff.xls'.</td>
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<td>Miscell 05</td>
<td>Test of corrosion of spent fuel. Release of hydrogen from uranium spheres calculated. Includes aerobic and anaerobic phases.</td>
<td>Hydrogen release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_SF.xls'.</td>
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<td>Miscell 06</td>
<td>Test of gas release from unvented containers by all processes except corrosion.</td>
<td>Timing of gas release and resaturation checked for consistency with time of container breaching (noting that radiolysis of water begins at repository closure, see file ‘testunvented.xls’).</td>
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<tr>
<td>Miscell 07</td>
<td>Test of gas release from unvented containers by corrosion of waste.</td>
<td>Hydrogen release rates and cumulative release checked against independent spreadsheet calculation in file 'testcorrosion_unvented.xls'.</td>
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<td>Miscell 08</td>
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<td>spreadsheet calculation in file 'testcorrosion_unvented2.xls'.</td>
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<td>Test of resaturation model characterised by a water inflow rate. Tests</td>
<td>Independent numerical calculation</td>
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<td>calculation of groundwater saturation (which depends on water inflow and</td>
<td>performed to determine total water contents and groundwater saturations</td>
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<td>consumption). Release of hydrogen by anaerobic corrosion of stainless steel</td>
<td>(see files in subdirectory 'SatCalc'). Hydrogen release rates and</td>
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<td>calculated.</td>
<td>cumulative release checked against values calculated from independent</td>
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<td>Miscell 10</td>
<td>Test of calculation of corrosion product volume, wasteform strain and</td>
<td>Corrosion product volumes corrosion reaction volume changes and</td>
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<td>critical times for physical containment.</td>
<td>wasteform strains checked against independent spreadsheet calculation in</td>
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<td>file 'testcontainment.xls'.</td>
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<td>Miscell 11</td>
<td>Test of corrosion for package grouted during calculation period. Release</td>
<td>Hydrogen release rate and hydrogen and water cumulative release checked</td>
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<td>of hydrogen from Magnox calculated. Pre-closure period only.</td>
<td>against independent spreadsheet calculation in file 'testcorrosion_grouting.xls'.</td>
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<td>Miscell 12</td>
<td>Test of output of bulk gas results in volumetric units. (Gas release as in</td>
<td>Results with bulk gas in molar units converted into equivalent volumetric</td>
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<tr>
<td></td>
<td>Simple 06.)</td>
<td>results in spreadsheet 'checkoutputunits.xls' and compared. (Note: Output</td>
</tr>
<tr>
<td></td>
<td></td>
<td>results from Simple 06 required as input.)</td>
</tr>
<tr>
<td>Miscell 13</td>
<td>Test of output of bulk gas results in volumetric units with temperature</td>
<td>Results with bulk gas in molar units converted into equivalent volumetric</td>
</tr>
<tr>
<td></td>
<td>defining output volumes specified in degrees Celsius. (Gas release as in</td>
<td>results in spreadsheet 'checkoutputunits.xls' and compared. (Note: Output</td>
</tr>
<tr>
<td></td>
<td>Simple 06.)</td>
<td>results from Simple 06 required as input.)</td>
</tr>
<tr>
<td>Miscell 14</td>
<td>Test of use of volumetric units for specification of amount of oxygen.</td>
<td>All results checked against expected results for Miscell 01 (see</td>
</tr>
<tr>
<td></td>
<td>(Input as in Miscell 01, but with moles of oxygen converted to equivalent</td>
<td>spreadsheet file 'checkmultipackage.xls').</td>
</tr>
<tr>
<td></td>
<td>volume.)</td>
<td></td>
</tr>
<tr>
<td>Miscell 15</td>
<td>Test of use of Kelvin for specification of temperatures in temperature</td>
<td>Hydrogen and radionuclide release rates and cumulative release checked</td>
</tr>
<tr>
<td></td>
<td>profile. (Input as in Simple 01a, but with temperatures in temperature</td>
<td>against expected results for Simple 01a (see spreadsheet file</td>
</tr>
<tr>
<td></td>
<td>profile converted to equivalent values in Kelvin.)</td>
<td>'testcorrosion_steel.xls').</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
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<tr>
<td>Miscell 16</td>
<td>Test of use of alternative units for specification of G-values. (Input as in Simple 06, but with G-values converted to equivalent values in molecules/100eV.)</td>
<td>Hydrogen, H-3 and C-14 release rates and cumulative release checked against expected results for Simple 06 (see spreadsheet file 'testradiolysis.xls').</td>
</tr>
<tr>
<td>Exhaust 01</td>
<td>Test of exhaustion of metal during corrosion.</td>
<td>Hydrogen release rates and cumulative release (before and after metal exhaustion) checked against independent spreadsheet calculation in file 'testmetal.xls'.</td>
</tr>
<tr>
<td>Exhaust 02a</td>
<td>Test of exhaustion of oxygen during organic degradation. (Parameters chosen so that gas production occurs only while oxygen is consumed, and so that no additional oxygen will enter the package.)</td>
<td>Consistency of cumulative gas production after oxygen exhaustion with initial oxygen available and rates of gas production after oxygen exhaustion checked (see file 'checkexhaust02.xls').</td>
</tr>
<tr>
<td>Exhaust 02b</td>
<td>Test of exhaustion of nitrate during organic degradation. (Parameters chosen so that gas production occurs only while nitrate is consumed.)</td>
<td>Consistency of cumulative gas production after nitrate exhaustion with initial nitrate available and rates of gas production after nitrate exhaustion checked (see file 'checkexhaust02.xls').</td>
</tr>
<tr>
<td>Exhaust 02c</td>
<td>Test of exhaustion of sulphate during organic degradation. (Parameters chosen so that gas production occurs only while sulphate is consumed.)</td>
<td>Consistency of cumulative gas production after sulphate exhaustion with initial sulphate available and rates of gas production after sulphate exhaustion checked (see file 'checkexhaust02.xls').</td>
</tr>
<tr>
<td>Exhaust 03</td>
<td>Test of limitation of water. (Aluminium sphere corrosion model used such that initial water exhausted before closure leaving only supply by diffusion, but no limitation after closure.)</td>
<td>Hydrogen release rates and cumulative release checked against independent spreadsheet calculation in file 'testwater.xls'.</td>
</tr>
<tr>
<td>Exhaust 04</td>
<td>Test of exhaustion of metal combined with limitation of multiple processes due to availability of water.</td>
<td>Hydrogen release rates and cumulative amounts of metals, water and hydrogen checked against Mathematica calculation in file 'testmetalwater.nb' (as processed in file 'checkmetalwater.xls').</td>
</tr>
<tr>
<td>MassBal 01</td>
<td>Test of mass conservation for corrosion, organic degradation and gas conversion under aerobic conditions.</td>
<td>Changes in molar quantities calculated and checked in spreadsheet file 'MassBalanceCheck(Aer).xls'.</td>
</tr>
<tr>
<td>MassBal 02</td>
<td>Test of mass conservation for corrosion, organic degradation and gas conversion under anaerobic, nitrate-rich conditions.</td>
<td>Changes in molar quantities calculated and checked in spreadsheet file 'MassBalanceCheck(Nitrate).xls'.</td>
</tr>
<tr>
<td>MassBal 03</td>
<td>Test of mass conservation for corrosion, organic degradation and gas conversion under anaerobic, sulphate-rich conditions.</td>
<td>Changes in molar quantities calculated and checked in spreadsheet file 'MassBalanceCheck(Sulphate).xls'.</td>
</tr>
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<td>Description</td>
<td>Checking</td>
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<tr>
<td>MassBal 04</td>
<td>Test of mass conservation for corrosion, organic degradation and gas conversion under anaerobic conditions.</td>
<td>Changes in molar quantities calculated and checked in spreadsheet file 'MassBalanceCheck(Anaer).xls'.</td>
</tr>
<tr>
<td>Driver 01</td>
<td>Test of Multirun Driver spreadsheet. 20 cases based on test case Miscell 10, with variations of parameters used for waste package integrity calculations.</td>
<td>Critical times for all cases checked against independent spreadsheet calculations in file 'testsimplemultirun.xls'.</td>
</tr>
<tr>
<td>Driver 02</td>
<td>Test of Multirun Driver spreadsheet. 4 cases containing extensive range of waste materials, with variations of a wide range of parameters to test correct transcription of data into main SMOGG spreadsheet.</td>
<td>Calculations rerun in main SMOGG spreadsheet with each case specified as a separate waste stream (see spreadsheet files 'manyparamcalcACD.xlsm' and 'manyparamcalcB.xlsm'), then all results compared with test case results in spreadsheet file 'testmanyparam.xls'.</td>
</tr>
<tr>
<td>Driver 03</td>
<td>Test of Multirun Driver spreadsheet. 600 cases based on Driver 01 cases (repeated 30 times).</td>
<td>Checked whether all calculations completed, to ensure a large number of calculations can be run in a single batch.</td>
</tr>
</tbody>
</table>