SMOGG (Version 5.0), a Simplified Model of Gas Generation from Radioactive Wastes: User Guide

A Report produced for United Kingdom Nirex Limited

BT Swift

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SMOGG (Version 5.0), a Simplified Model of Gas Generation from Radioactive Wastes: User Guide

BT Swift
Serco Assurance, Harwell

Abstract

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 5.0) 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 repository. 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. Repository 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.

October 2006
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 5.0) 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 repository. 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). Repository 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 unreactive metals (steels, Zircaloy and uranium) and reactive metals (Magnox and aluminium) to produce hydrogen.
b) Radiolysis of water and organic materials to produce hydrogen.
c) Microbial degradation of organic materials (following hydrolysis of cellulose) to produce carbon dioxide and methane, with the gas composition depending on conditions (e.g. aerobic vs. anaerobic).
d) Radioactive decay of radium to produce radon.
e) The release of tritium, $^{81}$Kr, $^{85}$Kr, $^{39}$Ar and $^{42}$Ar: all of these from metals (as a result of corrosion or solid state diffusion) and tritium also from tritiated water and graphite in the wastes.
f) The release of $^{14}$C labelled gases from the hydrolysis of activation products in some metals as the metal corrodes, from the microbial and radiolytic degradation of some organic wastes, and from graphite containing $^{14}$C.

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.

This user guide was prepared by Serco Assurance under contract to United Kingdom Nirex Limited between September and October 2006, in association with the implementation of the enhancements included in SMOGG version 5.0. The report is based upon, and solely refers to, information available at that time. The work forms part of the Nirex Safety Assessment Research Programme. The information contained in this report has been verified under arrangements established by Serco Assurance. These arrangements have been approved by Nirex and comply with ISO 9001.

The views expressed and conclusions reached are those of the authors and do not necessarily represent those of Nirex.
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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, United Kingdom Nirex Limited (Nirex) undertakes assessments of gas generation from packaged wastes in the UK radioactive waste inventory. Nirex 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 repository 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 repository vaults and final closure\(^1\). This period, which is also referred to as a care and maintenance period, may be several hundred years if a deferred repository closure strategy is adopted);

c) modelling the post-closure period of such a repository (that is, gas generation from the wastes following repository closure). For this phase of the repository 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 repository, for example, in the context of co-disposal with ILW and LLW.

Nirex 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. Nirex 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.

\(^1\) Surface storage of wastes prior to acceptance by Nirex is here termed “interim storage”.


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.

This revised user guide describes the operation and data requirements of the Nirex 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 5.0. It is anticipated that future enhancements to SMOGG will lead to a reissuing of this document to take account of the changes.

Operation of the main SMOGG model is described in Section 2, while operation of the SMOGG multi-run driver is described in Section 3. Finally, Section 4 discusses the verification performed for both the model and the driver.

This report was prepared by Serco Assurance under contract to United Kingdom Nirex Limited. The preparation of this report was carried out during September and October 2006 and the report is based upon, and solely refers to, information available at that time. The work forms part of the Nirex Safety Assessment Research Programme. The information contained in this report has been verified under arrangements established by Serco Assurance. These arrangements have been approved by Nirex and comply with ISO 9001.

The views expressed and conclusions reached are those of the authors and do not necessarily represent those of Nirex.
2 OPERATION OF THE MODEL

The main SMOGG model consists of two components: a C++ application which performs the calculation, and a customised Excel spreadsheet which handles the data input and output processing, including the production of graphs. The spreadsheet writes input data to temporary files that are subsequently read by the C++ application. The C++ application is launched from the spreadsheet, and results, written to temporary files by the C++ application, are loaded back into the spreadsheet.

An optional third component of the SMOGG model is another Excel spreadsheet that provides an automated interface to the main spreadsheet for sequentially performing large numbers of calculations. The main model is described in this section. The optional multi-run driver spreadsheet is described separately in Section 3.

2.1 Installation of SMOGG

The C++ application “SmoggApplication.dll” should be placed in the installation directory “C:\Program Files\Smogg\”. The intermediate temporary files “InputData.txt”, “CumulativeGas.txt”, “GasRates.txt” and “OtherResults.txt” will be written to this directory. The Excel spreadsheet “SmoggSpreadsheet.xls”, which provides the user interface for the Simple Model of Gas Generation 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.

2.2 Structure of the Spreadsheet User Interface

2.2.1 Introduction

As already indicated, SMOGG consists of two parts. The first is a user interface consisting of an Excel spreadsheet (SmoggSpreadsheet.xls) and the second is a pre-compiled C++ program (SmoggApplication.dll) that performs the calculations. Inventory, run-scenario and calculation parameters are entered into the spreadsheet. The spreadsheet 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 charts 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 repository operation under aerobic conditions. In this period it is assumed that there is a limited supply of water. The second time period is from repository closure to repository 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 repository 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 repository.

The models for gas generation are:

- Corrosion of Magnox, aluminium, stainless steel, carbon steel, Zircaloy and uranium to produce hydrogen.
- Release of radionuclides $\left( ^3H, ^{14}C, ^{81}Kr, ^{85}Kr, ^{39}Ar, ^{42}Ar \right)$ in gaseous form (i.e. incorporated into gaseous molecules in the case of $^3H$ and $^{14}C$) from Magnox, aluminium, stainless steel, carbon steel, Zircaloy and uranium due to corrosion and diffusion.
- Cellulose degradation to produce glucose or ISA, and subsequently microbial degradation of glucose or ISA to produce carbon dioxide and methane.
- $^{14}C$ release from microbial degradation of glucose or ISA.
- Radon production from radioactive decay of $^{226}Ra$ and its parents.
- Production of hydrogen by radiolysis of water, cellulose, polymers and oils and the release of $^{14}C$-containing gases by radiolysis of small molecules.
- Release in gaseous molecules of “trapped” $^3H$ 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.

### 2.2.2 Description of each worksheet

When the main SMOGG spreadsheet is initially opened it contains six visible worksheets. These worksheets contain cells for entering data (coloured light blue), cells containing calculated data (uncoloured), buttons that run Excel Visual Basic macros (blue text on grey backgrounds) and boxes for entering data or run options from fixed lists. Charts to display results can be generated by Excel Visual Basic macros initiated by buttons on a chart worksheet.

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.

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 and displays the package results and the totals of all the package results on separate worksheets.

After the macro is run the worksheets in the spreadsheet are protected (charts, subsequently generated, based on the results can be changed). 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 associated charts. Re-running the calculation will also delete all previous result worksheets and associated charts.

Each of the worksheets and generated charts are described below, followed by a description of a typical calculation in subsection 2.3. If invalid or inconsistent data are placed in any of the worksheets then an error message is displayed in a message box and the calculation is not performed. The user is required to re-enter permissible or consistent data.

**General Data**

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 “B3” and “B5” 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.

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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 SMOGG Excel workbook itself, which will provide a more readable and complete identification of the features being described.
The spreadsheet calculates the number of package worksheets (see below) included in the calculation and writes this to Cell “B7”. Package worksheets are added by the user but can be optionally excluded from the calculation. Cell “B7” 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 “B9” and “B10” specify the start and end times for the calculation. The end time must be greater than the start time. Cell “B12” specifies the time of repository closure. Cells “B13” and “B14” specify the rate of water inflow after closure and the time of repository resaturation; one of these values only must 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 “B16” to “B27” and beyond can be used to obtain the results of calculations at additional output times.

At cells “G8” to “G9” there is a box with a drop-down list to specify whether the results for the non-radioactive gases are output using moles or m$^3$. If a calculation has been run and result worksheets are present, the list is greyed-out and is inactive. Otherwise there is a choice of “mole” or “m$^3$”. If “m$^3$” is chosen, cells “G12” and “G13” 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 Kelvin appear in cell “G12” and 1.01325 $10^5$ Pascal (one atmosphere) in cell “G13”. The user can overwrite these default values.

On worksheet “General Data” there are seven buttons that launch macros. At cells “E17” to “H19” there are four buttons to alter the 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 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. The worksheet “DefaultPackageData” contains default rate data but no inventory data and can be used as a basis for constructing a new data worksheet. The user is required to enter new inventory data and can also edit the rate data.

- **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 “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).

- 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).

At cell “E2” 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. 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 worksheets and associated charts 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 worksheets in the spreadsheet are protected (charts, subsequently generated, based on the results can be changed). This preserves the relationship between the data entered into the worksheets and the results of the calculation.

At cell “H2” is one button labelled “Go to Charts sheet” which is a shortcut to display the “Charts” worksheet. The “Charts” worksheet is used to display graphs of the results based on user options.

At cells “E21” to “F23” 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 associated charts and unprotect the worksheets.

**DefaultPackageData**

The worksheet “DefaultPackageData” contains default rate data but no inventory data and can be used as a basis for constructing a new data worksheet. 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. The structure of all data worksheets is consequently the same as the structure of worksheet “DefaultPackageData”. Data worksheets are described below.
Data-############3

A data worksheet contains inventory and rate data for a specific type of waste package or waste stream. A screen-shot of a typical worksheet is given in Figure 2 (parts 1-7). 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 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 from 1 up to 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 “B7”. This cell should not be edited. (Note that all Excel worksheets require unique names.)

The buttons “Rename Sheet”, “New Sheet”, “Copy Sheet”, “Delete Sheet” and “Unprotect Data and Results for editing” at cells “D1” to “I1” are duplicates of the buttons appearing on worksheet “General Data” described above.

Cell “B3” 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 “B8” 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 “B10” to “B22” 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.

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3 The string “############” is used in this document to indicate a string of up to 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-############”, and in naming the chart sheets when these refer to a single package or waste stream.
• The initial mass of water in the package. This can be zero but must be less than 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 repository is closed.) If a time is set it must be between the start time of the calculation and the time of repository 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 backfill (excluding any water) associated with a package and the mass of water in the backfill at closure. These must be non-negative.

• The available oxygen in the package at closure. This must also 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 repository closure but becoming anaerobic “immediately” at closure, this value should be set to a small but non-zero number.

• The pore space in the waste and in the backfill. When multiplied by the water density (taken to be 1000 kg m\(^{-3}\)), the pore space in the waste 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 pore space 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 \(^{14}\)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. \(^{14}\)CO\(_2\) is also converted to \(^{14}\)CH\(_4\) in proportion to the amount of bulk carbon dioxide converted to methane. The reaction is assumed to be instantaneous on a timestep basis.

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 “C23:C24”, 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 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 at the time required is the product of the input corrosion rate and the rate-factor.

The packages in each waste stream can be placed in the repository 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 repository at a discrete number of times before repository closure. The default is to enter one emplacement time in cell “C25” and one associated number of packages (the total for the waste stream) in cell “C26”. If more pairs of emplacement times and numbers of packages are required, they are entered in the cells to the right of “C25” and “C26”.

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. 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 “B30” 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 “B36” to “no”. Magnox spent fuel wastes comprise of 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 “B37”.

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 “C26” 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 “B48” to “G52” and “B53” to “C54”. 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 from worksheet “DefaultPackageData”.
- The metal masses and initial sphere radii for the sphere components.
- The metal masses and initial plate thicknesses for the plate components.
- The metal masses and initial wall thicknesses for the container components. The container components are restricted to stainless or carbon steels.

In the section “Corrosion Rates”, parameters are entered in order to calculate the corrosion rates for each metal at each timestep. 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 are copied into the data worksheet from worksheet “DefaultPackageData”.

The first set of corrosion rate data is for Magnox. There are separate data required for the three time periods “atmospheric”, “before resaturation” and “after resaturation”. In the first of these periods a corrosion rate parameter and characteristic time are supplied in cells “B59” and “C59” 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 “B61” and “C61” 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 “E59” and “E60” (in order of ascending temperature), a temperature dependent rate-factor can be calculated and used to multiply the acute corrosion rate. 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 “E61” and “E62” (in order of ascending temperature).
The corrosion parameters can be similarly set for the “before resaturation” and “after resaturation” time periods for the Magnox metal. If required, parameters can also be set for aluminium, stainless steel, carbon steel, Zircaloy and uranium. 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 repository 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 repository 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 timestep 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, as $^{14}$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 CO₂ can be specified. By default it is assumed that none of the $^{14}$C is released as CO₂ (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 entering “1” in cell “B214”. 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 “B217” and “C217”. If either of these values is entered, the dissolution and hydrolysis rates in cells “D217” and “E217” must be positive. The second model is chosen by entering “2” in cell “B214”. 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 “B220” to “C221”. 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 “D220” to “F221”.

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 “B225”. The cellulose degradation model treats this as a mass of the intermediate corresponding to the model selected in cell “B214”. 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 repository 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 “C225” and/or “D225”. 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 “E225”. This will allow production of carbon dioxide and methane that contain $^{14}$C.

Non-zero values can be entered in cells “B228” to “B232” for the rates, under each of the conditions, of processes in the second phase of cellulose degradation during which glucose or ISA degrades to carbon dioxide and methane. If any of these rates 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 “C228” to “C231”. 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 “C232” and “D232”. 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.

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, $^{230}$Th, $^{234}$U, $^{238}$Pu, $^{242}$Pu, $^{242m}$Am, $^{242}$Cm and $^{246}$Cm in cells “B236” to “J236”. The hold-up factor entered in cell “B238” 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.

The section “Radiolysis” provides the data for the radiolysis model. The model can perform calculations of hydrogen gas generation from radiolysis of one or more of the following: water (within waste containers and in the associated backfill after repository closure), cellulose, other polymers and oils. 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. 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-factor.

To initialise the radiolysis model for any substance, a positive inventory for one or more of a comprehensive fixed set of radionuclides must be entered in appropriate cells in the region between cell “B241” and cell “I269”. 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-factors must also be non-zero. The mass of water is 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 polymers and of oils are not required in other models so are entered in cells “D272” and “E272”. The G-factors are entered in cells in the region between cell “B275” and cell “F283”. Separate G-factors are required for each type of decay ($\alpha$, $\beta$ and $\gamma$) and for each gas produced. 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 “B285”. Finally, for the radiolysis of water, 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 “B286” (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 cellulose, other polymers and oils are not modelled, as the fractions consumed by radiolysis are not expected to be significant.)

In the section “Radionuclide release from graphite”, the model to calculate active gas release from graphite is initialised by entering a non-zero value for the graphite mass in cell “B290” and an initial inventory for either or both of $^{14}$C and $^3$H in cells “B293” and “C293”. For each inventory added, a corresponding initial release rate must be entered in cells “B294” and “C294”. Finally, as $^{14}$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 entered in cell “B295”. By default it is assumed that none of the $^{14}$C is released as CO$_2$ (i.e. the fraction is zero).

**GasRates-############, CumulativeGas-############# and OtherResults-##############**

Pressing the button “Calculate” on worksheet “General Data” 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 for 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 repository (specified in cells to the right of “B25” 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, 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, 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 determined (by interpolation of the results for linear strain). The times for loss of wasteform and container integrity 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.

Charts

The “Charts” worksheet contains five boxes, with drop-down lists, and two buttons. A screen-shot of the “Charts” worksheet is shown in Figure 5. The purpose of the worksheet is to provide a simple method by which the user can generate a number of default graphs of the gas generation results on separate chart sheets. The default charts provided are all for rates or amounts of gases generated summed over all the gas generation processes (i.e. the default charts do not show results for individual gas generation processes such as corrosion, or for non-gas related results). For the active gases, rates are given in terms of the rates of release of activity of the various radionuclides, and cumulative amounts are given in terms of the amount of activity of the various radionuclides remaining in the released gas.

The five boxes provide options for:

- the type of result (cumulative amount or rate of gas generation),
- data source (the waste package or total from all waste packages),
- active or non-active gases to be plotted:
  - the plot of the production of a single, selected, gas,
  - plots of the production of all active gases or non-active gases on a single chart,
  - the plot of the sum of the production of all active gases or all non-active gases,
- the scale types for the axes (logarithmic or linear).

The graphs are generated by selecting the required options in each of the five boxes then pressing the button “Draw Chart”. A further button “Go to General Data sheet” provides a shortcut to the worksheet “General Data”. A screen-shot of an example generated chart is given in Figure 6.

It is also possible for the user to create additional charts manually from the data in the worksheets prefixed with “GasRates-”, “CumulativeGas-” and “OtherResults-”.
2.3 Running a Typical Calculation

The following describes the stages 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. Choose the amount unit ("m\(^3\)" or "mole") for the non-active gas results in the box on worksheet “General Data”.

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 “B3” to “yes”). Press button “Calculate” on worksheet “General Data”.

If there are pre-existing result worksheets or charts (see below) when the “Calculate” button is pressed then these will be deleted. The results will be calculated by the C++ application and displayed on results worksheets.

Three result 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, 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 result worksheets: “GasRates-AllPackages” and “CumulativeGas-AllPackages” containing the sum of the individual waste stream gas generation results; and “OtherResults-AllPackages” containing 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 go to worksheet “Charts”. If the user has the “General Data” worksheet on view (e.g. following the use of button “Calculate”)
there is a short-cut to worksheet “Charts” available by using button “Go to Charts sheet”. On worksheet “Charts” there are five boxes with drop-down lists containing graph plotting options:

- The “Result Type” can either be “Cumulative Amount” or “Rate” allowing charts to be plotted either of the cumulative amount of gas generated or of the gas generation rates.

- The “Data Source” box contains a list of the waste stream names “<name>” (i.e. the data worksheet names without the “Data-” prefix) and “AllPackages”. The chart will plot results from worksheet “CumulativeGas-<name>” or “CumulativeGas-AllPackages” if the “Cumulative Amount” option is chosen for the “Result Type” or results from worksheet “GasRates-<name>” or “GasRates-AllPackages” if the “Rate” option is chosen for the “Result Type”.

- The “Gas” box has the following options for displaying result sets for active or non-active gases: the total gas generated from all processes for a selected gas, the total gas generated from all processes for each gas plotted together, the sum of the amounts of all active gases or non-active gases produced.

- The “Y scale” box allows a choice of linear or logarithmic scale on the y-axis of the graphs. (Note: if a logarithmic scale is chosen, data points with value zero will not be plotted.)

- The “X scale” box allows a choice of linear or logarithmic scale on the x-axis of the graphs. (Note: if a logarithmic scale is chosen, data points at time zero will not be plotted.)

Once the five chart options have been chosen, the graph can be generated by using the button “Draw Chart”. A chart sheet will be added to the workbook. The name of the chart sheet is formed by combining “Chart-” with: the result type “Cm-” or “Rt-” (for cumulative amount or rate), the gas type (an individual gas, e.g. “H2-”, or all of the non-active gases, “NonActive-”, or all of the active gases, “AllActive-”, or the sum of all non-active gases, “SumNonAct-”, or the sum of all active gases, “SumAct-”), and the package name or “AllPackages”. An example is “Chart-Cm-H2-TestPackage”. If the same chart is re-plotted with a different choice of scale for the x- or y-axis the chart sheet will be overwritten.

8. The previous eight steps represent a complete modelling cycle. If revisions or additions to the data worksheets are now required a further cycle can be started. There is a shortcut from the “Charts” worksheet to the “General Data” worksheet by using the button “Go to General Data sheet”. Once the “Calculate” button has been pressed on worksheet “General Data” 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 and charts (the “GasRates-AllPackages”, “CumulativeGas-AllPackages” and “OtherResults-AllPackages” worksheets will be cleared of data).
3 OPERATION OF THE MULTI-RUN DRIVER

As described in Section 2, the main SMOGG model consists of two components: a C++ application which performs the calculation, and a customised Excel spreadsheet which handles the data input and output processing. In addition, an optional third component, a further Excel spreadsheet that provides an automated interface to the main spreadsheet for sequentially performing large numbers of calculations, is available. The use of SMOGG through this optional multi-run driver spreadsheet interface is described in the section.

3.1 Installation of SMOGG

The C++ application “SmoggApplication.dll” should be placed in the installation directory “C:\Program Files\Smogg\”. The intermediate temporary files “InputData.txt”, “CumulativeGas.txt”, “GasRates.txt” and “OtherResults.txt” will be written to this directory. To enable use of the main Excel spreadsheet “SmoggSpreadsheet.xls” by the multi-run driver, the main spreadsheet should also be placed in the installation directory “C:\Program Files\Smogg\”. The driver Excel spreadsheet “SmoggMultirunDriver.xls”, 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.

3.2 Structure of the Driver Spreadsheet User Interface

3.2.1 Introduction

As indicated, the driver spreadsheet for SMOGG is a spreadsheet 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 2), except that the driver automates the input of data and the running of calculations that otherwise would be performed by the user.

3.2.2 Description of each worksheet

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), buttons that run Excel Visual Basic macros (blue text on grey backgrounds) and a box for entering data from a fixed list.

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 of 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 and the calculations are aborted. The user is required to re-enter permissible or consistent data. If the error is detected during the processing of a calculation by the macros in the main SMOGG spreadsheet (rather than the macros in 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 is described below, followed by a description of a typical set of calculations in subsection 3.3.
**Calculation Control**

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 spreadsheet,
  - launches the macro in 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.

**General Data**

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 spreadsheet in subsection 2.2.2.

**Package Data**

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 varies 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 spreadsheet in subsection 2.2.2.

**Parameters**

The worksheet “Parameters” contains both general input and package data that varies 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. This 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 7.

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 spreadsheet to determine the number of variable parameters in the calculations, so no blank columns should be left between parameters. The maximum number of parameters that can be included is limited (by the size of a worksheet in Excel) to 254.

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 spreadsheet to determine the number of calculations in the set, so no blank rows should be left between calculations. The maximum number of calculations that can be included is limited (by the size of a worksheet in Excel) to 65530. (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-%%%%%%%%%%%%%%%%#” worksheets in subsection 2.2.2.

**Results**

Once a set of calculations have 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 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 packagesstreams.
3.3 Running a Typical Suite of Calculations

The following describes the stages in performing a typical suite of calculations with the 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 hasn’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 have been compiled, the calculation 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 SMOGG spreadsheet, which is constructed to perform each calculation, to be saved (for completeness, the spreadsheets 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 SMOGG spreadsheet will be constructed and the calculation run (and the 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 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.
4 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] (verification) is derived in two ways:

a) From the application of appropriate QA during the development of the program;

b) From the use of a comprehensive suite of test cases that have been developed to test the model.

Serco Assurance carries out its projects in accordance with the requirements of the BS EN ISO 9001:2000 standard. Its Business Management arrangements have been assessed by Lloyds Register Quality Assurance (LRQA) against the requirements of this standard and received certification of conformance to it (certificate Number LRQ 0964988). In particular, software development is carried out in accordance with the TickIT scheme.

SMOGG was developed following Serco Assurance’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 v5.0 is listed in Appendix B. Every effort was made to test the various models implemented in SMOGG against independent calculations. In most cases these calculations were carried out in Excel spreadsheets, in a few cases models implemented in Mathematica were used to derive the 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.
REFERENCES


FIGURES

Figure 1  Worksheet “General Data”
Figure 2  Worksheet Example “Data-TestPackage” (Part 1)
**Figure 2  Worksheet Example “Data-TestPackage” (Part 2)**
### Figure 2  Worksheet Example “Data-TestPackage” (Part 3)
Figure 2  Worksheet Example “Data-TestPackage” (Part 4)
Figure 2  Worksheet Example “Data-TestPackage” (Part 5)
Figure 2  Worksheet Example “Data-TestPackage” (Part 6)
Figure 2  Worksheet Example “Data-TestPackage” (Part 7)
Figure 3  Worksheet Example “GasRates-TestPackage”
### Figure 4  Worksheet Example “OtherResults-TestPackage”
Figure 5  Worksheet “Charts”
Figure 6  Example of Generated Chart
Figure 7  Driver Spreadsheet Worksheet “Parameters”
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 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$_4$ and $^{14}$CO$_2$ 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 v5.0.

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Description</th>
<th>Checking</th>
</tr>
</thead>
<tbody>
<tr>
<td>simple01a</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01b</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01c</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01d</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01e</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01f</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. (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>simple01g</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple01h</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. (Note: Spreadsheet requires oxygen exhaustion time as input.)</td>
</tr>
<tr>
<td>simple02a</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.</td>
</tr>
<tr>
<td>simple02b</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.</td>
</tr>
<tr>
<td>simple02c</td>
<td>Test of diffusion. Release of radionuclides from Zircaloy calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple02d</td>
<td>Test of diffusion. Release of radionuclides from Magnox calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple02e</td>
<td>Test of diffusion. Release of radionuclides from uranium calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple02f</td>
<td>Test of diffusion. Release of radionuclides from aluminium calculated.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple03a</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.</td>
</tr>
<tr>
<td>simple03b</td>
<td>Test of organic degradation to glucose and carbon dioxide production from degradation of glucose under aerobic (grouted) conditions.</td>
<td>Carbon dioxide release rate and cumulative release checked against Mathematica calculation.</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
<td>----------</td>
</tr>
<tr>
<td>simple03c</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.</td>
</tr>
<tr>
<td>simple03d</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.</td>
</tr>
<tr>
<td>simple03e</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.</td>
</tr>
<tr>
<td>simple04</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.</td>
</tr>
<tr>
<td>simple05</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.</td>
</tr>
<tr>
<td>simple06</td>
<td>Test of radiolysis of water, cellulose, polymers, oils and small organics 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.</td>
</tr>
<tr>
<td>simple07</td>
<td>Test of release of C-14 (in two forms) and H-3 from graphite.</td>
<td>C-14 and H-3 release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple08</td>
<td>Test of conversion of carbon dioxide and hydrogen to methane. Carbon dioxide generated from organic degradation as in test case simple03e with additional glucose as in test case simple011. Hydrogen generated from radiolysis as in test case simple06.</td>
<td>Methane, carbon dioxide, hydrogen and C-14 net release rates and net cumulative releases checked against independent spreadsheet calculation. (Note: Carbon dioxide, hydrogen and C-14 results from other processes required as input.)</td>
</tr>
<tr>
<td>simple09</td>
<td>Test of radionuclide release from corrosion with non-uniform radionuclide distribution in metal. Corrosion as in test case simple01a with aerobic period extended to end of calculation.</td>
<td>Radionuclide release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>simple10</td>
<td>Test of H-3 release from tritiated water via corrosion reactions. (Corrosion as in simple01d – Magnox only.)</td>
<td>H-3 release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>simple11</td>
<td>Test of C-14 release from degradation of ISA. (ISA production as in test case simple04.)</td>
<td>C-14 release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>massbal01</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 a spreadsheet.</td>
</tr>
<tr>
<td>massbal02</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 a spreadsheet.</td>
</tr>
<tr>
<td>massbal03</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 a spreadsheet.</td>
</tr>
<tr>
<td>massbal04</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 a spreadsheet.</td>
</tr>
<tr>
<td>miscell01</td>
<td>Test of the inclusion of multiple packages within a single waste stream.</td>
<td>Calculation rerun with a single package, then all results scaled and compared with test case results in a spreadsheet.</td>
</tr>
<tr>
<td>miscell02</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, then active gas and radiolysis results decayed by factor(s) corresponding to test case emplacement time and all results compared with test case results in a spreadsheet.</td>
</tr>
<tr>
<td>miscell03</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, then all results compared with test case results in a spreadsheet.</td>
</tr>
<tr>
<td>miscell04</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.</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
</tr>
<tr>
<td>----------</td>
<td>------------------------------------------------------------------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>miscell05</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.</td>
</tr>
<tr>
<td>miscell06</td>
<td>Test of gas release from unvented containers by all processes except corrosion.</td>
<td>Timing of gas release checked for consistency with time of container breaching (noting that radiolysis of water begins at repository closure).</td>
</tr>
<tr>
<td>miscell07</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.</td>
</tr>
<tr>
<td>miscell08</td>
<td>Test of gas release from unvented containers by corrosion of containers.</td>
<td>Hydrogen release rates and cumulative release checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>miscell09</td>
<td>Test of resaturation model characterised by a water inflow rate. Tests calculation of groundwater saturation (which depends on water inflow and consumption). Release of hydrogen by anaerobic corrosion of stainless steel calculated.</td>
<td>Independent numerical calculation performed to determine total water contents and groundwater saturations. Hydrogen release rates and cumulative release checked against values calculated from independent water and saturation data.</td>
</tr>
<tr>
<td>miscell10</td>
<td>Test of calculation of corrosion product volume, wasteform strain and critical times for physical containment.</td>
<td>Corrosion product volumes and critical times checked against independent spreadsheet calculation.</td>
</tr>
<tr>
<td>exhaust01</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.</td>
</tr>
<tr>
<td>exhaust02a</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.</td>
</tr>
<tr>
<td>Case ID</td>
<td>Description</td>
<td>Checking</td>
</tr>
<tr>
<td>-----------</td>
<td>------------------------------------------------------------------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>exhaust02b</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.</td>
</tr>
<tr>
<td>exhaust02c</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.</td>
</tr>
<tr>
<td>exhaust03</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.</td>
</tr>
<tr>
<td>driver01</td>
<td>Test of Multi-run Driver spreadsheet. 20 cases based on test case miscell10, with variations of parameters used for waste package integrity calculations.</td>
<td>Critical times for all cases checked against independent spreadsheet calculations.</td>
</tr>
<tr>
<td>driver02</td>
<td>Test of Multi-run Driver spreadsheet. 4 cases containing an 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, then all results compared with test case results in a spreadsheet.</td>
</tr>
</tbody>
</table>
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