Protocol for numerical models stored in the Science Model Warehouse

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Department of Environment, Water and Natural Resources

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Disclaimer

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Contents

1 Introduction

The Department of Environment, Water and Natural Resources (DEWNR) maintains a repository of numerical water models developed by [DEWNR](#) and the [Goyder Institute for Water Research](#). These numerical models are computer-based mathematical models that simulate hydrological and ecological processes, and have become essential tools for supporting water resource management.

This document provides guidance on how numerical models that are stored in the Science Model Warehouse can be used. It gives a clear and simple description of legal conditions for numerical models released from the warehouse, and also outlines standards for metadata, file directory structure and naming conventions.

1.1 Purpose of this protocol

This protocol will help to:

- Ensure the long-term integrity of numerical models developed by DEWNR and the Goyder Institute for Water Research, and all data and documentation associated with those models.

- Ensure that numerical models are version controlled and contain the best available scientific data.

- Ensure that modelling practitioners are provided with the most up-to-date numerical model for use in publically funded projects.

- Provide guidance on file structure and naming conventions for archiving numerical models in the Science Model Warehouse.

- Provide a clear and simple document, written in plain English, explaining the terms and conditions for the use of numerical models by external stakeholders.

- Outline the process that external stakeholders must follow to request numerical models from the Science Model Warehouse.

1.2 Audience

This protocol is written for specialist numerical water modelling practitioners and those managing numerical modelling projects. Predominantly this may include ecologists and surface and groundwater hydrologists working for government, research institutions and private industry.

1.3 Definitions

Term	Definition
Applicant	Private consultant or organisation applying to access and use the numerical model.
Archiving	A filing fold and rule for model storage, filing structure and model documentation.
Authorised Purpose	Purposes for a Local, State or Federal project which is named in the formal request.
Contract documents	List of detailed works and major processes that describe a numerical modelling project.
Document	Any embodiment of data, text or image related to numerical modelling works.
Goyder Institute	The [Goyder Institute for Water Research](). The Goyder Institute was established in 2010 for an initial term of five years as a partnership between the South Australian Government, CSIRO, the University of Adelaide, Flinders University and the University of South Australia to deliver expert advice to support water policy and water management in South Australia.
Intellectual Property Rights	Intellectual Property Rights are any patent, copyright, trademark, trade name, design, trade secret, know how or other form of intellectual property right whether arising before or after the execution of this Agreement and the right to registration of these rights.
Minister	Minister for Sustainability, Environment and Conservation Minister for Water and the River Murray Minister for Climate Change
Receiving Party	Applicant who has received the numerical model and has a permit to use it.
The model	Refers to the numerical model and associated data.
The Work	Numerical modelling work as described in the application for which the model is required.
Version control	A rule for model name convention.
Science Model Warehouse	The Science Model Warehouse is an ongoing data management service that maintains the integrity and accessibility of numerical models developed by DEWNR and the Goyder Institute. Includes protocols for developing, archiving, using and releasing numerical models.

2 Science model warehouse

2.1 Description

Numerical models developed by DEWNR and the Goyder Institute are housed in the Science Model Warehouse, an ongoing data management service that maintains the integrity and accessibility of numerical models. The systems and protocols established for the now superseded Groundwater Model Warehouse (a service provided by DEWNR's Science Unit from 2010-15), have been redeveloped and broadened for the Science Model Warehouse. The numerical models housed in the warehouse are discoverable publically via WaterConnect and within DEWNR via iShare.

There are four protocols that have been developed by DEWNR:

- *Protocol for developing numerical models* (DEWNR internal document)

- *Protocol for numerical models stored in the Science Model Warehouse* (public document)

- *Protocol for archiving numerical models* (DEWNR internal document)

- *Protocol for releasing numerical models* (DEWNR internal document)

2.2 Releasing models

This section describes the process Applicants must follow to request numerical models from the Science Model Warehouse.

The numerical models available from the Science Model Warehouse are shown on WaterConnect. For detailed information about each model, use the website links to view metadata and/or the model report. Before formally requesting model files and associated data, read the metadata/model report and legal conditions described in this document.

2.2.1 Formal request

To initiate the process of accessing a numerical model from the warehouse, a formal request is required. This request can be in the form of a pre-prepared email available on WaterConnect, or using the Letter of Request template in Section 6.

2.2.2 Project brief

A detailed outline of the project brief is required as an attachment with the formal request. The project brief must include details of authorised persons who will have access to the model and files and, if applicable, details of any third parties to whom modelling results and reports will be provided.

2.2.3 Declaration of agreement and participation

Prior to the release of a numerical model and the associated data files and documentation, a completed Declaration of Agreement and Participation form (Section 7) is required. This form must be co-signed by (1) the Applicant, or an authorised representative, and (2) DEWNR's Water Science Unit Manager.

Model files and input/output data files will be provided to the Applicant after the Declaration of Agreement and Participation form has been completed and signed by all parties.

2.2.4 Returning the model

All model files and data should be returned to DEWNR within the prescribed time frame (see Section 4). If the model is redeveloped, observe the following guidelines:

- All files (model and input/output data) are to be archived using the recommended filing structure and naming conventions described in Section 3.

- Model folder names must align with the recommended version control conventions (see Section 3.4).

2.2.5 Rights and responsibilities

Guidelines and policies detailed in Section 3 through Section 4 (inclusive) are to be followed during, at the conclusion, and after termination of the Work.

3 File structure and naming convention

All data and reports relevant to the numerical model should be archived in electronic format, using the guidelines in the following sections.

3.1 File directory structure

All modelling projects require a consistent, logical file directory structure to ensure file integrity, and allow for future replication and reuse for other applications. Modelling projects should use the standard modelling file directory examples shown in Figure 1. It is understood that model software or project specific requirements may result in minor amendments to this structure. Note that any files released from the Science Model Warehouse will not include project management or correspondence files.
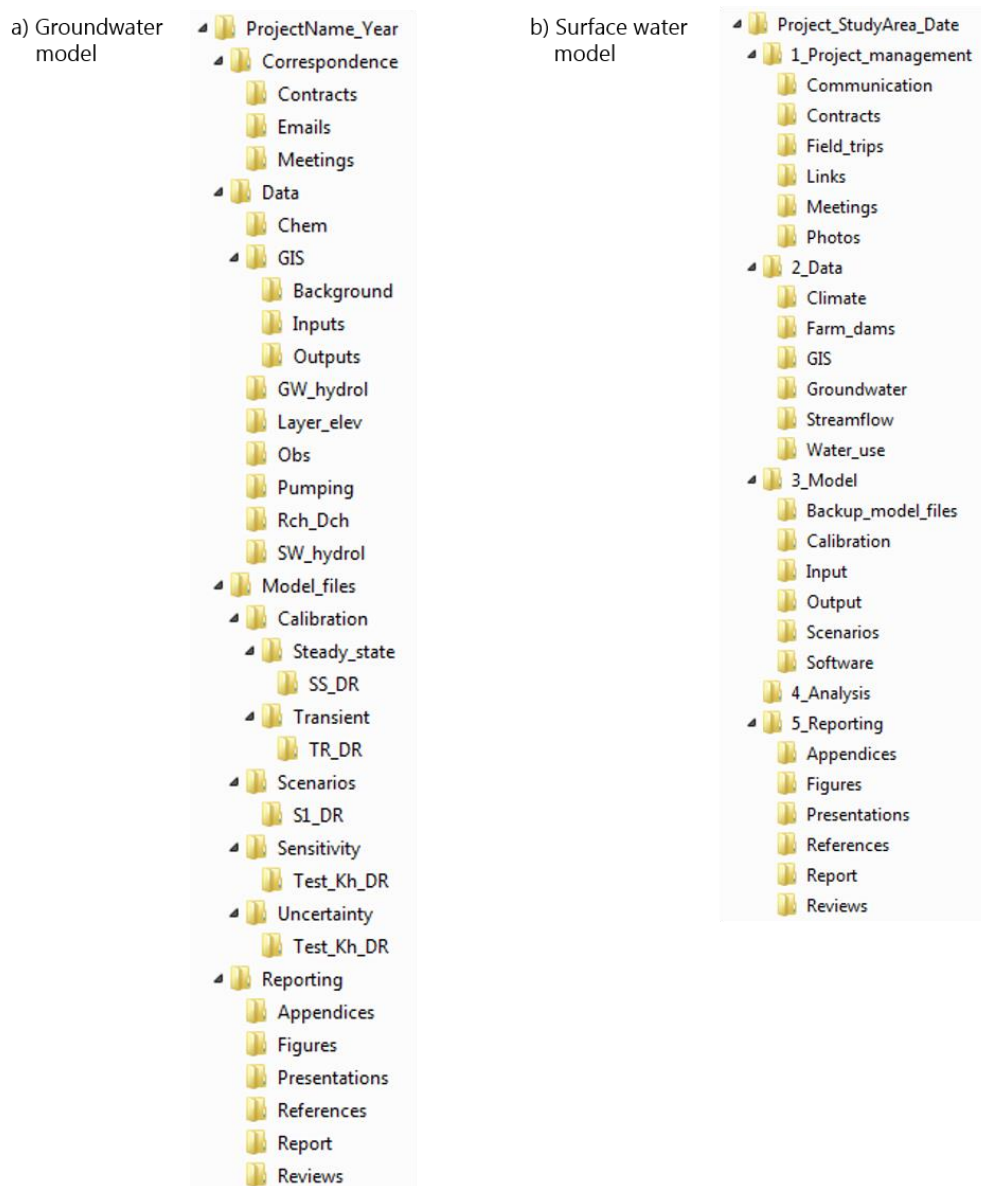

Figure 1. Example file directory structures for numerical models: a) groundwater model and b) surface water model. Ensure there are no spaces in the folder or file names (required for some software; helpful for later hyperlinking).

3.2 File naming conventions

3.2.1 Main folder

The name of the main folder should include the model name and year of the project. Including the year will assist with version control (Section 3.4). Some descriptive text can also be included. For example, the Adelaide Plains 2011 groundwater model could be named "AP2011".

3.2.2 Subfolders

The standard file directory structure in Section 3.1 provides guidance on naming conventions for project subdirectories. It is understood that model or project specific requirements may result in minor amendments to this structure.

3.2.3 Data and results

The data and results (DR) folder (Figure 1) is used to store input and output files for particular model runs. Examples of files that would be stored in a DR folder could include:

- Model initial head file (e.g. "AP2011_SS.hds") (where SS refers to a steady-state simulation).

  – If the model initial head file contains more than one stress period then a text file should be included to indicate which stress period is to be used.

- All inputs for transient model calibrations (e.g. recharge and pumping extraction rates) and model outputs (e.g. head levels and flux). Input and output files should be stored in separate folders.

- All inputs for prediction and scenario models (e.g. recharge and pumping extraction scenarios) and predicted outputs (e.g. head level and flux). Input and output files should be stored in separate folders.

3.2.4 Calibration

The final calibrated model files must have a filename that clearly indicates the modelling project name, followed by the model type (SS for steady state and TR for transient) and the year of completion. For example, the calibrated steady state groundwater model for the Adelaide Plains completed in 2011 could be named "AP2011_SS", and the calibrated transient model "AP2011_TR".

3.2.5 Scenario testing

When running scenarios using calibrated models, each scenario model must also be archived and named appropriately to indicate the calibrated model used and the scenario name. If the modelling project is to run scenarios using an already-existing model from a previous project, the completion date of the scenario run should also be included in the model name. As multiple scenario runs may occur in the same year, the month should also be included.

For example, if the calibrated Adelaide Plains transient model was developed in 2011 and was used to run a prediction scenario called Scenario 2, then the file name would be "AP2011_S2". If the same model was used to run another scenario called Scenario 3 in June 2012, then the file name would be "AP2011_S3_Jun2012".

3.3 Archiving files

At the completion of a modelling project, the following guidelines should be followed to archive model files:

- A text file called "READ_ME.txt" should be filed in the main project folder. This text file should document summary information about the modelling project.

- Final copies of all the model files should be zipped (to minimise the size and act as a preliminary backup) and archived in the appropriate Model_Files sub-folders (Section 3.1).

- All empty folders should be deleted to minimise the size of the directory.

- If the project involves changing an existing model, the changes are to be documented either in the model report or in the 'READ_ME.txt' text file mentioned above.

- Detailed model reports should accompany the model files.

- Metadata should be completed using the template in Section 5.

3.4 Version control

New versions of a numerical model will be treated as a new model. Including the year (and month, if necessary) in the name of the main folder will avoid confusion when archiving at the end of the project. For example, if the Adelaide Plains 2011 groundwater model was revised in 2013, a new project folder would be created ("AP2013") and the file directory structure and naming conventions described in the previous sections would be followed.

The superseded version of the numerical model will remain in the Science Model Warehouse for reference. A new text file will be filed in the main project folder directing future users to the new model version.

4 Legal rights

The Applicant (Receiving Party) is required to acknowledge their legal rights and responsibilities (as detailed below) by signing a Declaration of Agreement and Participation form (Section 7).

4.1 Copyright

Copyright applies to any Work produced by DEWNR or the Goyder Institute in the course of undertaking a modelling project, including any interim or incidental Documents produced during model development. These Works are owned by the Minister.

All Work by the Applicant that is produced using the Model, and/or using DEWNR/Goyder Institute model reports, and which is submitted for publication requires appropriate referencing, according to standard scientific conventions (e.g. references of the model from the department and model reports in the references list).

4.2 Receiving party's obligations

In consideration of the disclosure of the Model by DEWNR, the Receiving Party undertakes the following obligations:

a) The Receiving Party must only use the Model for the Authorised Purpose and in accordance with any conditions of use notified to the Receiving Party by DEWNR.

b) The Model shall not be used for any purpose in order to make financial gain, unless explicitly agreed to with IP holders.

c) The Receiving Party must promptly notify DEWNR if it is aware of any unauthorised disclosure of the Model.

d) During the course of the Work, the Receiving Party will not use the Model for any purpose that is not approved by the Minister as part of the Work.

e) The Receiving Party must promptly notify DEWNR if it is aware of any extension to the period of use of the Model which is greater than the duration originally proposed in the formal request.

f) Following completion of the Work, and following return delivery of the Documents and Models to DEWNR, the Receiving Party will not keep any copies of the model, nor use the Model for any subsequent purpose.

4.3 Documents

Upon termination or completion, and at any other time on demand by the Minister, the Receiving Party must deliver within fourteen days, all Documents and Models provided by, or originating from, the Minister and all Documents and Models produced by the Receiving Party, in the course of undertaking the Work, including:

a) Digital copies of data which related to model input/outputs

b) Working copies of all computer files required to run models

c) Data and reports supporting models.

4.4 Intellectual property rights

a) The Intellectual Property Rights of the Model will vest in the Minister. Those Rights are retained despite any disclosure to the Receiving Party.

b) DEWNR warrants that the use of the Model for the Authorised Purpose will not infringe the Intellectual Property Rights of the Model to any other party.

c) Additional data and new publications associated with the Work by the Receiving Party, pursuant to the Declaration of Agreement and Participation, will vest in the Minister and the Receiving Party.

d) The Goyder Institute Agreement grants the Government of South Australia a perpetual, royalty-free, non-exclusive licence to use, reproduce, adapt, communicate, publish and modify (but not commercialise) the Research Project Intellectual Property in South Australia, for the purpose of discharging the State's or an agency's role, function and responsibilities in and for the public interest in South Australia and to improve and further develop the Research Project Intellectual Property, for the agency's functions and responsibilities in and for the public interest in relation to water in South Australia. The State will own all such improvements to the Research Project IP.

5   Metadata

Table 1. Metadata template for numerical models. This metadata is to accompany all models archived in the Science Model Warehouse. This template is available for download on WaterConnect.

Metadata	Description
Model name / Version	Short, succinct, summary title that will be understood by multiple disciplines, including general public. Include year of publication and version.
Project name	Project name and organisation.
Project team	Names and email addresses.
Creator / Developer	Name, email address and organisation of model developers.
Key contact	Name, phone and email of key modeller who is able to provide technical advice.
Model location	Location of archived files.
Intellectual property / Confidentiality	Details of intellectual property issues or confidentiality agreements associated with the model and data (if applicable).
NRM Region	Natural Resources Management (NRM) region where domain is located (e.g. Eyre Peninsula).
Reporting region	Area/region of model domain (e.g. Scott River catchment, SA).
Description	Brief description of model.
Software package	Software package(s) (e.g. Modflow; Source). Include information on dependencies upon: 1) other models and/or platforms (including version) 2) essential data and data sources.
Platform / Language	Modelling platform used and computational requirements. Include skills/ resources required to run model (e.g. knowledge of C#, etc).
How model was used	Outline of model (construction; spatial and temporal discretisation; scenarios; parameterisation/validation; key assumptions; key limitations; sensitivity tests; uncertainty analysis; extensibility; peer review process).
Data sources	Inventory of data sources.
Publications / Reports	Citations. Include hyperlinks to published report(s) or articles where possible.
Collaborations / Acknowledgements	Collaborative partners, advisory groups and/or peer reviewers.
Keywords	Index terms or descriptors.
Model domain	Include a map of the model domain, or a shapefile with geographic coordinate system GDA 1994.

References: This metadata template was adopted from the Goyder Institute; with reference to Location SA, CSIRO's Data Access Portal and Research Data Australia (operated by the Australian National Data Service).

6   Template – Letter of request

[Insert date]

[Name of Applicant]
[Position]
[Organisation]
[Address]

Water Science Unit Manager
Science, Monitoring and Knowledge Branch
Department of Environment, Water and Natural Resources
GPO Box 1047
ADELAIDE SA 5001

To the Water Science Unit Manager,

RE: THE [INSERT MODEL NAME] – ACCESS AND USE

I am writing to you in relation to accessing the [insert model name] that was developed by, and is the intellectual property of [DEWNR; or insert name of Goyder Institute research partner]. This model was reported in [insert report title(s)].

The model will be used, and may be modified, as a part of the [insert project name]. This [insert funding partner, e.g. State or Commonwealth] funded project is to be conducted in collaboration with [insert name of collaborative organisation(s) e.g. NRM Board; SA Water; DEWNR]. A copy of the project brief and project contract are attached.

The project will run until [insert date], and it is requested that permission to use the model be granted over this period.

In signing the Declaration of Agreement and Participation form, I declare that I understand my rights and responsibilities, and the conditions of use of Department of Environment, Water and Natural Resources (DEWNR) numerical models, as outlined in DEWNR's *Protocol for numerical models stored in the Science Model Warehouse*.

Please contact [insert Applicant's Name] on [insert Applicant's phone number] or [insert Applicant's email address] if you have any queries in relation to this matter.

Yours sincerely

[SIGN HERE]

[Insert name]

[Insert position]

[Insert Organisation]

7 Form – Declaration of agreement and participation

<table>
<tr><td colspan="3">DECLARATION OF AGREEMENT AND PARTICIPATION

We agree to use the model in accordance with the conditions listed in the protocol, as listed in this document under sections below:</td></tr>
<tr><td></td><td>Applicant's name</td><td>Applicant's signature</td></tr>
<tr><td>Section 3 – File structure and naming convention</td><td></td><td></td></tr>
<tr><td>Section 4 - Legal rights</td><td></td><td></td></tr>
<tr><td colspan="3">DECLARATION OF AGREEMENT TO FOLLOW CONDITIONS

We agree to use the model in accordance with the conditions listed in the contract documents and protocols</td></tr>
<tr><td>ORGANISATION</td><td>Applicant</td><td>DEWNR</td></tr>
<tr><td>SIGNATURE</td><td></td><td></td></tr>
<tr><td>NAME</td><td></td><td></td></tr>
<tr><td>POSITION</td><td></td><td></td></tr>
<tr><td>DATE</td><td></td><td></td></tr>
</table>