



Mixing Cell Models

The mixing cell approach represents a method for the inverse calculation of groundwater fluxes and/or various sources of inflows from hydrochemical and isotopic data.

This approach is an extension of the simple mixing cell approach for the assessment of the relative influx of two end-members to complex flow systems with several compartments, each of which may have several sources of recharge. The mixing cell approach makes use of the mathematical theory and techniques for optimizing flow systems of quadratic water and mass balance objective functions with linear chemical mass balance constraints.

Method

The flow system is first conceptualized and then characterized by its chemical and/or isotopic compositions. Later, it has to be translated into mathematical expressions: a set of linear water and mass balance equations. In general, real hydrogeological systems tend to have 'fuzzy' hydrological parameters, and measured data are prone to errors. Therefore, optimization methods need to be applied for solving the system of linear mass balance equations describing the flow model structure.

In this site we provide the software (MIG) for running a compartment or mixing cell model for a steady flow system under the Excel© environment, together with information, explanations and examples on how and when to use this technique successfully. A comprehensive well documented „help manual“ and three examples are provided to assist the user to get acquainted with the Mixing Cell Model (MCM) approach.

Downloads

In this section we provide the latest versions of the mixing cell models.

- [install.txt](#) - first instruction on handling the installaton file
- [Mixing Cell Model for Excel, version 1.0](#)
- [Help file](#) for the Mixing Cell program for Excel (pdf)

The distribution also contains three examples that can be used for getting acquainted with the Mixing Cell method and program. As separate download:

- An example with 1 cell and 5 sources ([data_1_5.xls](#))
- An example with 4 cells and 12 sources ([data_4_12.xls](#))
- An examples with 12 cells, 17 sources ([data_12_17.xls](#))

Mixing Cell for Excel

At this stage there are two major lines of development. The Mixing Cell Model Generator a macro extension to Microsoft® Excel® is available for download. The latest version is MixCell 1.0.

Compiled MCMsf

Soon a stand alone version for Microsoft Windows© computer will be released. The suffix represent steady flow as we are also working on extending the MCM paradigm to unsteady low systems. The stand alone version has an extensive help documentation interface.

Documentation

The following MIG computer code is restricted to a steady flow and steady hydrochemical flow system. The code for a non-steady hydrological system is still heavily dependent on external optimization libraries, such as the NAG© Library. Therefore, a stand-alone “friendly” code or solver for a non-steady system has yet to be compiled. Readers looking to implement the mixing-cell approach in a non-steady hydrological flow system are encouraged to contact the authors. In order to simplify the procedure of preparing the data and running the Mixing-Cell Model for a steady flow system, a special Mixing Input Generator (MIG) has been programmed. MIG is a Visual Basic Microsoft© application that runs within Excel© (5.0 or newer version) via Windows 95® or a newer environment. The program has been tested and used successfully in Windows NT©, Windows 95©, Windows 98©, Windows XP© and Vista©, together with Excel 5.0, 7.0 & stand-alone Version MIG that runs on a Windows© system without Microsoft Excel© is also available. The following section 1 provides some clarifications of terms that are used in MCM in the MIG version. For elaboration of the basic assumptions and for further mathematical description, the user is referred to the explanations provided in the scientific publications provided in this manual.

Terminology

Sources

The term source refers to any flow component that contributes water and mass of dissolved constituents to any cell within the modeled aquifer. A source is used to represent external inputs into the flow system (for example: sources of groundwater recharge or any genuine contribution from outside the modeled aquifer or any other modeled flow system). It is considered to be a potential end-member with a constant chemical and/or isotopic composition. A source can also be used to simplify part of the modeled system, such that a complex subsystem can be introduced as a lumped source of inflow into the modeled area.

Cells

The modeled aquifer is discretized or subdivided into homogeneous compartments within which all the considered parameters are assumed to be constant for a specific time period, such as hydraulic

heads, isotopic composition and ionic concentrations. Mixing of various sources or contributors such as from upstream compartments and external sources, and dilution with water already existing in the cell, control the concentration of the characteristic chemicals and the isotopic compositions of each compartment. Therefore, every well-mixed or homogeneous aquifer section (cell or compartment) is characterized by a unique representative chemical concentration and/or isotopic composition.

A cell must have input fluxes, either from output flux from an upstream cell, from a source, or from several sources. Each cell must have an output flux, either into a downstream cell (or cells), via withdrawal of water (i.e. pumping), or via natural subsurface groundwater flow leaving the system, so that the water balance is maintained.

Every cell can have a number of sources and can contribute water to several downstream cells. Any hydrological connection between two cells will have a unique flow direction. Fluxes into and out of cells are proposed along the downstream hydraulic head gradients. Possible hydraulic connections among cells based on groundwater head gradients are proposed prior to the optimization process, i.e., the assigned flow vector cannot change its direction during the period for which the optimization is performed. As a result of the optimization process a flow rate (≥ 0) is attributed to each potential flow component. Some fluxes might end up with an effective rate of 0. This means that this specific component has been considered as a potential contributor, but in reality it is not active and does not contribute a substantial flux into the specific cell. In addition, in cases where a cell is assigned a potential source that has a very similar chemical concentration to another source which was also assigned to the same cell, or has a specific chemical composition that is (or close to) a linear combination of another source, the solver will combine the contribution of these two sources into one. In other words, one of these sources will be given the entire flux of the two, and the other will be assigned zero flux. The solver of this model cannot assign flux values to missing flow components that were not identified or introduced into the model.

Requirements

A PC with Windows® operating system (Windows 95® or newer) is needed. MIG itself is an Excel® file that contains a number of “macro” routines for processing other Excel® files. Therefore, Excel 5.0® or a newer version is needed, such as Excel 2000®. The language of the system (English, German, International versions) does not seem to make any difference to the program execution. All the comments and commands of MIG, however, are in English.

Installation

The installation file MixCell_setup.exe contains the necessary software. The file is an archive containing compressed files. It is recommended to create a folder c:mixel in which the unzipped files can be stored. You may, however, choose any other folder. Activate (double-click) MixCell_setup.exe to start the decompression. A window will open asking you for the target directory. Please confirm or choose an alternative directory using the ‘Browse’ button. Clicking the ‘Unzip’ button will start the extraction of files to be inserted in the selected directory. After extraction of the data files, MIG can be operated directly from the Excel-data-file.

Please also refer to the detailed instructions file help_MIG.pdf that come with the installed package.

Publications

- ADAR E. M. (1984): Quantification of aquifer recharge distribution using environmental isotopes and regional hydrochemistry. Doctoral thesis, Univ. of Arizona, Tucson, United States, 269 p.
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- KÜLLS, C. (2000) Groundwater of the North-Western Kalahari, Namibia. (PhD/Dissertation), Fakultät of Geosciences, University of Würzburg, 2000. (Online Document at the German Library)
- KÜLLS C., ADAR E., GEYH M. & UDLUFT P. (1999) Identification of Subsurface Fluxes into the North-Western Kalahari Basin Using Environmental Tracers. J. Conf. Abstr., 4(1): p. 584

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