A Guide to Using the Basin2 Software Package

Basin Modeling with Basin2

Release 5.0.1

Craig M. Bethke
Ming-Kuo Lee
Jungho Park

Hydrogeology Program
University of Illinois

Printed August 18, 2007
This document was prepared for the research affiliates of the Hydrogeology Program, who sponsored this work:

- Amoco Production Company
- ARCO Oil and Gas Company
- British Petroleum Research
- Chevron Oil Field Research Company
- Conoco, Incorporated
- Du Pont Company
- ExxonMobil Upstream Research Company
- Idaho National Engineering and Environmental Laboratory
- Hewlett Packard, Inc.
- Illinois State Geological Survey
- Japan National Oil Company
- Lawrence Livermore National Laboratories
- Marathon Oil Company
- Mobil Research and Development
- Sandia National Laboratories
- SCK-CEN
- SiliconGraphics Computer Systems
- Texaco, Incorporated
- Union Oil Company of California
- United States Geological Survey

© Copyright 2002 by the authors and The Board of Trustees of the University of Illinois; previous editions © Copyright 1993, 1999. This document may be reproduced freely to support any licensed use of the Basin2 software. All other rights reserved.

The software programs described in this document were developed over many years by the staff and students of the Hydrogeology Program in the Department of Geology at the University of Illinois at Urbana-Champaign, in collaboration with a large number of affiliate researchers. The software authors thank all those who gave us guidance in designing the codes, suggested improvements, and reported flaws.

Mary Glockner edited this Users Guide and Joan Apperson prepared the cover design; Amy Berger, Jeffrey Biesiadecki, Melinda Legg, and Wanbing Li checked facts and content.

Software copyright notice: Programs Basin2 and B2plot © Copyright 1982–2002 by The Board of Trustees of the University of Illinois. An unpublished work distributed via trade secrecy license. All rights reserved under the copyright laws.

Software Restricted Rights Legend: Use, duplication, or disclosure by the Government is subject to restrictions as set forth in subparagraph (c)(1)(ii) of the Rights in Technical Data and Computer Software clause at DFARS 252.227-7013. The Board of Trustees of the University of Illinois, Urbana, Illinois.

CGM is a standard of the American National Standards Institute; Canvas™ is a trademark of Deneba Systems; Microsoft®, MS®, Windows 95®, Windows 98®, and Windows NT® are registered trademarks of Microsoft Corporation; The Geochemist’s Workbench® is a registered trademark of The Board of Trustees of the University of Illinois; PostScript® is a registered trademark of Adobe Systems, Inc.; Silicon Graphics® is a registered trademark of Silicon Graphics, Inc.; SPARCstationTM is a trademark of Sun Microsystems, Inc.; UNIX® is a registered trademark of AT&T Bell Laboratories; X Window System™ is a trademark of the Massachusetts Institute of Technology. Other products mentioned in this document are identified by the trademarks of their respective companies; the authors disclaim responsibility for specifying which marks are owned by which companies.
Contents

1 Introduction 1
   About Basin2 ......................................................................................................................1
   Origin of the programs ......................................................................................................2
   Modeling goals and expectations ......................................................................................3
   Constructing a basin model ...............................................................................................4
   Input conventions ..............................................................................................................6
   Gridding and the numerical solution ..................................................................................7
   Input and output .................................................................................................................9
   Displaying your results .....................................................................................................10
   Further reading ................................................................................................................12
   Users’ group ......................................................................................................................12
   Software distribution .......................................................................................................12
   Getting further help .........................................................................................................13

2 Setting Rock Properties 15
   About rock properties ....................................................................................................15
   Porosity evolution ............................................................................................................16
   Permeability .....................................................................................................................21
   Thermal conductivity .......................................................................................................23
   Rock density and heat capacity .......................................................................................24
   Diffusion and dispersion .................................................................................................25
   Built-in rock types and default values .............................................................................26

3 Fluid Properties 29
   About fluid properties .....................................................................................................29
   Fluid density .....................................................................................................................29
   Viscosity ..........................................................................................................................31
   Heat capacity ...................................................................................................................32
   Halite saturation .............................................................................................................33

4 Defining Basin Stratigraphy 35
   About basin stratigraphy ...............................................................................................35
   Stratigraphic units and wells ...........................................................................................35
   Rules of scope ................................................................................................................37
   Deposition and erosion, uplift and subsidence ...............................................................39
   Volume averaging ..........................................................................................................41
Hydraulic faults.................................................................................................................................................... 43

5 Transient and Steady State Solutions ............................................................................................................. 45
   About transient and steady state solutions ........................................................................................................ 45
   Transient solutions ............................................................................................................................................. 45
   Time stepping ..................................................................................................................................................... 48
   Time weighting .................................................................................................................................................. 49
   Numerical stability ........................................................................................................................................... 50
   Steady-state solutions ....................................................................................................................................... 51

6 Configuring and Running Basin2 ........................................................................................................................ 55
   About configuring and running Basin2 ................................................................................................................ 55
   Groundwater flow .............................................................................................................................................. 55
   Heat transfer ....................................................................................................................................................... 57
   Organic maturation ........................................................................................................................................... 58
   Salinity distributions ......................................................................................................................................... 59
   Isotope transport .............................................................................................................................................. 60
   Hydrologic residence time ................................................................................................................................. 61
   Cementation ....................................................................................................................................................... 62
   Radial flow and wedging .................................................................................................................................... 63
   Gridding ............................................................................................................................................................. 64
   Running the programs ....................................................................................................................................... 64
      From the Basin2 control panel .......................................................................................................................... 65
      From the command prompt ............................................................................................................................ 66
      On a Unix workstation .................................................................................................................................. 67
   Output tables ..................................................................................................................................................... 68
   Plot interface ..................................................................................................................................................... 71
   Debugging variables ........................................................................................................................................ 72

7 Compaction, Pressure, and Groundwater Flow ............................................................................................... 73
   About compaction-driven flow ........................................................................................................................... 73
   Rate of groundwater flow .................................................................................................................................. 74
   Hydraulic potential ............................................................................................................................................ 75
   Compaction in one dimension ............................................................................................................................ 76
   Compaction of the Niger Delta .......................................................................................................................... 79

8 Groundwater Flow due to Topographic Relief ................................................................................................. 85
   About topography-driven flow ........................................................................................................................... 85
   Flow in homogeneous basins .............................................................................................................................. 86
   Flow in heterogeneous basins ............................................................................................................................. 89

9 Erosion and Groundwater Flow .......................................................................................................................... 93
   About the effect of erosion on flow...................................................................................................................... 93
   One-dimensional model ................................................................................................................................... 93
   Western Canada Sedimentary basin ................................................................................................................... 95
10 Heat Transfer and Thermal Convection

About heat transfer.................................................................99
Rate of heat transfer .................................................................99
Thermal convection.................................................................100

11 Organic Maturation

About modeling organic maturation .................................103
Lopatin model........................................................................103
Arrhenius model................................................................104
LLNL vitrinite model..............................................................105
Effect of heat flow.................................................................106
Organic maturation of Niger basin...........................................108

12 Mass Transport and Salinity

About modeling salt transport............................................111
Rate of mass transport........................................................111
Infiltration of a surface brine..................................................113
Buried halite layer.................................................................115

13 Groundwater Flow and Cementation

About modeling cementation.............................................119
Mineral solubility.................................................................119
Mathematical model............................................................121
Linkage to React.................................................................122
Cementation in a sloping aquifer........................................123
Cementation near a fault zone............................................124

14 Isotope Transport

About modeling isotope transport........................................127
Source rates of the isotopes................................................127
Neutron production............................................................127
Production of 3He...............................................................128
Production of 4He ...............................................................129
Decay and production of 36Cl .............................................130
Production of 40Ar.............................................................131
Helium distribution in a basin................................................131

15 Using B2plot

About B2plot.................................................................135
“File” menu.................................................................136
“Plot” menu.................................................................136
Cross-section plots............................................................137
Plots versus distance, depth, or time .......................137
Global keystroke commands........................................138
Appendix 1  Glossary of Basin2 Keywords 143

About Basin2 keywords ........................................................................................................ 143
Keyword glossary.................................................................................................................. 144

A1_3He, A1_36Cl ................................................................. 144
A1_4He, A2_4He, A1_40Ar .............................................. 144
A1_nflux, A2_nflux .......................................................... 145
A_mk, B_mk, C_mk, D_mk, E_mk ..................................... 145
A_perm ............................................................................ 145
A_tc ................................................................................. 146
act_eng ........................................................................... 146
alpha_L ........................................................................... 146
alpha_T ........................................................................... 146
arrrhenius ...................................................................... 147
Axsect ............................................................................ 147
Axsect_6Li, Axsect_35Cl ............................................... 147
B_perm ............................................................................ 147
B_tc ................................................................................. 148
balance .......................................................................... 148
beta_por ........................................................................... 148
beta_ul ............................................................................ 149
bottom_conc .................................................................. 149
bpor ................................................................................ 149
bpor_ul ............................................................................. 150
bulk_density .................................................................... 150
cbase_isol, cbase_iso2 .................................................. 150
cementation ..................................................................... 151
column ............................................................................ 151
compaction ...................................................................... 151
conc_increase .................................................................. 152
conv_conc ....................................................................... 152
conv_isol, conv_iso2 ...................................................... 152
conv_press ....................................................................... 152
conv_temp ....................................................................... 153
conv_tres ....................................................................... 153
csurf_isol, csurf_iso2 .................................................... 154
delta_z .............................................................................. 154
density ............................................................................. 154
diff_con ........................................................................... 155
diff_isol, diff_iso2 ........................................................ 155
diff_T ............................................................................... 155
diff_tres ........................................................................... 156
diffpt_isol, diffpt_iso2 .................................................... 156
diff_tres

disequilibrium

disp_tensor

dt_max

dump_end

dump_start

dz0

dz

dump_start

dump_end

equilibrum

eustat

equilibrum

eustat

explain

fault

fault_begin

fault_bottom

fault_end

fault_position

fault_top

fault_xperm

fault_zperm

feedback

flip

flow

halite_sat

halite_solubility

heat_flow

include

initial

initial_step

isol_flux, iso2_flux

isol_increase, iso2_increase

isol_equation, iso2_equation

isol_type, iso2_type

iterations

left

left_table

max_iter

max_passes

max_steps

min_nodes

meteoric_conc

nx

nz_max

p_kxxkz

passes

perm_max

phi0
1 Introduction

About Basin2

Basin2 is a numerical model designed to trace through geologic time the evolution of groundwater flow regimes within sedimentary basins. You, the modeler, provide data on the arrangement of basin strata along a vertical cross section, the timing of sediment deposition and erosion, and the physical and hydrologic properties of sediments and rocks in the basin. From these data and equations describing flow and transport, the model reconstructs basin development.

The results may be presented in table form, but most commonly you display and interpret results graphically using the program B2plot, which is included in the Basin2 workbench. Basin2 and B2plot work on PCs under MS Windows. The Basin2 program may also be compiled to run on various types of computers running the Unix operating system.

Depending on how you configure your input, output from the program can include the evolution of:

- **Porosity and permeability** of strata across the basin, as calculated from overburden stress, fluid pressure, and stress history.
- **Fluid pressure** in basin strata, accounting for the effects of sediment compaction during burial and rebound during unloading, the development of topographic relief, thermal expansion, and fluid migration.
- **Flow patterns** of groundwaters through the basin in response to sediment compaction and rebound, buoyant forces, and topographic relief.
- **Temperature** throughout the basin as controlled by heat conduction, groundwater advection, and the crustal heat flux.
- **Thermal maturation** of organic matter in basin strata, including the timing of oil and gas generation and the distribution of mature petroleum sources through geologic time.
- **Salinity** of basin groundwaters, accounting for diffusion, hydrodynamic dispersion, advection, and the presence of evaporites.
- **Cementation** of basin strata, including the rates at which cements precipitate and minerals dissolve as a result of the migration of
groundwaters over flow paths along which temperature and pressure vary.

- **Radioactive and radiogenic isotopes** in basin groundwater, including the distribution of isotopes in the systems $^4\text{He}/^3\text{He}$, $^{36}\text{Cl}/\text{Cl}$, and $^{40}\text{Ar}/^{36}\text{Ar}$. These isotopes are used in basin hydrology to estimate the residence time (or "age") of groundwater in sedimentary basins.

Later chapters in this guide explain how the program calculates each of these aspects of basin evolution.

## Origin of the programs

The Basin2 software package was developed over more than fifteen years in a cooperative project between industry and the Hydrogeology Program at the University of Illinois at Urbana-Champaign. Craig Bethke, sponsored by Exxon Production Research Company and ARCO Oil and Gas Company, wrote the original versions of Basin2 and B2plot in 1982. Since then, under the sponsorship of more than a dozen companies and laboratories (Table 1.1), programmers and graduate students in the Hydrogeology Program have extensively revised and expanded the original codes.

### Table 1.1 Members of the consortium that sponsored Basin2 development (* indicates sponsors of Release 4).

<table>
<thead>
<tr>
<th>Company/Multinational Organization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amoco Production Company</td>
</tr>
<tr>
<td>ARCO Oil and Gas Company*</td>
</tr>
<tr>
<td>British Petroleum Research</td>
</tr>
<tr>
<td>Chevron Oil Field Research Company*</td>
</tr>
<tr>
<td>Conoco, Incorporated*</td>
</tr>
<tr>
<td>Du Pont Company</td>
</tr>
<tr>
<td>Exxon Production Research*</td>
</tr>
<tr>
<td>Idaho National Engineering and Environmental Laboratory*</td>
</tr>
<tr>
<td>Hewlett Packard, Inc.</td>
</tr>
<tr>
<td>Illinois State Geological Survey</td>
</tr>
<tr>
<td>Japan National Oil Company*</td>
</tr>
<tr>
<td>Lawrence Livermore National Laboratories*</td>
</tr>
<tr>
<td>Marathon Oil Company</td>
</tr>
<tr>
<td>Mobil Research and Development*</td>
</tr>
<tr>
<td>Sandia National Laboratories*</td>
</tr>
<tr>
<td>SCK-CEN*</td>
</tr>
<tr>
<td>SiliconGraphics Computer Systems*</td>
</tr>
<tr>
<td>Texaco, Incorporated*</td>
</tr>
<tr>
<td>Union Oil Company of California</td>
</tr>
<tr>
<td>United States Geological Survey*</td>
</tr>
</tbody>
</table>

Thomas Corbet developed a method of simulating the effects of surficial erosion, Kurt Larson coded the mass transport equations that describe the movement of dissolved salt, and Ming-Kuo Lee programmed the algorithms for modeling cementation. Jeffrey
Biesiadecki wrote the modules that read user input in free form, and added the routine that allows Basin2 to take input in a variety of units.

Charles Norris and Thomas Dirks developed the first interactive version of B2plot (the original was designed for batch computers and floor-model plotters in use around 1980). Brian Healy wrote a library used by B2plot to display graphics on a variety of output devices, and Walter Kreiling revised it to work under X Window System. Bethke rewrote the entire B2plot program as a menu-driven program offering the current plot options; Kreiling, Jeffrey Biesiadecki, and Daniel Hayba added new features. Kreiling developed an improved version of B2plot, implemented with its point-and-click interface. Bethke, Kreiling, Hernán Quinodoz, and Lee developed the third generation of the package, which was released in 1993.

Since then, the package has been ported to the PC platform under MS Windows, primarily through the efforts of Corey Steffen, Tren Haselton, Ester Soriano, and Rick Hedin. Quinodoz, Xiang Zhao, Theresa Fritzel, Jungho Park, and Bethke expanded the code to account for the transport of radiogenic and radioactive isotopes, as well as a number of other new features. Steffen and Haselton once again replaced the B2plot program with an improved version, using a graphics library designed and largely written by David Solt. The current release of Basin2, representing the package’s fifth generation, was developed with the assistance of Lalita Kalita, Rick Hedin, Jungho Park, and David Solt.

Modeling goals and expectations

A model may be defined as “a simplified version of reality that is useful as a tool.” By this definition, a model should not be so simple that it fails to resemble reality and hence is not useful. Neither should a model be so complex in its attempt to approach reality that it becomes too cumbersome to evaluate.

In basin modeling, the data available to constrain models are invariably insufficient to describe the full complexity of the basin subsurface. Even if data were available in such detail, modern computers would be incapable of manipulating and displaying it. A basin model, therefore, can not be expected to mirror reality because information about the real system is always incomplete. Even though some information used to construct a model comes from direct observation, a considerable amount of input data represents assumptions about the unknown details of the system. There are, therefore, subjective aspects to each model because modelers make different assumptions about those details.

The process of modeling is iterative by nature. The modeler runs the model, analyzes results, changes some assumptions or asks for more data, and runs the model again. This process continues until the modeler considers that his or her results represent reality reasonably well, given the information available. In making this judgment, the modeler considers what the results will be used for and what type of questions
they will be expected to answer. A simple model, for instance, can be used for a preliminary screening of alternatives, but a more detailed one is needed to make operational decisions in later stages of a project. In other words, modeling goals largely affect the modeling results.

Basin modelers use programs like Basin2 to investigate how hydrologic processes operate and interact in the subsurface, to understand how transport phenomena operate on basin scales, and to visualize how basins have evolved through geologic time. Goals might include providing insight into where and when petroleum accumulated in a basin, how ore deposits formed, or what factors influenced the distribution of diagenetic cements. Using Basin2, you can pose questions, test ideas quantitatively, and investigate the factors controlling subsurface processes. By performing tests under a spectrum of conditions, you can develop an intuitive feeling about complex aspects of basin hydrology. You will probably find inappropriate theories to reject. At the end of the day, you can present diagrams showing the results of your tests.

The practice of modeling lies in these pursuits and is not complicated. The art of modeling, however, is bridging the gap between computer output and reality. A first-hand knowledge of reality, therefore, is an integral part of modeling. Scientists with mathematical or computing skills may excel at modeling practice, but geologists who study basins directly many times make the best modelers.

Constructing a basin model

To calculate a basin model, you provide Basin2 with three types of information. First, you specify the physical and hydrologic properties of the various types of rock and sediment that make up the strata in the basin you are studying. Properties of three rock types are already built into Basin2. The predefined rocks are a generic sandstone, shale, and carbonate. Instead of relying on the built-in values, however, you will probably want to use data taken from the basin under study.

You can, for example, define a rock type with the properties of a dolomite formation, labeled dol, with statements such as

```
rock dol
phi0 = 35%; phi1 = 5%
A_perm = 8; B_perm = -5 log_darcy
```

Here, \( \phi_0 \) is the reducible porosity present at deposition, \( \phi_1 \) is the irreducible porosity that will persist even after deep burial, and \( A_{\text{perm}} \) and \( B_{\text{perm}} \) are coefficients in the correlation that defines permeability. The program automatically assigns default values to the other variables used to describe the rock type. Chapter 2 gives complete details on setting rock properties.

Second, you tell Basin2 about the arrangement of strata in the basin and the evolution of the basin through time. You can divide the basin into as many stratigraphic units as you wish, subject to practical
considerations and the size of program arrays. It is advisable to begin
with the simplest possible model and then add complexity as you go
along.

At a minimum, you specify when each stratigraphic unit in the basin
was deposited, how thick it is, and the rock type or types of which it is
composed. Each unit can vary in thickness and composition (i.e., undergo
facies changes) along the cross section. You can also describe how strata
uplift or subside through time and how quantities such as heat flow vary
over time and along the cross section.

To describe a sandstone of constant thickness along the cross section
that contains 10% shale interbeds, for example, you can enter the
statements

```
strat 'Triassic sandstone'
t_dep = -195 m.y.
thickness = 250 m
X(ss) = 90%; X(sh) = 10%
```

Here, \( t_{\text{dep}} \) is the time, 195 million years ago, at which deposition of the
sandstone was complete. You might, on the other hand, describe a
formation that varied in thickness and composition with the input

```
strat 'Mississippian dolomite/shale'
t_dep = -310 m.y.
column     thickness(ft)  X(dol)   X(sh)
well(1)       220         1/3      2/3
well(2)       180         .55      .45
well(3)       170         .75      .25
well(4:6)     175         .95      .05
```

In this block, the formation’s thickness and composition are set at six
positions or wells well(1), well(2), etc., across the basin. (You set
positions of the wells separately in the input, as described later.) The last
line sets values at wells four through six. The program automatically
interpolates among wells when it grids the basin prior to beginning a
calculation. Chapter 4 gives complete details on how to define the
basin’s stratigraphy.

Finally, as described in Chapters 5 and 6, you enter keywords telling
the program how to proceed in the calculation. For example, if you wish
Basin2 to hold fluid pressure to values along a hydrostatic gradient, you
enter

```
pressure = hydrostatic
```

Similarly, to start the simulation at the end of the Cambrian, 500 million
years ago, you enter

```
start = -500 m.y.
```

or

```
start = -500e6 years
```

As you can see, Basin2 considers time to be an increasing quantity, so
the points in the geologic past are negative and the future is positive.
Input conventions

Input to Basin2 is based on assigning values to keywords and is free of formatting rules. You use the equal sign (=) to make an assignment; the keyword goes to the left and the value assigned to it to the right. Blank spaces and tabs between keywords are not significant and blank lines may appear anywhere. You can enter comments at any point; comments start with a pound sign (#) and continue to the end of the line. In the following block, for example,

```plaintext
# This is a comment.
run = transient  # set a transient run
```

the program scans the assignment run = transient and ignores the rest of the input. Basin2 also ignores any lines beginning with a period (.), which it takes as directives for word processing.

Input is not case sensitive, so you may mix upper and lower case letters within the keywords as you wish. You can insert the underscore character (_) within keywords to improve clarity. The keywords aperm, Aperm, and A_perm are treated identically. As well, when assigning a literal value to a keyword, you need type only enough letters to uniquely identify the entry. The following commands work the same.

```plaintext
x_average = harmonic
X_average = H
```

Basin2 recognizes as numerical entries real numbers (3.14159 and 5.e-3), integers (-8), fractions (2/3), percentages (30%), and exponents (10^-5.5). The program also recognizes a number of units in common use (see Appendix 2). You enter the unit after the numerical value in an assignment. If you omit the unit, Basin2 assumes a default. Appendix 1 gives the default unit for each variable. Multiple assignments may appear separated by semicolons (;) on a single line. You may use the comma (,) or plus sign (+) to join arguments

```plaintext
tables = porosity, permeability
cementation = chalcedony + anhydrite
```

for clarity; the backslash (\) continues one line onto the next.

You use a column block, as shown in the previous section, to specify in tabular form how values vary across the basin. The double quote (") serves as a ditto sign. Within a column block, this character causes Basin2 to copy the value in the previous statement. The ampersand (&) causes the program to linearly interpolate between the previous and following entries, accounting for the well positions. In the following example, where we follow the common practice of abbreviating well to w,
water depth is set to a constant 100 m. The formation’s thickness varies linearly from 700 m at well one to 500 m at well five, and then remains invariant across the remaining wells. Note that because of the special meaning of the double quote as the ditto sign, you use the single quote (‘) to delimit character strings:

```
title 'Paleozoic evolution of the Paris basin'
strat 'Devonian/Mississippian source rock'
```

You should avoid enclosing character strings in double quotes, as this will confuse the program.

Basin2 has a facility for including external files in the input stream. You might maintain a list of rock types and their properties in a file `Rock.library`. Rather than repeating the list in each input file you create, you can refer to the file with an `include` statement

```
(Various statements)
include 'Rock.library'

(cont’d)
```

In this case, Basin2 reads through the input until it encounters the `include` statement. At this point, it reads through file `Rock.library` until the end and then returns to read the remaining lines in the original input file. You can nest `include` statements within included files, and refer to files residing anywhere in your computer’s file structure.

Finally, Basin2 allows you to set variables in your input file, the values of which you can assign later, when you run the simulation. You might, for example, include in your input file the entry

```
A_perm = $AP, B_perm = $BP
```

Here, the dollar sign marks an argument that serves as a variable. Variables can have numeric or string values; if you leave a variable undefined, Basin2 gives an error message and stops. You set values for the variables at run time, as described in Chapter 6 (see “Running the programs”). By setting variables in this way, you can make a series of related runs without editing your input file.

**Gridding and the numerical solution**

Basin2 works within a curvilinear coordinate system that follows basin stratigraphy. The x direction lies along stratigraphic time lines and hence curves to follow the dip of basin strata. This choice is important because it helps maintain an axis of the coordinate system along the direction of greatest permeability (i.e., the principal axis of the permeability).
which in unfractured basin strata is commonly along stratigraphy.

The z direction is treated as if it were normal to x, but it actually lies along the vertical; it is positive downward with its origin at sea level. The fact that the coordinate system is not truly orthogonal, except when considering flat-lying sediments, introduces an error into the calculations. At dips typical of basin strata, this error is rather small, especially when compared to the error that would be introduced if the coordinate system were orthogonal but skewed with respect to the axes of the permeability ellipsoid.

A 10° dip, for example, introduces an error of less than 2%, which is negligible compared to the uncertainty in estimating permeability (see Chapter 2). Note that the dips apparent on basin cross sections, such as B2plot renderings, are greatly magnified due to the vertical exaggeration at which such diagrams are drawn. Vertical exaggerations of thirty-fold or more are common in plotting basin cross sections.

In order to solve its governing equations, Basin2 maps the basin cross section in curvilinear coordinates onto a finite-difference grid, as shown in Figure 1.1. The grid consists of nodal blocks arranged vertically in columns and along stratigraphy in rows. A nodal point at the center of each nodal block represents the properties of the entire block. Basin2 calculates pressure, temperature, and so on, only at the nodal points, so the gridding density limits the resolution possible in a run.

**Figure 1.1** Mapping an irregular basin cross section into a finite difference grid. Cross section is drawn to vertical exaggeration. The x direction is curvilinear along stratigraphic time lines. The properties of nodal blocks are projected onto nodal points (dots) for the numerical solution. Bold lines show boundaries and stratigraphic contacts.

Each nodal point is identified by a column index $i$ along $x$, and a row index $j$ along $z$. Points with indices $1 \leq i \leq N_x$ and $1 \leq j \leq N_z$ are interior nodes at which Basin2 seeks values for the unknown variables. A layer of nodal blocks surrounds the interior nodes; these boundary nodes are used to set the boundary conditions. Boundary nodes to the left and right
of the domain have indices \( i \) of 0 and \( N_x + 1 \); \( j \) indices of 0 and \( N_z + 1 \), respectively, denote those along the top and base of the cross section.

The user controls the density of the numerical grid by specifying the number of rows and columns, as described in Chapter 6. The columns have a uniform width \( \Delta x \), which is simply the width of the cross section divided by \( N_x \). The block height \( \Delta z \) varies along the cross section with the thickness of the stratigraphic unit. A block’s height changes over the course of the simulation as the sediments within it compact and rebound.

You should be aware that the results of a Basin2 simulation, as is the case for any finite-difference calculation, incorporate inaccuracies known as truncation errors (see also “Time weighting”, Chapter 5). Peaceman (1977) gives a thorough discussion of errors of this type. An important type of truncation error known as numerical dispersion arises in calculations that account for transport of heat or salinity by advection.

The magnitude of the numerical dispersion is proportional to the grid’s block size, so you can reduce error by refining the finite-difference grid. In doing so, of course, you increase the computing requirements for the calculation. There are no easy rules for choosing an appropriate grid density. After you have calculated an apparently satisfactory model, it is good practice to double the density and repeat the calculation. If the results change little, then truncation error can be taken to be acceptably small.

**Input and output**

Basin2 takes user input from a file named `B2in.txt` by default, and produces several output streams (Figure 1.2). In some cases (see Chapter 13), the program also reads as input data a table of mineral solubilities calculated by the geochemical model React. React, a software module in The Geochemist’s Workbench®, was also developed within the Hydrogeology Program at the University of Illinois.

**Figure 1.2** Basin2 reads user input, and optionally cementation tables produced by the program React, and produces output to the user’s Basin2 window, datasets `B2_output.txt` and `B2_plot.dat`, and optionally to table datasets. The `B2_plot.dat` dataset serves as input to the graphics program `B2plot`. 

---

**Basin2 Release 5**

9
Basin2 produces several output streams. It writes messages showing progress in the calculation to a window on screen of the computer from which it is being run, and writes a more complete overview of the calculation to the file `B2_output.txt`. Optionally, Basin2 writes a summary of the calculation results in table format to a series of files `B2_tab1.txt`, `B2_tab2.txt`, etc.

Most importantly, the program writes into a file `B2_plot.dat` a detailed log of the calculation results at intervals that you specify. The `B2_plot.dat` file provides the link between Basin2 and the graphics program B2plot. This dataset is most commonly in binary instead of character format, so you should not try to list or print it. Once Basin2 has completed writing the `B2_plot.dat` file at the end of a run, you use B2plot to read `B2_plot.dat` and display the calculation results.

**Displaying your results**

Basin2 produces results in such volume and detail that it is seldom convenient to plot the results by hand. It is better to use the program B2plot to render the results in the `B2_plot.dat` dataset in graphic form. B2plot can display the results in several ways.

First, you can use it to plot the simulation results for any point in time as a diagram in cross section. On the diagram, you can contour a field variable such as pressure, temperature, or thermal maturity, map one or two variables to a color scale and map another to a color mask; you can also represent as a vector field the patterns and rates of fluid migration.

Second, B2plot can plot the profile, at a chosen point in time, of a variable against depth in the basin. Finally, the program can plot the variation over time of a variable at a chosen point in the basin, or the variation of the maximum or minimum value of a variable against time. *Table 1.2* shows the field variables that are available to B2plot, depending on how you configure the calculation. Note that Basin2 only writes into `B2_plot.dat` results for variables that you tell it to calculate, as described in Chapter 6. The dataset, for example, will not contain data for vitrinite reflectance if you have not set the `vitrinite` option to `on`. 
### Table 1.2

Field variables that may be available to B2plot for plotting (depending on how the Basin2 simulation is configured), and their default units.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>$T$</td>
<td>°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>$P$</td>
<td>atm</td>
</tr>
<tr>
<td>Overpressure</td>
<td>$P - P_0$</td>
<td>atm</td>
</tr>
<tr>
<td>Pressure gradient</td>
<td>$P/Z$</td>
<td>atm/km</td>
</tr>
<tr>
<td>Hydraulic potential</td>
<td>$\Phi$</td>
<td>atm</td>
</tr>
<tr>
<td>Effective stress</td>
<td>$\sigma_k$</td>
<td>atm</td>
</tr>
<tr>
<td>Total stress</td>
<td>$\sigma_T$</td>
<td>atm</td>
</tr>
<tr>
<td>Subsidence velocity</td>
<td>$v_{zm}$</td>
<td>cm/yr</td>
</tr>
<tr>
<td>Fluid salinity</td>
<td>$C$</td>
<td>mol</td>
</tr>
<tr>
<td>Fluid velocity along x</td>
<td>$v_x$</td>
<td>cm/yr</td>
</tr>
<tr>
<td>Fluid velocity along z</td>
<td>$v_z$</td>
<td>cm/yr</td>
</tr>
<tr>
<td>Specific discharge along x</td>
<td>$q_x$</td>
<td>cm/yr</td>
</tr>
<tr>
<td>Specific discharge along z</td>
<td>$q_z$</td>
<td>cm/yr</td>
</tr>
<tr>
<td>Depth below sea level</td>
<td>$z$</td>
<td>km</td>
</tr>
<tr>
<td>Burial depth</td>
<td>$Z$</td>
<td>km</td>
</tr>
<tr>
<td>Rock types in strata</td>
<td>$X_{rk}$</td>
<td>volume fraction</td>
</tr>
<tr>
<td>Sediment porosity</td>
<td>$\phi$</td>
<td>volume fraction</td>
</tr>
<tr>
<td>Porosity of each rock type</td>
<td>$\phi_k$</td>
<td>volume fraction</td>
</tr>
<tr>
<td>Bulk density of sediment</td>
<td>$\rho_m$</td>
<td>g/cm$^3$</td>
</tr>
<tr>
<td>Fluid density</td>
<td>$\rho$</td>
<td>g/cm$^3$</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>$\mu$</td>
<td>centipoise</td>
</tr>
<tr>
<td>Permeability along stratigraphy</td>
<td>$k_x$</td>
<td>darcy</td>
</tr>
<tr>
<td>Permeability across stratigraphy</td>
<td>$k_z$</td>
<td>darcy</td>
</tr>
<tr>
<td>Permeability of each rock type</td>
<td>$k_{rk}$</td>
<td>darcy</td>
</tr>
<tr>
<td>Thermal conductivity along stratigraphy</td>
<td>$K_x$</td>
<td>cal/cm s °C</td>
</tr>
<tr>
<td>Thermal conductivity across stratigraphy</td>
<td>$K_z$</td>
<td>cal/cm s °C</td>
</tr>
<tr>
<td>Coefficient of hydrodynamic dispersion, along stratigraphy</td>
<td>$D_x$</td>
<td>cm$^2$/s</td>
</tr>
<tr>
<td>Coefficient of hydrodynamic dispersion, across stratigraphy</td>
<td>$D_z$</td>
<td>cm$^2$/s</td>
</tr>
<tr>
<td>Organic maturity</td>
<td>$TTI$</td>
<td>time-temperature index</td>
</tr>
<tr>
<td>Oil generated</td>
<td>$X_o$</td>
<td>fraction of capacity</td>
</tr>
<tr>
<td>Vitritine reflectance</td>
<td>$R_o$</td>
<td>% in oil</td>
</tr>
<tr>
<td>Cumulative cement volume, mineral $k$</td>
<td>$Y_k$</td>
<td>% of bulk rock</td>
</tr>
<tr>
<td>Cementation rate for mineral $k$</td>
<td>$dY_k/dt$</td>
<td>%/m.y.</td>
</tr>
<tr>
<td>Hydrologic residence time</td>
<td>$\tau$</td>
<td>yr</td>
</tr>
<tr>
<td>Concentrations of isotopes 1 and 2</td>
<td>$C_i$</td>
<td>molal</td>
</tr>
<tr>
<td>Isotopic ratio, isotope 1/isotope 2</td>
<td>$C_{i1}/C_{i2}$</td>
<td>atomic ratio</td>
</tr>
</tbody>
</table>
In addition to still images, B2plot allows you to animate simulation results, so you can watch how the basin develops and how field variables change over geologic time. You can record the frames in the animation on disk and then use them to produce a videotape of the results of your simulation. B2plot is described in more detail in Chapter 15.

Further reading

This guide is intended as an introduction to basin modeling using the programs in the Basin2 workbench, not as a text or general reference. Appendix 5 lists literature references that provide starting points for further reading.

Users’ group

Basin2_users is an independent group of users who share comments and results and answer questions of general interest over the Internet. The group also serves as a bulletin board for posting announcements, bug notices, and other current information about the software.

To join the users’ group (there is no charge), unsubscribe from the group, or post a message, select “Basin2 Users’ Group” from the Windows “Start” menu (Start → Programs → Basin2 5.0 → Basin2 Users’ Group), or the “Help” pulldown in any of the Basin2 programs. Alternatively, you can visit the group’s home page at www.geology.uiuc.edu/Hydrogeology/basin2_usergroup.html.

Software distribution

The Basin2 software package is distributed as source code and as a self-installing executable for MS Windows computers under the co-sponsorship of the Hydrogeology Program at the University of Illinois and the U.S. Geological Survey. The package may be downloaded over the Internet from Hydrogeology Program and USGS web sites.

The distribution to non-members of the Hydrogeology consortium is subject to a license agreement that is displayed when installing the software. The agreement may be viewed at any time from the Windows “Start” menu (Start → Programs → Basin2 5.0 → View Basin2 license agreement).

Briefly, the license agreement allows a user to download, modify, and apply the code freely for a wide variety of purposes, commercial and academic. The user, however, is prohibited from redistributing the code or any portion or derivative of it without written permission from the University of Illinois. Interested users should be directed to the web sites from which the software may be downloaded.
Getting further help

The Hydrogeology Program is pleased to provide the Basin2 software package to users at no cost. We are a small group with limited resources and, as such, regret that we can no longer provide user assistance or consulting services to users who are not members of the consortium. Non-consortium users who require assistance should contact the Basin2 Users’ Group (see “Users’ group”).
2 Setting Rock Properties

About rock properties

In configuring a basin model, you specify a list of the types of rock and sediment present in the stratigraphic section and set the physical and hydrologic properties of each. You might, for example, divide the basin fill into sandstone, siltstone, shale, limestone, dolomite, and so on. Each stratigraphic unit in the basin may be composed of a single rock type or a mixture of two or more types.

Basin2 traces strata from deposition through burial and lithification, so we do not always distinguish between sediment and rock; for convenience, we refer to classes of both sediments and rocks as rock types. There is no limit to the number of rock types you can define, except for practicality and the dimension of program arrays.

You define many of the properties for each rock type in terms of empirical correlations. Basin2, for example, uses correlations to track how porosity evolves through time and how permeability and thermal conductivity change with porosity. You supply the coefficients in these correlations. You use keywords to directly set other properties, such as the density of rock grains and the diffusion constant and dispersivity value appropriate for the rock type. In general, you enter data in forms that are commonly compiled in basin analysis or readily available in the literature.

You assign to each rock type a label of one to three letters. Three rock types are already defined in Basin2 arrays. The built-in types and their labels are sandstone (ss), shale (sh), and carbonate (cn). You may use these types directly, alter any of their properties, or ignore them and work only with rock types that you define.

As mentioned in the previous chapter, you use a block of input statements to define a rock type. The first statement is rock followed by the label of the rock type in question. You follow this statement with a list of keywords and values. Table 2.1 shows the keywords used to set rock properties. Basin2 will assign a default value for each keyword that you omit from the input.
Table 2.1  Keywords used to set properties of each rock type.

<table>
<thead>
<tr>
<th>Property</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>Reducible porosity present at deposition.</td>
</tr>
<tr>
<td>phi0</td>
<td>Irreducible porosity.</td>
</tr>
<tr>
<td>phi1</td>
<td>Compressibility of the reducible pore volume.</td>
</tr>
<tr>
<td>beta_por</td>
<td>Pore compressibility during unloading.</td>
</tr>
<tr>
<td>beta_ul</td>
<td>Exponential coefficient describing compaction.</td>
</tr>
<tr>
<td>bpor</td>
<td>Exponential coefficient for rebound during unloading.</td>
</tr>
<tr>
<td>bpor_ul</td>
<td></td>
</tr>
</tbody>
</table>

(Set beta_por or bpor; beta_ul or bpor_ul)

<table>
<thead>
<tr>
<th>Permeability</th>
<th>Slope of permeability correlation with porosity.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_perm</td>
<td>Intercept of permeability correlation with porosity.</td>
</tr>
<tr>
<td>B_perm</td>
<td>Anisotropy in permeability.</td>
</tr>
<tr>
<td>p_kxxz</td>
<td>Maximum allowed value of permeability.</td>
</tr>
<tr>
<td>perm_max</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thermal conductivity</th>
<th>Slope of thermal conductivity correlation with porosity.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_tc</td>
<td>Intercept of thermal conductivity correlation with porosity.</td>
</tr>
<tr>
<td>B_tc</td>
<td>Anisotropy in thermal conductivity.</td>
</tr>
<tr>
<td>t_kxxz</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Grain density</th>
<th>Average density of rock grains.</th>
</tr>
</thead>
<tbody>
<tr>
<td>rho_rk</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Heat capacity</th>
<th>First coefficient in Maier-Kelley equation.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_mk</td>
<td>Second coefficient.</td>
</tr>
<tr>
<td>B_mk</td>
<td>Third coefficient.</td>
</tr>
<tr>
<td>C_mk</td>
<td>Fourth coefficient.</td>
</tr>
<tr>
<td>D_mk</td>
<td>Fifth coefficient.</td>
</tr>
<tr>
<td>E_mk</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Diffusion and dispersion</th>
<th>Diffusion coefficient for salt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>diff_con</td>
<td>Diffusion coefficient for isotope 1.</td>
</tr>
<tr>
<td>diff_iso1</td>
<td>Diffusion coefficient for isotope 2.</td>
</tr>
<tr>
<td>diff_iso2</td>
<td>Diffusion coefficient for residence time.</td>
</tr>
<tr>
<td>diff_t</td>
<td>Temperature dependence of diffusion coefficient for salt.</td>
</tr>
<tr>
<td>diff_t_iso1</td>
<td>Temperature dependence of diffusion coefficient for isotope 1.</td>
</tr>
<tr>
<td>diff_t_iso2</td>
<td>Temperature dependence of diffusion coefficient for isotope 2.</td>
</tr>
<tr>
<td>diff_t_tres</td>
<td>Temperature dependence of diffusion coefficient for residence time.</td>
</tr>
<tr>
<td>alpha_L</td>
<td>Longitudinal dispersivity.</td>
</tr>
<tr>
<td>alpha_T</td>
<td>Transverse dispersivity.</td>
</tr>
</tbody>
</table>

Porosity evolution

Basin2 calculates porosity from the vertical stress balance on a sediment and the compressibility of the sediment’s pore volume. The program considers the average porosity of each rock type within a nodal block, which is the smallest division of the basin recognized within Basin2. For this reason, there is no provision for portraying variation in porosity.
within the nodal block, as might be seen on the scale of a hand sample or thin section. Basin2 by nature expresses porosity as a fraction, so a value of .5 represents a rock composed of one-half, not half a percent, pore volume.

Porosity is important to the calculation for two reasons. First, changes in porosity occurring as sediments compact during burial (Chapter 7) or rebound when erosion exhumes them (Chapter 9) drive groundwater flow. Second, the program uses the calculated porosity to assign permeability and thermal conductivity values to each rock type.

The program, by default, calculates porosity from the effective stress acting on a sediment. Effective stress \( \sigma_E \) is the difference

\[
\sigma_E = \sigma_T - P
\]

between the total stress \( \sigma_T \) and fluid pressure \( P \). Total stress, the weight applied by the overburden per unit area, is given

\[
\sigma_T = P_{atm} + \rho_s g Z
\]

Here \( P_{atm} \) is atmospheric pressure, \( \rho_s \) is the density of the saturated medium, averaged over the sediment column, \( g \) is the acceleration of gravity, and \( Z \) is burial depth.

Unless you set a value directly using the bulk_density keyword, Basin2 calculates \( \rho_s \) from porosity and rock and fluid densities in overlying strata. By Equation 2.2, total stress typically increases about 225 atm/km with burial. Hydrostatic pressure, on the other hand, increases along a gradient of about 100 atm/km.

The concept of effective stress holds that the weight of the overburden is borne jointly by sediment framework and pore fluid. A sediment in an overpressured basin is likely to be more porous than one buried to the same depth in a basin with normal fluid pressure, because the framework of the overpressured sediment supports less of the total stress. Such sediments are said to be in a state of disequilibrium compaction. For this reason, the default technique for calculating porosity is known as the disequilibrium method.

Basin2 can also calculate porosity according to an equilibrium method, in which pressure is taken to be the hydrostatic value corresponding to a sediment’s burial depth. In this case, sediments maintain a state of equilibrium compaction regardless of the fluid pressure. You invoke the equilibrium model by setting the keyword equilibrium = on (or disequilibrium = off).

The equilibrium and disequilibrium methods are equivalent in simulations where fluid pressure remains near hydrostatic. In such runs, use the equilibrium method, which is easiest to compute. In runs in which significant overpressures develop, it is important to use the disequilibrium method.

The program calculates porosity \( \phi \) from effective stress according to the relationship
\[ \phi = \phi_o \exp(-\beta \sigma_x) + \phi_i \]  \hspace{1cm} (2.3)

Here, \( \phi_o \) is the reducible porosity present when the sediment is deposited and \( \phi_i \) is the irreducible porosity that persists throughout burial. Coefficient \( \beta \), which has units of reciprocal pressure, is the compressibility of the reducible pore volume. The compressibility, defined as
\[ \beta = -\frac{1}{(\phi - \phi_i)} \frac{\partial \phi}{\partial \sigma_x} \]  \hspace{1cm} (2.4)

controls how quickly porosity is lost during burial. You can set the values of these variables for each rock type with the \texttt{phi0}, \texttt{phi1}, and \texttt{beta_por} keywords. For example, the statement

\begin{verbatim}
beta_por = 0.004 /atm
\end{verbatim}

sets \( \beta \) in reciprocal atm.

In basin analysis, it is often easier to describe compaction in terms of a porosity profile than in terms of the pore compressibility. Porosity profiles, commonly compiled in basin studies, are the easiest way to observe how rocks respond to burial in nature. Measurements of rock compressibility, on the other hand, are made on laboratory time frames and poorly predict the compaction that is observed to occur over geologic time. You can enter compaction curves of the form
\[ \phi = \phi_o \exp(-b Z) + \phi_i \]  \hspace{1cm} (2.5)

directly into Basin2. Here, \( Z \) is burial depth and \( b \) is the compaction coefficient, which has units of reciprocal depth.

**Figure 2.1 (a)** shows the form of Equation 2.5. The surface porosity is \( \phi_o + \phi_i \). With depth, porosity decreases and asymptotically approaches the value of \( \phi_i \). Large values of \( b \) describe sediments that compact rapidly with burial, whereas small values represent sediments whose porosity is preserved to greater depth. A typical value for \( b \) is one-half km\(^{-1}\). As a rule, as can be seen by manipulating Equation 2.1, a sediment buried to a depth equal to about \( 0.7/b \) has lost half of its reducible porosity.
To fit observed porosity-depth pairs to Equation 2.5, it is easiest to recast the equation as
\[ \ln (\phi - \phi_1) = -bZ + \ln \phi_o \]  
which has the form of a line. Assume a value for \( \phi_1 \) and plot the observed porosities \( \phi \) on coordinates \( \ln (\phi - \phi_1) \) versus \( Z \), as shown in Figure 2.1 (b). A least-squares fit through the plotted data gives a line whose negative slope is \( b \) and whose intercept is \( \ln \phi_o \).

In regressing porosity data from basins with nonhydrostatic pressures, you must replace burial depth \( Z \) in the analysis above with an effective depth \( Z_E \). To determine effective depth, figure the effective stress at the point of interest and then find the burial depth that would correspond to this effective stress, if pore pressure were hydrostatic. You can quickly convert from \( Z \) to \( Z_E \) by subtracting 100 meters of burial depth for each 10 atm (~1 MPa) that fluid pressure exceeds hydrostatic. Where fluid pressure lies below hydrostatic, you apply a negative correction of the same magnitude.

You set \( b \) for each rock type with the \texttt{b\_por} keyword in lieu of specifying a value for \( \beta \). If you have not set a value of \texttt{beta\_por} for a rock type, Basin2 converts the compaction coefficient that you have set, or its default value, to a compressibility according to the relation
\[
\beta = \frac{b}{(\rho_{sm} - \rho)g}
\]  

(2.7)

In the conversion, the program takes \(\rho_{sm}\) to be 2.3 g/cm\(^3\) or the value of variable \texttt{bulk\_density}, if you have set it, and the fluid density \(\rho\) to be 1 g/cm\(^3\).

Basin2 gives you the option of treating compaction as a reversible or irreversible process. The program normally calculates porosity directly from the equations above, and thus treats compaction as reversible. This treatment is of little consequence in runs in which sediments are buried and not exhumed, since stress tends to increase over the simulation. In runs accounting for erosion, however, \(\sigma_E\) is likely to decrease.

In this case, you should specify that the program treat compaction as an irreversible process so that rocks, once compacted, do not revert to their pre-compaction porosities, which would be unrealistic. The irreversible model may also be required in runs in which fluid pressure increases sharply, since an increase in \(P\) decreases the value of \(\sigma_E\).

You specify the compaction model with the keywords

```
compaction = reversible
```

or

```
compaction = irreversible
```

Basin2 by default treats compaction as reversible. In general, the reversible model is less tricky for Basin2 to compute and is likely to execute more quickly than the irreversible model.

To model the irreversible nature of compaction, Basin2 tracks \(\sigma_{max}\), the maximum effective stress seen at each nodal block, as well as \(\phi_{min}\), the porosity that corresponds to this depth. Whenever the current effective stress is greater than or equal to \(\sigma_{max}\), the program computes porosity in the usual way. When effective stress is less than the maximum, however, porosity is determined from the decompaction equation

\[
\phi = (\phi_{min} - \phi_l) e^{b_{ul}(\sigma_E - \sigma_{max})} + \phi_l
\]  

(2.8)

Here, the unloading compressibility \(\beta_{ul}\) describes the rebound of porosity.

You may specify the unloading compressibility directly using keyword \texttt{beta\_ul}, or set an unloading coefficient \(b_{ul}\) with keyword \texttt{bpor\_ul}. By setting \(\beta_{ul}\) to a value smaller than \(\beta\) or equivalently, by setting \(b_{ul}\) smaller than \(b\), the porosity gained when a rock is exhumed is less than the porosity it originally lost during compaction. A typical value for \(\beta_{ul}\) or \(b_{ul}\) might be just 10\% or 20\% of the value of \(\beta\) or \(b\).

Finally, Basin2 can track the effect of cementation on sediment porosity. This option is described in Chapter 6.
Permeability

Sediment permeability is not only the most critical variable in a hydrologic simulation but also the most difficult parameter to constrain. The permeability of sediments and sedimentary rocks varies over many orders of magnitude (Figure 2.2), and individual datasets commonly fall into log-normal distributions. For this reason, estimates of permeability are generally uncertain on logarithmic rather than linear scales.

Figure 2.2 Ranges in the permeability of sediments and rocks, as compiled by Freeze and Cherry (1979).

Permeability, furthermore, is broadly recognized to vary with the scale on which it is observed. Even in the absence of measurement error, values determined by laboratory or well tests can not necessarily be applied on a basin scale. The way you set permeability in a simulation represents an important assumption and is likely to be the principal cause of uncertainty in your modeling results.

Basin2 computes the permeability of each rock type by a correlation to porosity. There is in general no functional relationship between these two quantities. A tightly compacted sandstone, for example, may be more permeable than a porous shale. An uncompacted clay, as well, may be less permeable than a fully compacted but fractured shale deep in a basin.

Linear trends between the logarithm of permeability, nonetheless, are commonly observed for suites of related rocks, such as sandstones within a certain formation or basin. Figure 2.3 shows such a trend for Cambrian and Ordovician sandstones of the Illinois basin. Basin2 calculates permeability along strata (i.e., in the \( x \)-direction) from the computed value of porosity according to the correlation

\[
\log k_i = A\phi + B
\]
You set the coefficients $A$ and $B$ using the keywords $A_{\text{perm}}$ and $B_{\text{perm}}$. Note that coefficient $B$ has units of log permeability, but $A$ is unitless; to see why, recast the equation in linear form.

In order to prevent the correlation from predicting unrealistic values near the basin surface, Basin2 carries for each rock type a maximum value that it will assign to permeability. The value by default is 1 darcy, but you can assign another value with the $\text{perm\_max}$ keyword.

Permeability in basin sediments generally is anisotropic — that is, it varies with direction. Anisotropy in permeability arises from a number of factors, including the alignment of flat grains within sediments, the interlayering of laminae of varying permeability, and the orientation of fractures and joints. The program determines permeability in the vertical or $z$-direction from the permeability anisotropy $J_z$, which is defined as

$$J_z = \frac{k_x}{k_z} \quad (2.10)$$

You set the anisotropy directly with the $p_{\text{xkxkz}}$ keyword. If, for example, Basin2 calculates an $x$-direction permeability $k_x$ of 10 mdarcy using Equation 2.9 and you have set the anisotropy for this rock type to 5, then the program will assign a value of 2 mdarcy to the vertical permeability $k_z$.

You should note that in strata composed of more than one rock type, the overall anisotropy in permeability depends not only on the $p_{\text{xkxkz}}$ values set for the rock types, but the averaging method you use to determine overall permeability. Averaging techniques are discussed in Chapter 4 (see “Volume averaging”).
Thermal conductivity

The thermal conductivity of basin sediments is important when modeling a basin’s thermal history, because the value chosen determines the geothermal gradient for a given heat flux beneath the basin. Thermal conductivity also affects simulations of heat transport by groundwaters, as discussed in Chapter 10.

Basin2 correlates thermal conductivity, like permeability, to porosity. The variation in conductivity with porosity arises because minerals are more conductive than water. Well compacted rocks are more conductive than porous rocks, which are better thermal insulators. In Basin2 runs in which thermal conductivity varies with porosity, you will notice that the temperature profile with depth is somewhat curved because of this effect.

Basin2 uses the correlation function

\[ K_x = A \phi + B \]  

(2.11)

to set thermal conductivity as a function of porosity. You set the coefficients directly using the \texttt{A_{tc}} and \texttt{B_{tc}} keywords. Figure 2.4 shows the default regression for all rock types and the data from which it was derived.

**Figure 2.4** Least-squares fit of thermal conductivity to sediment porosity, from data of Sclater and Christie (1980) for shale and chalk from the North Sea basin. The regression line shown is the default in Basin2 for all rock types.

Basin2 allows for anisotropy in conductivity. The anisotropy \( J_K \) is defined

\[ J_K = \frac{K_y}{K_z} \]  

(2.12)

By default, the program takes the conductivity of each rock type to be isotropic, but you can set \( J_K \) with the \texttt{\_k\_kz} keyword.
Rock density and heat capacity

The average density of the minerals that make up a rock type enters into calculation of the overburden weight, and the heat capacity of the rock framework affects how quickly transients in temperature propagate through the basin. Choice of these values presents a minor source of uncertainty in a Basin2 simulation because the densities and heat capacities of common minerals are known rather precisely in comparison to other input, such as the correlations defining porosity and permeability.

The rock density is the density of the rock framework (i.e., the rock excluding its pore space). You determine the rock density as the average of the densities of each mineral in the rock, weighted by the minerals’ volume fractions. Enter the density value with the \textit{rho\_rk} keyword.

Basin2 uses an extended form of the Maier-Kelley equation as commonly applied in chemistry to set the rock’s heat capacity as a function of temperature. Here, $T_K$ is temperature in Kelvins, and $A$, $B$, $C$, $D$ and $E$ are empirical coefficients.

\begin{equation}
C_p = A + BT_K + CT_K^2 + \frac{D}{\sqrt{T_K}} + \frac{E}{T_K^2}
\end{equation} 

Equation 2.13 is unnecessarily precise, but Basin2 carries it in this form for convenience because thermodynamic compilations such as Robie et al. (1978) use it to present heat capacities for a large number of minerals. To determine the coefficients for a rock type, average by mass fraction the coefficients for the individual minerals that make up the rock. Lacking data, you can generally get adequate results by setting heat capacity to a single value $A$ or to a linear function $A + BT_K$.  

![Figure 2.5 Heat capacity functions for the rock framework in built-in rock types sandstone (ss), shale (sh), and carbonate (cn). The function for sandstone serves as the default for rock types defined by the user.](image-url)
Diffusion and dispersion

The diffusion coefficient and the dispersivity control the rate of solute diffusion through basin strata and the effect of hydrodynamic dispersion on solute distribution. Diffusion, the molecular process of solute transport, is described mathematically by the porous medium diffusion coefficient $D^*$, which is the coefficient in water divided by the tortuosity of the medium. Dispersion, a process of mechanical transport that operates in groundwater flow systems, results from the irregular nature of flow through porous media. Microscopic irregularities, such as the branching and rejoining of flow paths around rock grains, and macroscopic heterogeneities, such as channeling along permeable laminae and fractures, contribute to hydrodynamic dispersion.

The dispersivity coefficient, which has units of length, describes the effectiveness of hydrodynamic dispersion. Basin2 carries a longitudinal and a transverse dispersivity, $\alpha_L$ and $\alpha_T$, for each rock type. These terms describe, respectively, dispersion along and across the direction of flow. In general, $\alpha_L$ is larger than $\alpha_T$.

You set the diffusion coefficient with the `diff_con` keyword, and the longitudinal and transverse dispersivities with the keywords `alpha_L` and `alpha_T`. In modeling isotope transport, you can set distinct diffusion coefficients for isotopes 1 and 2 with the `diff_iso1` and `diff_iso2` keywords; use the `diff_tres` keyword to set the diffusion coefficient to be used in calculating hydrologic residence time (see Chapter 6).

You can set the various diffusion coefficients to vary with temperature according to

$$D^* = D_o e^{-\frac{1}{C} \left( \frac{1}{T} - \frac{1}{T_o} \right)}$$

(2.14)

where $D_o$ is the diffusion coefficient at the reference temperature (25°C, 298.15 K), coefficient $C$ describes temperature dependence, $T_K$ is absolute temperature, and $T_o$ is the reference temperature. For salt transport, you use keyword `diff_T` to set $C$ and `diff_con` to set $D_o$. For isotopes 1 and 2 and residence time, use keywords `diff_iso1`, `diff_iso2`, and `diff_tres` to set $C$, and `diff_iso1`, `diff_iso2`, and `diff_tres` to set $D_o$. By default, the values of $C$ for the various diffusion coefficients are set to zero, so $D^*$ and $D_o$ are equivalent.

As described in Chapter 12, Basin2 multiplies the dispersivity by the groundwater flow velocity to determine the coefficient of hydrodynamic dispersion, which has the same units (cm$^2$/sec) as the diffusion constant. The diffusion constant is a small number, on the order of $10^{-6}$ cm$^2$/sec, and dispersivities are commonly rather large, perhaps hundreds to thousands of cm.

For this reason, the effect of dispersion in Basin2 will overwhelm that of diffusion wherever groundwater flows more rapidly than about a cm per year. The value of the diffusion coefficient, therefore, is a significant source of uncertainty only where groundwater flow is very slow. The
values of $\alpha_L$ and $\alpha_T$, however, are difficult to estimate on basin scales because dispersivity tends to increase markedly with the scale on which it is observed. The settings for these variables, therefore, represent significant sources of uncertainty in the study of solute distributions within sedimentary basins.

**Built-in rock types and default values**

Basin2, as already mentioned, contains three built-in rock types: sandstone, shale, and carbonate. The properties of these rock types (Table 2.2, Figure 2.6) are those used in studies of interior basins in North America. There is, however, no special significance to the properties, and the authors urge you to work with data appropriate to the basin you are studying rather than relying on the built-in values.
Table 2.2 Properties of the built-in rock types in Basin2.

<table>
<thead>
<tr>
<th>Property</th>
<th>ss</th>
<th>sh</th>
<th>cn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\phi_0$</td>
<td>.4</td>
<td>.55</td>
<td>.4</td>
</tr>
<tr>
<td>$\phi_1$</td>
<td>.05</td>
<td>.05</td>
<td>.05</td>
</tr>
<tr>
<td>$b_{\text{por}}$ (km$^{-1}$)</td>
<td>.5</td>
<td>.85</td>
<td>.55</td>
</tr>
<tr>
<td>$b_{\text{por_ul}}$ (km$^{-1}$)</td>
<td>.1</td>
<td>.17</td>
<td>.11</td>
</tr>
<tr>
<td>Permeability</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_{\text{perm}}$</td>
<td>15</td>
<td>8</td>
<td>6</td>
</tr>
<tr>
<td>$B_{\text{perm}}$ (log darcy)</td>
<td>-3</td>
<td>-7</td>
<td>-4</td>
</tr>
<tr>
<td>$p_{kxkz}$</td>
<td>2.5</td>
<td>10</td>
<td>2.5</td>
</tr>
<tr>
<td>$\text{perm_max}$ (darcy)</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_{\text{tc}}$ (cal/cm sec °C)</td>
<td>-4.40×10$^{-3}$</td>
<td>-4.40×10$^{-3}$</td>
<td>-4.40×10$^{-3}$</td>
</tr>
<tr>
<td>$B_{\text{tc}}$ (cal/cm sec °C)</td>
<td>5.35×10$^{-3}$</td>
<td>5.35×10$^{-3}$</td>
<td>5.35×10$^{-3}$</td>
</tr>
<tr>
<td>$t_{kxkz}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Grain density</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_{\text{rk}}$ (g/cm$^3$)</td>
<td>2.65</td>
<td>2.74</td>
<td>2.75</td>
</tr>
<tr>
<td>Heat capacity (cal/g K)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_{\text{mk}}$</td>
<td>.2198</td>
<td>.4210</td>
<td>.3444</td>
</tr>
<tr>
<td>$B_{\text{mk}}$</td>
<td>123.3×10$^{-6}$</td>
<td>7.229×10$^{-6}$</td>
<td>8.454×10$^{-6}$</td>
</tr>
<tr>
<td>$C_{\text{mk}}$</td>
<td>2.652×10$^{-9}$</td>
<td>5.193×10$^{-9}$</td>
<td>15.70×10$^{-9}$</td>
</tr>
<tr>
<td>$D_{\text{mk}}$</td>
<td>-.7218</td>
<td>-3.979</td>
<td>-1.972</td>
</tr>
<tr>
<td>$E_{\text{mk}}$</td>
<td>-3.292×10$^{-3}$</td>
<td>-.402×10$^{-3}$</td>
<td>-3.060×10$^{-3}$</td>
</tr>
<tr>
<td>Diffusion and dispersion</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\text{diff_con}$ (cm$^2$/sec)</td>
<td>1×10$^{-6}$</td>
<td>1×10$^{-6}$</td>
<td>1×10$^{-6}$</td>
</tr>
<tr>
<td>$\text{diff_iso1}$ (cm$^2$/sec)</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>$\text{diff_iso2}$ (cm$^2$/sec)</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>$\text{diff_tres}$ (cm$^2$/sec)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\text{diff_T}$ (K)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\text{diff_iso1}$ (K)</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>$\text{diff_iso2}$ (K)</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>$\text{diff_tres}$ (K)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\alpha_L$ (cm)</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$\alpha_T$ (cm)</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

*Defaults to values set for keywords $\text{diff\_con}$ and $\text{diff\_T}$
Figure 2.6 Default correlations for the built-in rock types of (a) porosity with burial depth or effective depth, and (b) permeability with porosity.

You may alter the properties of the built-in types or define your own rock types. To alter, for example, the permeability correlation for the built-in sandstone, you use the commands

```
rock ss
B_perm = -4 log_darcy
```

To define a new rock type, you enter

```
rock ss1
phi0 = 35%; phi1 = 5%; bpor = .6 /km
A_perm = 10; B_perm = -4 log_darcy; perm_max = 2 darcy
(etc.)
```

If you define a new rock type but omit keywords describing some properties, Basin2 will automatically assign to those properties the default values for the built-in sandstone shown in Table 2.2.
3 Fluid Properties

About fluid properties

Basin2 calculates fluid properties directly from the values of temperature, pressure, and fluid salinity computed at each point in the basin, using built-in correlations. The following sections show how Basin2 calculates fluid properties, including density, compressibility, thermal expansivity, viscosity, heat capacity, enthalpy, and the salinity corresponding to halite saturation. The sections also show how to set density, viscosity, and halite solubility to constant values.

Fluid density

Fluid density enters into each of the governing equations in Basin2, but it is especially important in determining how buoyant forces drive groundwater migration and in predicting subsurface pressures. Basin2 calculates the density $\rho$ from a correlation developed by Phillips et al. (1981) for NaCl solutions. The correlation is

$$\rho = A + B \chi + C \chi^2 + D \chi^3$$

(3.1)

where

$$\chi = c_1 e^{m_1} + c_2 e^{m_2} + c_3 e^{m_3}$$

Here, $\rho$ is in g/cm$^3$, $m$ is the molal salinity, $T$ is temperature in °C, and $P$ is pressure in bars. The remaining variables are regression constants with values

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>-3.033405</td>
</tr>
<tr>
<td>$B$</td>
<td>10.128163</td>
</tr>
<tr>
<td>$C$</td>
<td>-8.750567</td>
</tr>
<tr>
<td>$D$</td>
<td>2.663107</td>
</tr>
<tr>
<td>$a_1$</td>
<td>-0.004539</td>
</tr>
<tr>
<td>$a_2$</td>
<td>-0.0001638</td>
</tr>
<tr>
<td>$a_3$</td>
<td>0.0002551</td>
</tr>
<tr>
<td>$c_1$</td>
<td>-9.9559</td>
</tr>
<tr>
<td>$c_2$</td>
<td>7.0845</td>
</tr>
<tr>
<td>$c_3$</td>
<td>3.9093</td>
</tr>
</tbody>
</table>

(Coefficient $c_1$ is listed in error in Phillips et al., 1981.) Figure 3.1 shows the form of the function.
Figure 3.1 Density (g/cm³) of NaCl solutions as a function of salinity (molal) and depth in a basin (vertical axis), computed from the correlation of Phillips et al. (1981). The calculation assumes a surface temperature of 10°C, a temperature gradient of 25°C/km, and a pressure gradient of 100 atm/km.

The correlation is known to be valid for $10 < T < 350$ °C, $0.25 < m < 5$ molal, and $P < 50$ MPa and greater than the fluid's vapor pressure. For reference, the salinity of seawater is about one-half molal. The function provides a smooth but not necessarily accurate extrapolation to higher salinities and pressures. Basin2 calculates density from Equation 3.1 using temperatures in the range 0°C to 350°C, salinities from 0 molal to 12 molal, and the pressure of interest.

You have the option of setting the fluid density to a constant value using the `density` keyword:

```
density = 1 g/cm³
```

In this case, the fluid maintains its density under all conditions, and hence has zero compressibility and thermal expansivity.

The fluid’s isothermal coefficient of compressibility $\beta_f$ and isobaric coefficient of thermal expansion $\alpha_f$ follow directly from the density correlation. The compressibility can affect how rapidly pressure varies in basin strata. Thermal expansivity affects convective flow regimes and the extent to which aquathermal pressure (i.e., pressure from thermal expansion of the pore fluid during burial) develops. Equations giving $\beta_f$ and $\alpha_f$

\[
\beta_f = \frac{1}{\rho} \frac{\partial \rho}{\partial P} = \frac{1}{\rho} \left( B + 2C \chi + 3D \chi^2 \right) a_3 c_5 e^{\alpha_f \rho} \quad (3.2)
\]

and

\[
\alpha_f = -\frac{1}{\rho} \frac{\partial \rho}{\partial T} = -\frac{1}{\rho} \left( B + 2C \chi + 3D \chi^2 \right) a_2 c_5 e^{\beta_f \rho} \quad (3.3)
\]

are derived by differentiating Equation 3.1. Basin2 sets $\beta_f$ and $\alpha_f$ to zero if the `density` keyword has been set.
Alternatively, you can set Basin2 to calculate fluid density using the correlation of Batzle and Wang (1992)

\[
\rho = 1 + 10^{-6} \left( -80T - 3.3T^2 + .00175T^3 + 489P \\
-2TP + .016T^2P - .002TP^2 \right) + S \left( .668 + .44S + 10^{-6} \left( 300P - 2400PS + T \\
(80 + 3T - 3300S - 13P + 47PS) \right) \right)
\] (3.4)

where \( T \) is temperature (°C), \( P \) is pressure in MPa, and \( S \) is the weight fraction NaCl in the fluid. The Batzle-Wang equation is fit over a temperature range of 20 to 350°C and over salinities of 0 to 8 molal; Basin2 extrapolates linearly beyond this salinity range.

You set the Batzle-Wang option with the command

\[
\text{density = batzle-wang}
\]

In this case, the coefficients of compressibility \( \beta_f \) and thermal expansion \( \alpha_f \), obtained by differentiating Equation 3.4, are given as

\[
\beta_f = \frac{1}{\rho} \frac{\partial \rho}{\partial P} = \frac{10^{-6}}{\rho} \left( 489 - 2T + .016T^2 - 1.3 \times 10^{-5}T^3 - .666P \\
- .004TP + S \left( 300 - 2400S - 13T + 47ST \right) \right)
\] (3.5)

and

\[
\alpha_f = -\frac{1}{\rho} \frac{\partial \rho}{\partial T} = -\frac{10^{-6}}{\rho} \left( -80 - 6.6T - .00525T^2 \\
+ P \left( -2 + .032T - 3.9 \times 10^{-5}T^2 - .002P \right) \right) + S \left( 80 + 6T - 3300S - 13P - 47PS \right)
\] (3.6)

## Viscosity

Fluid viscosity affects how rapidly groundwater migrates under a given potential gradient through basin strata. The viscosity of aqueous fluids varies with temperature and to a lesser extent with salinity; the effect of pressure is small. Viscosity is commonly expressed in units of centipoise (100 cp = 1 poise = 1 g/cm sec). For reference, the viscosity of pure water at 20°C is almost exactly one cp. Viscosity appears in the flow equations in a ratio to permeability. Since the error in determining viscosity is much smaller than that in estimating permeability, assigning values to fluid viscosity adds little to the uncertainty in the calculation.

Basin2 maintains a look-up table of the viscosities of water and NaCl solutions from 0°C to 350°C and 0 to 5 molal, as compiled by Phillips et al. (1980); these data are plotted in Figure 3.2. Basin2 determines viscosity from the fluid’s temperature and salinity by interpolating from...
the tabulated data. When temperature or salinity falls outside the range of the data, Basin2 extrapolates linearly to the conditions of interest.

As an alternative to the tabulated data, you can have Basin2 calculate fluid viscosity with the Batzle and Wang (1992) correlation

\[
\mu = 1 + 0.333 S + (1.65 + 91.9 S^2) e^{-\left(4.21 + 7.64 S + 0.44\right) T}
\] (3.7)

Here, \(\mu\) is in cp, \(T\) is in °C, and \(S\) is the weight fraction of NaCl. This equation is valid at temperatures less than 250°C and salinities less than 5 molal, although the program will follow a linear extrapolation to salinities as great as 12 molal. You set this method with the command

\[\text{viscosity} = \text{batzle-wang}\]

You can alternatively set viscosity to a constant value with the \textit{viscosity} keyword (e.g., \textit{viscosity} = 1 cp). This feature is sometimes useful when working with data expressed in terms of hydraulic conductivity \(K_H\) (e.g., in cm/sec) instead of permeability. The relation between the quantities is

\[K_H = \frac{\rho g k}{\mu}\] (3.8)

where \(\rho\) is fluid density and \(g\) is the acceleration of gravity. Setting \(\rho\) and \textit{viscosity} \(\mu\) constant gives a direct proportionality between the two variables.

**Heat capacity**

The fluid’s heat capacity affects the fluid’s ability to redistribute heat within the basin, and it affects to a lesser extent how quickly temperature transients can migrate through basin strata. In the former case, the
primary uncertainty is the rate of fluid flow, which is seldom as well constrained as the heat capacity.

Basin2 determines heat capacity from the rate at which fluid enthalpy, which is tabulated within the program, changes with temperature. The tabulated enthalpies, taken from Phillips et al. (1981) for a one-half molal NaCl solution, are given

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Enthalpy (cal/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°C</td>
<td>0.00</td>
</tr>
<tr>
<td>25°C</td>
<td>24.04</td>
</tr>
<tr>
<td>50°C</td>
<td>48.18</td>
</tr>
<tr>
<td>75°C</td>
<td>72.38</td>
</tr>
<tr>
<td>100°C</td>
<td>96.62</td>
</tr>
<tr>
<td>125°C</td>
<td>121.11</td>
</tr>
<tr>
<td>150°C</td>
<td>145.80</td>
</tr>
<tr>
<td>175°C</td>
<td>170.82</td>
</tr>
<tr>
<td>200°C</td>
<td>200°C 196.30</td>
</tr>
<tr>
<td>225°C</td>
<td>225°C 222.30</td>
</tr>
<tr>
<td>250°C</td>
<td>250°C 249.02</td>
</tr>
<tr>
<td>275°C</td>
<td>275°C 276.67</td>
</tr>
<tr>
<td>300°C</td>
<td>300°C 305.34</td>
</tr>
<tr>
<td>325°C</td>
<td>325°C 325.37</td>
</tr>
<tr>
<td>350°C</td>
<td>350°C 350.38</td>
</tr>
<tr>
<td>375°C</td>
<td>375°C 375.39</td>
</tr>
<tr>
<td>400°C</td>
<td>400°C 400.41</td>
</tr>
<tr>
<td>425°C</td>
<td>425°C 425.42</td>
</tr>
<tr>
<td>450°C</td>
<td>450°C 450.44</td>
</tr>
<tr>
<td>475°C</td>
<td>475°C 475.46</td>
</tr>
<tr>
<td>500°C</td>
<td>500°C 500.48</td>
</tr>
</tbody>
</table>

in cal/g. Basin2 extrapolates to temperatures outside the range 0°C to 300°C. The program does not currently account for the variation of enthalpy with salinity.

### Halite saturation

The solubility of halite enters into Basin2 calculations when you specify that this variable controls the fluid salinity along the basin’s basal boundary or within a formation. Significantly, Basin2 does not check to see whether fluid elsewhere in the basin has become supersaturated with respect to this mineral.

The program stores, in tabular form, data for the molal solubility of halite versus temperature

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (molal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25°C</td>
<td>6.1581</td>
</tr>
<tr>
<td>50°C</td>
<td>6.2786</td>
</tr>
<tr>
<td>75°C</td>
<td>6.4432</td>
</tr>
<tr>
<td>100°C</td>
<td>6.6538</td>
</tr>
<tr>
<td>150°C</td>
<td>7.2233</td>
</tr>
<tr>
<td>200°C</td>
<td>8.0148</td>
</tr>
<tr>
<td>250°C</td>
<td>9.0701</td>
</tr>
<tr>
<td>300°C</td>
<td>10.451</td>
</tr>
<tr>
<td>350°C</td>
<td>12.251</td>
</tr>
</tbody>
</table>

as compiled by Phillips et al. (1981); Figure 3.3 shows the data graphically.

Alternatively, you can set the solubility to a constant value (in molal) with the `halite_solubility` keyword. In this case, solubility in the simulation does not vary with temperature.
Figure 3.3 Solubility of halite (molal) versus temperature (Phillips et al., 1981).
4 Defining Basin Stratigraphy

About basin stratigraphy

The second step in running Basin2, after you have set properties for the rock types you wish to use, is to define your basin’s stratigraphy. To do so, you divide the basin’s stratigraphic section into time-stratigraphic units. The stratigraphic units commonly correspond to formations in the basin, but you should be careful that the formation tops are indeed time lines. In other words, you should not confuse rock stratigraphy with time stratigraphy.

You specify each unit’s thickness, the rock types of which it is composed, and other pieces of information. Unit thickness can vary along the cross section, so you can model basins with irregular geometries. You set composition by specifying the fraction of each rock type within the unit. The fractions can also vary along the cross section, so long as they sum to one. In this way you can account for facies changes within formations.

Basin2 can also account in a limited way for the hydraulic effects of faults. Hydraulic faults affect the flow of groundwater, but strata are not displaced across them, as they would be across structural faults. You can sometimes model a structural fault by setting an abrupt facies change across a hydraulic fault. Even then, however, Basin2 will not account for movement along the fault over geologic time.

Stratigraphic units and wells

You specify a minimum of three pieces of information for each stratigraphic unit: the unit’s thickness, composition, and time of deposition. The corresponding keywords are thickness, X_rock (usually abbreviated to x), and t_dep. The t_dep keyword defines the point in time at which the last of the unit was deposited.

Basin2 assumes that each unit is deposited at a uniform rate beginning immediately after completion of the previous unit (i.e., the t_dep of the underlying formation) and continuing to the t_dep of the unit in question. You can define hiatuses in deposition and even intervals of erosion that separate periods of deposition. By convention, you begin by defining the oldest stratigraphic unit and progress upward through the
section to the youngest unit. Basin2, however, is forgiving in this regard: it will rearrange your units in time sequence if you fail to enter them in proper order.

You set the properties of each unit within a strat block. A strat block starts on a line with the `strat` keyword followed by a label (within single quotes) for the unit; the block ends with an `end_strat` entry or the start of a new strat block. The example

```
strat 'lowermost formation, sandstone'
  X(ss) = 1; t_dep = -200 m.y.
  thickness = 1 km
strat 'middle formation, carbonate'
  X(cn) = 1; t_dep = -100 m.y.
  thickness = 1500 m
strat 'gravels of uppermost formation'
  X(grv) = 1; t_dep = -50000 years
  thickness = 100 m
end_strat
```

defines a simple basin containing three stratigraphic units of uniform thickness and composition. The final `end_strat` keyword is optional. As noted in the next section (“Rules of scope”), you can assign values globally by placing assignments outside strat blocks.

To model a realistic basin, of course, the thicknesses and compositions of the stratigraphic units need to vary across the basin. You accomplish this by setting a number of wells across the cross section. The wells may be the actual wells from which you obtain data, or imaginary wells at points where it is convenient to constrain the calculation. In any case, you tell Basin2 where the wells are located with the `x_well` command. For example, you can specify the locations of five wells across the basin with the command

```
x_well(km)  10  100  125  220  270
```

The positions represent distance, in this case in kilometers, from the left side of the cross section. The wells are numbered one at 10 km through five at 270 km.

You can use the `well_name` command to give each well a name. In this case, the well names are passed to B2plot to be used in labeling cross-section plots. The format is the same as the `x_well` command, except that each name should appear within single quotes.

Basin2 does not require you to specify the wells in order from left to right. Since the wells are referred to by number within column blocks, we encourage you to arrange the wells by position. In creating a new well in the middle of the cross section, on the other hand, you may find it convenient to append the new well to the well list. In this way, you need not alter the indices of existing wells.

You assign values such as the unit’s thickness and composition at each well within a column block. Such blocks begin with a `column` statement listing the variables to be defined and their units, and continue
with a series of \texttt{well} (or \texttt{w}) statements. For example, you could set a stratigraphic unit with the statements

\begin{verbatim}
strat 'sandstone/shale wedge'
t,dep = -31 m.y.
column X(ss) X(sh) thickness(m)
w(1)  .7     .3        1100
w(2)  .5     .5        870
w(3)  .25    .75        430
w(4,5) .15    .85        310
\end{verbatim}

The form that the well index takes in the \texttt{well} statement is flexible. You may set a single index (e.g., \texttt{w(2)}), two or more indices separated by commas (\texttt{w(1,2,4)}), or a range of indices (\texttt{w(1:4)}); the syntax \texttt{w(4:)} refers to wells with indices of four and greater.

The cross section extends in the $x$-direction from zero at the left to the position of the right-most well. You can extend it farther to the right by setting the \texttt{width} keyword:

\begin{verbatim}
width = 300 km
\end{verbatim}

In this example, the basin extends 30 km to the right of the fifth well, the position of which we set above in the \texttt{x_well} statement. You can reverse the well positions with the command

\begin{verbatim}
flip = on
\end{verbatim}

In this case, the left-most well appears farthest to the right, and so on.

Basin2 grids the basin in an even mesh, without regard for the positions of wells. To set the unit’s thickness or composition, for instance, along the cross section, the program finds the well immediately to the left and to the right of the nodal point in question. The program then interpolates from the values at these wells. Nodal points to the left of the left-most well take values directly from that well, and those to the right of the right-most well are treated similarly. If you set three wells closely together, the properties of the middle well will be ignored in the gridding unless a nodal point happens to fall within the group.

**Rules of scope**

Many of the variables in Basin2 can vary along the cross section and from stratigraphic unit to stratigraphic unit. Other variables can change with geologic time. Basin2 lets you set values to such variables in a number of ways: globally, by stratigraphic unit, by position along the cross section, or by unit and position. To take advantage of this flexibility, you should be aware of two rules of scope that Basin2 follows. These rules apply not only to variables discussed to this point, but to those presented in later sections.

The first rule is that assignments made within strat blocks apply only to the stratigraphic unit in question, whereas those made outside strat blocks apply to all strata remaining to be defined. For example, in the input
Defining Basin Stratigraphy

\[ X(ss) = 1 \]
\[ \text{strat 'one'} \]
\[ \ldots \]
\[ \text{strat 'two'} \]
\[ \ldots \]
\[ \text{strat 'three'} \]
\[ X(ss) = 0; X(sh) = 1 \]
\[ \ldots \]
\[ \text{strat 'four'} \]
\[ \ldots \]
\[ \text{end_strat} \]

Units one, two, and four are composed of sandstone, but unit three is made of shale. In the example

\[ X(ss) = 1 \]
\[ \text{strat 'one'} \]
\[ \ldots \]
\[ \text{strat 'two'} \]
\[ \ldots \]
\[ \text{end_strat} \]
\[ X(ss) = 0; X(sh) = 1 \]
\[ \text{strat 'three'} \]
\[ \ldots \]
\[ \text{strat 'four'} \]
\[ \ldots \]
\[ \text{end_strat} \]

Units one and two are sandstone, and units three and four are shale.

The second rule of scope is that simple assignments apply at all wells along the cross section, but assignments made in column blocks apply to individual wells.

\[ \text{strat 'one'} \]
\[ X(sh) = 1 \]
\[ \ldots \]
\[ \text{strat 'two'} \]
\[ X(cn) = 1 \]
\[ \ldots \]
\[ \text{strat 'three'} \]
\[ \begin{array}{ll}
\text{column} & X(sil) & X(dol) \\
\text{w(1)} & 1 & 0 \\
\text{w(2)} & 2/3 & 1/3 \\
\text{w(3)} & 1/3 & 2/3 \\
\text{w(4)} & 0 & 1 \\
\end{array} \]
\[ \ldots \]
\[ \text{strat 'four'} \]
\[ X(ss) = 1 \]
\[ \ldots \]
\[ \text{end_strat} \]

In this example, units one, two, and four, respectively, are composed of shale, carbonate, and sandstone. Unit three, however, varies across the cross section from siltstone \((sil)\) to dolomite \((dol)\).

Note that the first rule applies to column blocks as well as simple assignments. In other words, a column block that appears within a strat...
block pertains only to that unit. A column block outside of a strat block, on the other hand:

```
column     X(ss)  X(cn)  X(sh)
w(1:3)     .9      0     .1
w(4:6)     .8     .1     .1
w(7:)      .6     .4      0
strat 'one'
  ...
strat 'two'
  ...
strat 'three'
  ...
end_strat
```

applies to all strata remaining to be defined.

As you can see, the rules of scope provide you with considerable flexibility in configuring your input. We might as easily have cast the examples above in terms of any variable from thickness to heat_flow, the heat flow conducted into the basin from the underlying crust. For example, you could set a single value for heat flow for the entire simulation and then define a single interval of higher heat flow within a strat block. You could also set heat flow to vary across the cross section, to vary over time, or to vary with both position and time.

### Deposition and erosion, uplift and subsidence

You control the deposition, erosion, uplift, and subsidence of basin strata with the `thickness` and `water_depth` keywords. As already mentioned, Basin2 deposits the sediment in a stratigraphic unit at a uniform rate beginning at the `t_dep` of the underlying unit and continuing until the `t_dep` of the unit in question.

The thickness of a stratigraphic unit, of course, changes as sediments compact over the course of a simulation. If the rock types compact differentially, the volume fractions `X_rock` for each unit also vary. For these reasons, it is important to specify the state of compaction to which your input refers. You do so with the `reference` keyword, which you can set globally or separately for each unit.

Basin2 offers two choices of reference state. You can enter thicknesses and rock fractions that refer to uncompacted sediment with

```
reference = uncompacted
```

In this case, the program uses the surface porosity $\phi = \phi_s + \phi_t$ as the reference porosity in interpreting the thicknesses and rock fractions you enter. Setting a unit’s thickness to one kilometer, for example, will cause a total of a kilometer of uncompacted sediment to be deposited. The unit itself will never quite reach this thickness, however, since the first sediments deposited will have compacted under the weight of overlying
Defining Basin Stratigraphy

Sediments in the unit by the time the top of the unit is laid down. With time, the unit will continue to compact and hence decrease in thickness.

Alternatively, you can enter values that refer to the unit in its compacted state with the keywords

```
reference = compacted
```

This is the default reference state in Basin2. Basin2 figures the maximum burial depth that the center of the unit will experience over the run. The program then uses the porosity corresponding to this depth, calculated as an equilibrium value by **Equation 2.1**, as the reference porosity. In this case, you enter thicknesses that correspond to present-day values. The thicknesses in Basin2 output may differ somewhat from your input if the unit is very thick (in which case the porosity at its center may not reflect the average porosity) or if erosion exhumes the unit in a run that assumes reversible compaction.

To set a hiatus in deposition, you define a stratigraphic unit with zero thickness:

```
strat 'hiatus'
  thickness = 0 m; t_dep = -60 m.y.
end_strat
```

Basin2 will not deposit sediment during the time interval from the \( t_{dep} \) of the previous unit to –60 million years. You deposit a unit that pinches out along the cross section in a similar way. In this case, set the unit’s thickness to zero

```
strat 'pinch out'
  column  thickness(ft)
  w(1)    150
  w(2)    80
  w(3)    25
  w(4)    0
end_strat
```

at the wells where it is not deposited.

You define an interval of erosion by setting a sediment thickness to a negative value. For example, the block

```
strat 'pleistocene erosion'
  t_dep = -50000 years
  column  thickness(m)  X(grv)
  w(1)    -760          0
  w(2)    -480          0
  w(3)    -150          0
  w(4)    -60           1
end_strat
```

causes underlying units to be eroded at wells one through three, and 60 meters of gravel (grv) to be deposited at well four.

You use the `water_depth` keyword, which you can set individually for each unit and well, to control the uplift and subsidence of basin strata.
Water depth is the elevation below sea level of the unit’s top surface. Basin2, by default, assumes a water depth of zero. The program changes water depth gradually over a unit’s interval of deposition. At the beginning of the interval, the program assumes the water depth specified for the previous unit. The value varies linearly until it reaches the setting for the current unit as deposition is complete.

You specify topographic relief by setting `water_depth` to negative values. For example, the surface of a unit defined by

```plaintext
strat 'Tuscarora formation'
column water_depth
  w(1)  -40
  w(2)  -20
  w(3)   30
  w(4)  200
end_strat
```

is, at the end of its interval of deposition, elevated above sea level along wells one and two, but subsea at wells three and four.

You can globally adjust either the water depths within a unit or for all units (see “Rules of scope”) by setting the `eustat` keyword. Setting a positive value raises sea level, and negative values cause sea level to fall. For example, the assignment

```plaintext
eustat = 20 m
```

causes Basin2 to add 20 meters to each value of water depth. By default, `eustat` is set to zero. You can suppress topographic relief over the simulation with the statement

```plaintext
relief = off
```

Setting this flag causes Basin2 to interpret all negative values of water depth as zero. You may find it convenient to suppress topography for runs in which relief drives groundwater flow rapidly near the surface, because rapid flow can cause the program to take small time steps and hence execute slowly.

### Volume averaging

When a stratigraphic unit is composed of a single rock type, the values assigned to permeability, thermal conductivity, and the coefficient of hydrodynamic dispersion are simply those determined for the rock type. For units containing a mixture of two or more rock types, however, it is necessary to average in some way the values for the rock types over the volume of the nodal block.

The averaging technique that you choose is very often critical to the results of the model. Three choices are built into Basin2: arithmetic, harmonic, and geometric averaging. Given rock types 1, 2, 3, and so on in volume fractions $X_1, X_2, X_3, \ldots$, the permeability $k_{\text{ave}}$ calculated as the arithmetic average of the permeabilities $k_1, k_2, k_3, \ldots$ is given

$$k_{\text{ave}} = X_1 k_1 + X_2 k_2 + X_3 k_3 + \cdots$$  \hspace{1cm} (4.1)
The permeability calculated by geometric average, on the other hand, is
\[ k_{ave} = (k_1)^{x_1} (k_2)^{x_2} (k_3)^{x_3} \cdots \] (4.2)
whereas the harmonic average would be
\[ \frac{1}{k_{ave}} = \frac{X_1}{k_1} + \frac{X_2}{k_2} + \frac{X_3}{k_3} + \cdots \]
or, expressed in another form,
\[ k_{ave} = \frac{1}{X_1/k_1 + X_2/k_2 + X_3/k_3 + \cdots} \] (4.3)

The averaging techniques give very different results when the values to be averaged vary over a broad range. Figure 4.1, for example, shows the results of averaging the permeabilities of two rock types by the arithmetic, geometric, and harmonic methods. The arithmetic method gives values near the larger of the two permeabilities over a wide range of compositions, and the harmonic average predicts permeabilities near the smaller of the two values. The geometric average appears as a straight line when plotted in logarithmic coordinates.

**Figure 4.1** Average permeability of a stratum composed of two rocks types, as calculated by different averaging techniques. The rock types occupy fractions \( X_1 \) and \( X_2 \) of the stratum \((X_1 + X_2 = 1)\) and have permeabilities of \( k_1 = 10^{-3} \) and \( k_2 = 10^{-1} \) darcy.

You commonly assign different averaging techniques along the \( x \) and \( z \) directions. Since the methods give such divergent results, the averaged properties of basin strata composed of more than one rock type can be highly anisotropic. In many cases, the formation anisotropy that results from averaging is much more significant than the anisotropy you set (i.e., with the \( p_{kxz} \) keyword) for the individual rock types within the formation.

The averaging techniques you choose depend on how you envision the arrangement of rock types within the stratigraphic unit. If the rocks are layered, you set an arithmetic average along the layering (along \( x \)), and a harmonic average across the layers (\( z \)). On the other hand, if the more permeable rock type is present in isolated pods, you set a geometric
average along the unit and most commonly a harmonic average across it. If the strata are strongly deformed, you might set a geometric average in each direction.

Many real formations do not fall clearly into any of these categories. Unfortunately, considering the importance of volume averaging on the modeling results, there is currently little guidance to offer in such cases. In one study, Fogg (1986) considered the Wilcox aquifer system of the Gulf of Mexico basin in east Texas. The Wilcox is a fluvial system composed of channel-fill sands in a complex intermixture with interchannel sediments. The channel sands serve as the aquifers in the formation, but the degree to which they are hydraulically interconnected is not known. Fogg found that where channel sands make up at least 20% of the formation’s volume, horizontal permeability is best calculated as an arithmetic average.

You set the average in both the $x$ and $z$ directions with the $X_{\text{average}}$ and $Z_{\text{average}}$ keywords, either globally or by unit

\[
X_{\text{average}} = \text{arithmetic}; \quad Z_{\text{average}} = \text{harmonic}
\]

or by well within a column block

<table>
<thead>
<tr>
<th>column</th>
<th>$X_{\text{average}}$</th>
<th>$Z_{\text{average}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1:3)</td>
<td>A</td>
<td>H</td>
</tr>
<tr>
<td>w(4)</td>
<td>G</td>
<td>H</td>
</tr>
<tr>
<td>w(5)</td>
<td>G</td>
<td>G</td>
</tr>
</tbody>
</table>

In the latter case, Basin2, when assigning averaging techniques to a nodal block, checks to see which well is closest to the node. It then assigns to the node the $x$ and $z$ averaging techniques assigned at that closest well.

**Hydraulic faults**

You define hydraulic faults within fault blocks. At a minimum you set a position for the fault and its vertical permeabilities; you can also set the fault’s horizontal permeability. For example, the block

```plaintext
fault 'Spindletop fault zone'
  fault_position = 250 km
  fault_xperm = 10 md; fault_zperm = 1 darcy
end_fault
```

sets a hydraulic fault 250 km from the basin’s left side.

Basin2 takes the column of nodal points closest to the position you specify and treats it as a fault zone. Hence, the fault zone has a width equal to the width $\Delta x$ of nodal blocks in the grid. The program, instead of calculating permeability in the usual way for the nodal blocks in this column, assigns for $k_z$ the value specified in the fault block. You may leave $k_x$ for the fault unset, in which cases the program calculates it in the usual way, or explicitly assign a value.

You can use the `fault_bottom` and `fault_top` keywords to specify that a fault penetrate only certain formations. For example, including the line
within a fault block sets the fault to pass through stratigraphic units 3, 4, and 5. The index of the oldest stratigraphic unit in the basin is one, and the overlying units are numbered two, three, and so on, up to the basin’s youngest unit.

You can also specify a time interval over which a hydraulic fault exists using the `fault_begin` and `fault_end` keywords. Remembering that Basin2 considers that time in the past is negative, you could include within a fault block

```
fault_begin = -220 m.y.; fault_end = -200 m.y.
```

This line causes the fault to be hydraulically conductive for an interval of 20 million years.
5 Transient and Steady State Solutions

About transient and steady state solutions

Basin2 can seek either transient or steady-state solutions to groundwater flow problems. A transient solution, as the name implies, shows how the basin and its groundwater flow regime evolve through time. Transient solutions are needed to model flow regimes that vary in time, including flows occurring in response to sediment compaction. A transient solution is also required for tracing thermal history and organic maturation.

A steady-state solution, on the other hand, shows the basin at a single point in time. The subsurface flow predicted by the model is one that would exist if the flow regime had sufficient time to adjust to the basin configuration. Steady-state solutions, which are generally easier for Basin2 to calculate, can be useful for studying thermal convection and flow due to topographic relief.

This chapter shows how to set transient and steady-state runs and how to control the way Basin2 seeks numerical solutions.

Transient solutions

Transient solutions follow the evolution of a sedimentary basin through geologic time. The results show not only the response to conditions at a point in time, but also whatever effects of past conditions might remain from earlier times. For example, overpressures predicted in a transient run might reflect the effects of whatever pressures have not dissipated from earlier periods of sedimentation and compaction as well as the effects of the current rate of compaction.

Transient runs can model groundwater flow driven by sediment compaction and rebound, topography, and buoyant forces. The runs can also trace changes in the distributions of temperature and solute concentration (salinity and isotopes 1 and 2) within the basin over time in response to fluid migration, conduction, diffusion, and hydrodynamic dispersion. The transient mode must also be used to trace the thermal maturation of organic matter (Chapter 11) and to calculate the
cumulative volumes of cements deposited by groundwaters in basin strata (Chapter 13).

The main disadvantage to transient runs is that they can consume considerable amounts of computing time, especially when topography or buoyant forces drive rapid groundwater flow in models that account for advective transport. In cases of very rapid flow, you might consider whether a suitable model might be constructed at steady state or by neglecting the effects of groundwater advection (see Chapter 6). Alternatively, you might simply leave the program running overnight or longer.

Figure 5.1 shows how Basin2 traces a transient run. The program begins by reading your input, gridding the domain, and setting initial conditions. The program then steps forward in time by an interval $\Delta t$, which it chooses automatically (see following section on “Time stepping”), by depositing a small amount of sediment in the nodal blocks along the basin’s top surface. In making the time step, the program solves differential equations that give (1) porosity $\phi$ and nodal block heights $\Delta z$, (2) fluid pressure $P$, (3) temperature $T$, (4) salinity $C$ and the isotope distributions, and (5) hydrologic residence time over the domain. Since the solutions to these equations affect each other to varying degrees, the program can make an arbitrary number of iterations through the solution process at each time step, as specified by the user.

Figure 5.1 Procedure followed by Basin2 to trace a transient model, as discussed in text.
simulation should be written to the B2_plot.dat file, and returns to make another time step. When the program has taken enough time steps to fill the top row of nodal blocks with sediment, it creates a new, almost empty row of nodes. In this way, Basin2 continues until it reaches the end point of the simulation.

You set Basin2 into transient mode with the keywords

```
run = transient
```

The program, in fact, is in transient mode by default, so you may omit this entry if you wish. You set the points in time to start and end the run with the `start` and `end` keywords. For example, assignments

```
start = -550 m.y.; end = -250 m.y.
```

set a simulation to begin in the Cambrian and end in the Permian.

The starting times must match the `t_dep` value of one of the stratigraphic units in the basin, so at least one stratigraphic unit must be present at the onset of a run. If you do not set a starting time, the program begins the simulation at the `t_dep` value for the lowermost stratigraphic unit. Similarly, a Basin2 simulation runs by default to the `t_dep` of the last unit deposited.

Basin2 normally makes two passes through the iteration cycle (Figure 5.1) for each time step in the simulation. You can control the number of passes with the `passes` keyword. The assignment

```
passes = 1
```

sets a single pass per time step. Increasing the number of passes decreases numerical error created by solving the governing equations independently, and can sometimes improve numerical stability in a run. At the same time, increasing `passes` adds to the computing time required for each time step.

You will find that a single pass suffices for most purposes and that two passes are commonly more than adequate. In this case, you might be able to reduce computing time by almost half if you set `passes` to one. For problem runs, however, increasing `passes` over at least part of the simulation may make Basin2 run faster by increasing stability and thereby allowing the program to take larger time steps.

Basin2 also has the capability of continuing to pass through the solution cycle at each time step until each of the governing equations has converged to within a small tolerance. You specify that Basin2 should iterate to convergence by setting `passes` to zero

```
passes = 0
```

Depending on how you set the convergence tolerances, this option can be quite useful, sometimes allowing you to run problems that would otherwise be unstable. You can set the tolerances with the `tol_press`, `tol_temp`, `tol_conc`, `tol_iso1`, `tol_iso2`, and `tol_tres` keywords, which may be set globally or by stratigraphic unit. Default values,
respectively, are .01 atm, .01°C, .01 molal (for the three concentration variables), and the time span of the simulation divided by 10⁶.

Variable `max_passes` controls the greatest number of passes the program will attempt in traversing a single time step. By default, this number is 99. If the program still has not converged after this number of passes, it will write a warning message to `B2_output.txt` and attempt to continue the simulation.

A choice of methods is built into Basin2 to solve the matrix equations that result from finite difference approximations to the governing equations. The current options are L-U decomposition and a sparse matrix solver. You set the solution method with the `solution` keyword

```
solution = LU
```

the arguments of which can be `LU` or `sparse`.

L-U decomposition, a direct method for factoring band matrices, is generally quite fast. The sparse matrix solver is relatively slow but uses less memory to store the matrix arrays. The sparse solver was implemented when computer memory was expensive, and is seldom used today.

**Time stepping**

Basin2 works in transient mode by a time marching algorithm, repeatedly stepping forward through time until it has moved from the beginning point to the end of a simulation. The size of the steps the program takes in this process controls the stability of the solution process, as well as the amount of computing time required to complete the simulation.

The program automatically determines the size of its time steps, but you can closely control its decision process. The program sets the time step at the beginning of the simulation, as well as each step beginning deposition of a new stratigraphic unit, to a small value. The initial step size is stored in variable `initial_step`, which you can set in the input file. For example,

```
initial_step = 1 year
```

The default value of this variable is the time range of the simulation divided by 10⁶.

In the succeeding steps, Basin2 seeks to increase the size of the time step, subject to a number of criteria. First, the program does not allow itself to deposit more sediment in a top nodal block than already exists, nor erode more than this amount of sediment. Second, the program limits the ratio of the sizes of the current step to the previous time step. The limiting ratio, by default two, is stored in variable `step_increase`. Third, the program chooses a step so that the increases in pressure, temperature, solute concentration, and residence time, as projected from the rates of change over the previous step, do not exceed specified values. The
limiting values are stored in variables `press_increase`, `temp_increase`, `conc_increase`, `isol_increase`, `iso2_increase`, and `tres_increase`. You can set these variables in your input; the default values are 1 atm, 1°C, 0.05 molal (for the three concentration variables) and the value set for keyword `dt_max`.

In runs that consider advective transport, Basin2 constrains the step to be no longer than the time required for fluid in any nodal block to traverse either the block’s width or height. This constraint is widely applied in finite difference calculations to help assure numerical stability. Unfortunately, in runs in which groundwater moves rapidly, the constraint can lead to quite small time steps. You can relax this constraint at your own risk with the `relax` variable. The variable by default is set to one. Setting it to a larger value will allow larger time steps. A value of two, for example, allows fluid to traverse a distance twice the width or height of nodal blocks. You should use this variable with care, however, because setting it too large will cause the run to become unstable and actually decrease the step sizes that the program takes.

The program also honors a maximum time step `dt_max`, and will not pass a designated point for writing results to the `B2_plot.dat` file. By default, the program takes `dt_max` to be the time span of the simulation divided by 10^7, but you can set it directly in the input. You set the time interval between writing results to the `B2_plot.dat` file with the `print_step` keyword. Be careful that you do not set the value too small, or the `B2_plot.dat` file will become unwieldy. If you do not set a value for `print_step`, the program will write results after each stratigraphic unit has been deposited (i.e., at each value of `t_dep`).

Variable `max_steps` is the maximum number of time steps that Basin2 will take before giving up. The default value is 99999, which is quite large. You may set this value smaller to stop your simulation should it take too many steps to complete. Finally, you can set the keyword `explain` to cause the program to tell you which of the above factors limits each time step. The format is

```
explain = on
```

The program writes its explanation for each step into the `B2_output.txt` dataset.

**Time weighting**

Finite difference solutions to transient problems can be posed with different time weightings. To understand why time weighting arises, consider that the governing equations in Basin2 contain time derivatives, which at each point in the basin give each variable’s rate of change, and derivatives in space. The spatial derivatives, for example, appear in Darcy’s law, which relates groundwater discharge to gradients in hydraulic potential, and in Fourier’s and Fick’s laws, which relate the conductive heat flow and diffusive solute flux to gradients in temperature and concentration. Hence, they control transport through the medium.
As Basin2 marches forward in time, it can calculate the space
derivatives either at the beginning or end of the time step. In fact, the
program takes a weighted average of the two values; the time weighting
variable $\theta$ controls how it takes this average. Taking $n$ to refer to the
time level at the beginning of the step, and $n+1$ as the end, the averaging
technique applied along $x$ and $z$ is

$$
\frac{\partial}{\partial x} = (1-\theta) \left( \frac{\partial}{\partial x} \right)^n + \theta \left( \frac{\partial}{\partial x} \right)^{n+1}
$$

and

$$
\frac{\partial}{\partial z} = (1-\theta) \left( \frac{\partial}{\partial z} \right)^n + \theta \left( \frac{\partial}{\partial z} \right)^{n+1}
$$

Setting $\theta$ to zero causes Basin2 to consider only derivatives at the
beginning of the step, and a value of one sets the program to use
derivatives calculated at the end of the time step. Values of $\theta$ between
zero and one result in spatial derivatives that are averaged in time.

The value you choose for $\theta$ exerts an important control on the
solution’s stability and accuracy. $\theta$ values less than one-half are almost
certain to give unstable solutions, and a value of one puts the greatest
weight on stability. On the other hand, $\theta$ values near one-half produce
solutions that give the least amount of a numerical inaccuracy known as
truncation error.

Basin2 by default assumes a value for $\theta$ of 0.7, but you can use the
theta keyword to set it to any value from zero to one. Keep in mind,
however, that values less than one-half are unlikely to give stable
solutions. In practice, the truncation error produced by Basin2 is
probably small compared to the necessary errors in configuring the run,
estimating permeability, and so on. Confronted with a problem run, you
should not hesitate to set theta to one, at least for the interval of the
simulation in which the program experiences difficulty.

**Numerical stability**

Numerical stability is the ability of a numerical model to attenuate error.
In an unstable model, error grows and the calculation becomes erratic. In
Basin2, instability will manifest itself through the choice of very small
time steps or an error message reporting that a variable is out of range.
Porosity, for example, might attain a value less than zero or greater than
one during an unstable run, causing the program to stop.

Basin2, fortunately, is quite stable, so the average user need not
worry about the numerics. If you encounter an unstable run, however,
you should not respond to the small steps the program begins to take by
relaxing the constraints on the time step. Instead, try to limit the step size,
especially over the period of the simulation when the instability began.
By maintaining small steps, the program will be more likely to remain stable and complete in a reasonable time.

The following steps may help if you are confronted with an unstable transient run:

- From the B2_output.txt dataset, find how large the time step was just before the run became unstable. Then set $dt_{\text{max}}$ to be smaller than this value. Note that you can set this variable just for the troublesome stratigraphic unit.

- Decrease the values of variable $step_{\text{increase}}$, $press_{\text{increase}}$, $temp_{\text{increase}}$, or $conc_{\text{increase}}$. By setting $\text{explain} = \text{on}$, you can get an idea of which of these variables is most important in controlling the time step.

- Increase the value of $\theta$ to one.

- Make sure that $\text{relax}$ is set to one.

- Sometimes the problem is caused by poor coupling among the governing equations. In this case, try increasing the value of $\text{passes}$. You can set this value by stratigraphic unit. You can also try setting this variable to one, which sometimes helps by allowing you to take smaller time steps in the same amount of time. Or, set $\text{passes}$ to zero, which forces convergence at each step.

- Finally, we notice that many instances of instability arise when users specify overly complicated models. In an effort to get these monsters to run quickly, they adjust parameters controlling the time step until the program becomes unstable. A good strategy is to begin with a simple model, and then add complexity as you go along.

---

**Steady-state solutions**

Steady-state models differ from transient runs in that they consider conditions in the basin to be invariant in time. In calculating a steady-state model, you are in effect assuming that conditions in the basin have been constant for so long that the groundwater flow regime, temperature distribution, and solute distribution have reached an invariant state. You can also use a steady-state solution as the starting point for a transient run, as discussed in the Chapter 6.

Steady-state runs are faster for Basin2 to calculate than transient runs, and can provide good models of groundwater flow in response to topography and convective forces. It may be necessary to assume a steady state to calculate models that account for very rapid groundwater flows, since rapid flow rates can lead to small time steps in transient runs, as discussed above. Steady-state models, however, cannot account for the effects of sediment compaction in driving groundwater flow, the development of overpressures in compacting basins, or the thermal maturation of organic matter. The models can predict cementation rates (e.g., the amount of a cement formed per million years), but not cumulative cement volumes.
Figure 5.2 shows how Basin2 calculates a steady-state model. As with a transient run, the program reads your input and builds a numerical grid. It sets initial guesses to the porosity, pressure, temperature, and solute concentration fields in the basin. The program then proceeds to repeatedly solve the governing equations that define these variables. By iterating in this way, it eventually converges to the solution, at which time it writes the results to the B2_plot.dat file.

You set a steady-state run with the statement

\[ \text{run = steady} \]

To specify the point in time of the simulation, you use the start keyword; there is no need to set the completion time (i.e., the end keyword) in a steady-state run. As before, you set the numerical solution technique with the solution keyword.

The keyword iterations controls the number of iterations taken through the solution cycle. By default, this variable is zero, which causes the program to continue iterating until (within small tolerances) pressure, temperature, solute concentration, and residence time cease changing. You can set these tolerances with the keywords conv_press, conv_temp, conv_conc, conv_isol, conv_iso2, and conv_tres. The default values for these variables are $10^{-4}$ atm, $10^{-4}$ °C, and $10^{-4}$ molal (for each of the three concentration variables), and $10^{3}$ years. Variable max_iter, set to 9999 by default, sets the maximum number of iterations allowed.

If you encounter a solution that oscillates instead of converging, you can use the under_relax keyword to set under-relaxation for the iteration. Under-relaxation is a technique that limits the amount of change applied to each variable over an iteration. Specifically, if the value of a variable $\psi$, which can represent either temperature or salinity,
after the previous iteration is $\psi^{(k)}$, and solving the governing equations gives a value $\psi^*$, the program assigns a new value $\psi^{(k+1)}$ at the current iteration level according to the scheme

$$
\psi^{(k+1)} = \psi^{(k)} + \chi_{UR} (\psi^* - \psi^{(k)})
$$

(5.2)

The under-relaxation parameter $\chi_{UR}$ can range from zero to one. A value of one, the default, sets $\psi^{(k+1)}$ directly, and hence applies no under-relaxation. Smaller values of $\chi_{UR}$ decrease the correction made at each step, but hopefully improve the overall rate of convergence.
6 Configuring and Running Basin2

**About configuring and running Basin2**

The final step in setting up a Basin2 run, once you have defined rock properties and basin stratigraphy, is to configure the simulation. To do so, you tell the program how to calculate distribution of pressure, temperature, and salinity. These variables, once known, allow the program to calculate the groundwater flow regime in the basin. You can also set the program to model the thermal maturation of organic matter in petroleum source rocks, and to predict the quantities of cement precipitated from migrating groundwaters.

This chapter shows how to select the governing equations for a model and how to set the boundary conditions and initial conditions. Subsequent chapters (Chapters 7–13) show examples of applying Basin2 to a variety of problems in basin modeling.

**Groundwater flow**

Basin2 calculates the fluid pressure distribution and corresponding groundwater flow regime that result from topographic relief across the basin surface, changes of porosity in basin sediments, the expansion and contraction of pore fluids, and buoyant forces arising from gradients in fluid density. Chapters 7–9 summarize the physical basis and mathematical model for making these calculations.

You can calculate the fluid pressure in various ways. In the simplest method, you tell Basin2 to maintain pressure along the hydrostatic gradient corresponding to the fluid density. The program in this case sets groundwater flow rates to zero. You might employ this method if you are interested in studying organic maturation but not groundwater flow. You can also specify that Basin2 consider only vertical flow (which might occur in a compacting shale basin where lateral flow is unlikely) or calculate a full model of groundwater flow in two dimensions.

You set the flow model with the `flow` (or, equivalently, `pressure`) keyword. The values you can assign are

- **hydrostatic**: Hydrostatic model, flow not considered.
- **vertical or 1_D**: Vertical flow only.
- **full or 2_D**: Vertical and lateral flow.
For example, you could set the one-dimensional flow model with the entry

```
flow = vertical
```

A two-dimensional calculation is the default.

Basin2 assumes that the top surface of the sediment pile is open to groundwater flow. Where the surface is subsea, the program sets a boundary pressure at each point corresponding to hydrostatic pressure at the specified water depth. Basin2 calculates the boundary pressure assuming that the density of the overlying seawater is the same as the density of the pore fluid at the basin top surface. You can, however, set seawater density directly with the `sw_density` keyword. If, for example, you set

```
sw_density = 1.03 g/cm3
```

the program will use this value to determine the subsea boundary pressure.

At points above sea level, the program assumes that the water table corresponds to the basin surface and that pressure along the water table is one atmosphere. The program takes the bottom of the cross section as a barrier to groundwater flow.

The sides of the basin, by default, also act as barriers to flow. As such, no groundwater can enter or leave through the left sides of nodal blocks in column one, or through the right sides of blocks in the right-most column. You can set either or both side boundaries to be open to flow with the entries

```
left = open
right = open
```

You can set the `left` and `right` keywords globally or by stratigraphic unit, so that the boundaries along only certain units are open to flow.

When you set a boundary open, groundwater flows across the boundary in response to pressure differences across it. Basin2 fixes pressure in the column of boundary nodes along the side of the cross section. By default, pressure in this column follows a hydrostatic gradient extending to sea level or the basin surface, whichever is higher. You can, however, explicitly set the position of the water table to be other than that of the land surface with the `left_table` and `right_table` keywords. In setting these keywords, remember that positions above sea level are negative.

In transient simulations, the program by default takes the initial condition to be a hydrostatic pressure distribution. In some cases, you may wish to begin a calculation with the steady-state solution to the flow problem corresponding to conditions at the starting time. You do so with the entry

```
flow = vertical
```
The default setting for this keyword is hydrostatic.

**Heat transfer**

Basin2 can model heat transfer by conduction through basin sediments and by groundwater advection. The model does not account for thermal dispersion. You can set the heat transfer model in several ways using the **temperature** keyword. The simplest way is to set a single value for all basin strata:

```
initial = steady
```

You set more realistic models with the arguments

- `temperature = 20 C`
- `vertical or 1_D`
- `conductive or 2_D`
- `full or advective`

For example:

```
temperature = conductive
```

The `vertical` method, which is the default, takes the temperature distribution to fall along the equilibrium gradient between the bottom and top boundaries. The `conductive` and `full` options give solutions for heat transfer that, respectively, neglect and account for advective transport. In transient runs, these selections differ from the `vertical` option in that they account for the transient aspects of heat flow, including heat storage in fluid and rock and moving boundary effects, rather than assuming equilibrium conditions.

Each of the latter three methods requires you to set a surface temperature and a heat flow from beneath the basin. You set these values with the `surface_temp` and `heat_flow` keywords. The default values, respectively, are 20°C and 1.5 heat flow units (HFU; 1 HFU = \(10^{-6}\) cal/cm² sec).

These parameters can change along the cross section and with time, as described in Chapter 4. You might, for example, wish to set one value of surface temperature for the subsea portion of a cross section, and another for where the basin surface rises above sea level. You might also account for climate change by varying surface temperature with time.

When you set a boundary condition such as heat flow or surface temperature for a stratigraphic unit, Basin2 assigns the condition to the unit’s `t_dep` (Figure 6.1). When the unit begins to be deposited, the boundary condition is the value corresponding to the `t_dep` of the previous unit. Basin2 then linearly varies the condition so that at the end of the interval of deposition it matches the value for the current unit. If, for example, you set a heat flow of 1 HFU for one unit and 2 HFU to a second unit, then rather than suddenly changing the heat flow when the
second unit begins to be deposited, the program will gradually increase heat flow over the unit’s interval of deposition.

**Figure 6.1** Boundary conditions set by stratigraphic unit apply at the ends of deposition intervals. In this plot, heat flow during deposition of Unit 2 varies linearly from the value set for Unit 1 (HF₁ at t_\text{dep}_1), reaching the value for Unit 2 (HF₂) at the end of the interval of deposition (t_\text{dep}_2).

Boundary conditions along the side of the basin depend on whether you have set these boundaries closed or open to groundwater flow. In either case, Basin2 assumes that no heat leaves or enters the basin by conduction across the side boundaries. Heat, however, can be carried across these boundaries by advection if they are left open to groundwater flow.

The manner in which the program determines the initial temperature distribution depends on how you set the temperature and initial options. If you set temperature to a constant value, of course, this value serves as the initial temperature. Otherwise, if you have set the initial keyword to hydrostatic, which is the default, Basin2 sets the initial temperature to the vertical conductive profile resulting from the boundary conditions at the starting time. For steady initial conditions, on the other hand, the program calculates temperature from the initial flow regime according to the setting of the temperature keyword.

**Organic maturation**

Basin2 can model the maturation of organic matter, a key variable in delineating petroleum sources, in several ways. The first model is Lopatin’s method, a simple model that is widely applied in the petroleum industry. The method is based on the assumption that the maturation rate doubles with each 10°C increase in temperature. Maturity is expressed non-dimensionally as a time-temperature index, or \( TTI \), which can be interpreted as described in Chapter 11. According to the model, for example, a sediment generates oil when the \( TTI \) is in the range of 15 to 160, with peak generation occurring at a value of 75.

You tell Basin2 to calculate maturity in this way by setting the \( TTI \) keyword.
The equation used to calculate $T TI$ treats temperature in discrete blocks of 10°C rather than continuously, so contour plots of this function tend to be jagged and plots against time can appear with small valleys and bumps. The argument *discrete* is synonymous with *on*. You can specify that the program calculate $T TI$ using the continuous function of Wood (1988), as explained in **Chapter 11**. The entry $T TI = \text{continuous}$ produces smooth contours and plotted curves.

Second, Basin2 can calculate source bed maturation using the Arrhenius model of Lewan (1985). According to this model, oil generation is governed by the Arrhenius equation, which employs an activation energy and pre-exponential factor to calculate $X_o$, the oil generated by a bed as a fraction of its capacity. To activate this model, set keyword *arrhenius* to *on*. You can set the activation energy and pre-exponential factor either globally or by stratigraphic unit with the *act_eng* and *pre_fac* keywords.

Finally, the program can trace the evolution of vitrinite reflectance using the parallel reaction model of Sweeney and Burnham (1990). Activate this model with the entry $\text{vitrinite} = \text{on}$

**Chapter 11** gives complete details on using these methods to trace organic maturation.

### Salinity distributions

Basin2 calculates the salinity distribution in a basin by solving an equation of solute transport that accounts for the effects of molecular diffusion, hydrodynamic dispersion, and groundwater advection. The program treats basin groundwaters as NaCl solutions of varying concentration. If you want to assume a uniform concentration and bypass the salinity calculation altogether, specify a numerical value for the *concentration* (or *salinity*) keyword. For example, the entry $\text{concentration} = 0.5 \text{ molal}$ sets the fluid to the approximate salinity of seawater.

There are several options for calculating salinity. You specify the calculation method by setting the *concentration* keyword to one of the following arguments:

- vertical OR 1_d: Vertical diffusion (equilibrium model).
- diffusive OR 2_d: Vertical and lateral diffusion.
- full OR advective: Diffusion, dispersion, and advection in 2-D.

Basin2 by default assumes a uniform salinity of one-half molal.
The boundary conditions for solute transport are like those for heat transfer. You set the surface salinity with the `surface_conc` keyword, and the salt flux from basement (in mol/cm² sec or mol/cm² yr) with `salt_flux`. Keyword `meteoric_conc` set to `on` invokes the special case in which the program assumes a surface salinity of zero wherever the basin surface is exposed above sea level. Setting `salt_flux` to zero gives a sealed basal boundary. Basin2 by default sets a surface concentration of one-half molal and a sealed basal boundary. The program treats the side boundaries as barriers to diffusion and dispersion, although salt may be advected across them if they are left open to groundwater flow.

You can also specify that the basal boundary be held at a fixed salinity by setting the `bottom_conc` keyword. For example, the entry

```
bottom_conc = 3 molal
```

holds concentration along the basal row of boundary nodes to three molal. The entry

```
bottom_conc = halite
```

sets the basal concentration to halite saturation. Set either the `salt_flux` or `bottom_conc` keyword, but not both.

When concentration is allowed to vary, the program determines the initial salinity distribution in much the same manner as it determines temperature. When the `initial` keyword is set to `hydrostatic`, initial salinities are those that fall along a vertical diffusive gradient. For steady initial conditions, the program finds the steady-state distribution of salinity that corresponds to the initial flow regime, according to the setting of the `salinity` keyword.

You can also set interior nodes in the basin to the salinity corresponding to halite saturation. Basin2 assumes that a nodal block set in this way contains halite that dissolves (or precipitates) rapidly enough to maintain an equilibrium salinity throughout the block. To set such nodes, define a rock type that is present only where you want to maintain halite saturation. Then, set the `halite_sat` keyword to the label for this rock type. For example, the entry

```
halite_sat = ev
```

causes Basin2 to hold salinity at halite saturation in each nodal block that contains rock type `ev`. There is currently no provision for tracking the amount of halite that dissolves through time.

**Isotope transport**

Basin2 can simulate the transport of the radiogenic and radioactive isotopes $^3$He, $^4$He, $^{36}$Cl, and $^{40}$Ar in groundwater flow regimes, accounting for boundary conditions and the rates at which the isotope is generated and/or decays. The program reports the concentrations of up to two of these isotopes, as well as ratios such as $^3$He/$^4$He, $^{36}$Cl/$^{35}$Cl, and $^{40}$Ar/$^{36}$Ar.
You identify the isotopes to be considered in a simulation with the \texttt{isol\_type} and \texttt{iso2\_type} keywords. For example, you might set
\begin{verbatim}
isol\_type = 3He; iso2\_type = 4He
\end{verbatim}
in which case the program will report the distribution of $^3$He and $^4$He in the basin, as well as the $^3$He/$^4$He atomic ratio. Setting $^{36}$Cl or $^{40}$Ar as an argument in these commands similarly causes the program to consider the transport of $^{36}$Cl or $^{40}$Ar. You can also set as arguments Cl and $^{36}$Ar. In the case of Cl, the program takes the “isotope” concentration to be groundwater salinity, as determined by solving the salinity equation. This feature allows the program to report the $^{36}$Cl/Cl ratio. Similarly, $^{36}$Ar is set to allow the $^{40}$Ar/$^{36}$Ar ratio to be determined. This isotope neither is produced nor decays at significant rates in the subsurface; hence its concentration in a Basin2 simulation simply reflects the boundary conditions you set.

Like the salinity equation, you can solve for the distribution of each isotope in one of several ways, including (1) a full solution considering advection, dispersion, and diffusion, (2) a solution considering diffusion alone, (3) a vertical solution, or (4) setting a constant value. You set the solution type with the \texttt{isol\_equation} and \texttt{iso2\_equation} keywords:
\begin{verbatim}
isol\_equation = full; iso2\_equation = full
\end{verbatim}
Other keywords include \texttt{diffusive, vertical, on} or \texttt{off}, or a real value representing the isotope’s molal concentration.

The boundary conditions for isotope transport parallel those used in solving the salinity equation. You set surface concentration with the \texttt{csurf\_isol} and \texttt{csurf\_iso2} keywords. You can set the basal boundary as a specified flux condition (keywords \texttt{isol\_flux} and \texttt{iso2\_flux}) or as a fixed concentration condition (\texttt{cbase\_isol} and \texttt{cbase\_iso2}).

The source and decay rates are calculated differently for each isotope. In each case, you can control the rates using various keywords; the rate calculations and corresponding keywords are described in detail in Chapter 14.

\section*{Hydrologic residence time}

Basin2 can calculate over the simulation the residence time or “age” of groundwater across the basin. The residence time is the average interval of time that has elapsed since water at a nodal block recharged the subsurface (or the beginning of the simulation, for water present in the subsurface at the initial condition). The program figures hydrologic residence time from the rates of advection and hydrodynamic dispersion (but, by default, not molecular diffusion) in basin strata. We refer to this quantity as the “hydrologic” residence time to avoid confusion with residence time as might be calculated using isotopic methods.

By default, Basin2 does not figure hydrologic residence time. To cause it to do so, set
Configuring and Running Basin2

residence_time = on

In the input. Depending on how you wish to conceptualize residence
time, you may wish to consider diffusion in solving for this variable. To
do so, you set a diffusion coefficient equal to the self-diffusion
coefficient of water, using the **diff_tres** keyword.

Cementation

In transient runs, Basin2 can trace the volumes of cements that
precipitate in basin strata from migrating groundwater as well as the
volumes of minerals that dissolve; in steady-state runs it can calculate
instantaneous rates of cementation and dissolution. The calculation
technique is straightforward. The program assumes that mineral
solubility varies only with temperature or with temperature and pressure,
and that groundwater maintains local equilibrium with the minerals
considered.

There is no provision for many factors that can affect mineral
precipitation and dissolution, such as changes in pH due to addition or
loss of CO₂, mixing of groundwaters of differing compositions, and
kinetic controls on reaction rates. By linking the program to the React
geochemical model, however, you can account for common-ion effects
among the dissolution and precipitation reactions.

Basin2 has built-in correlations for the solubilities of five minerals:
quartz, chalcedony, cristobalite, amorphous silica, and anhydrite. The
correlations, shown in **Chapter 13**, give the solubilities of the first four
minerals as functions of temperature, and the solubility of anhydrite as a
function of temperature and pressure. There is no provision in the built-in
correlations for considering the effect of salinity on mineral solubility.

You set the program to track cementation with the **cementation**
 keyword. The keyword takes the arguments **quartz**, **chalcedony**, **cristobalite**, **amorphous**, and **anhydrite**. For example,

\[
cementation = \text{quartz} + \text{anhydrite}
\]

The argument **all** tells the program to track each of these minerals.

Keep in mind, however, that the built-in correlations treat the reaction
for each mineral independently. You should not, for this reason, add the
volumes of the silica minerals together. Rather, interpret the results as,
for example, the volume of amorphous silica that would form or dissolve
if the groundwater maintained equilibrium with this mineral. A good
practice is to consider one silica mineral at a time.

As an alternative to the built-in correlations, you can use program
React in The Geochemist’s Workbench® software package to determine
mineral solubilities. In this case, you can account for interaction among
the precipitation and dissolution reactions. First, use React to trace a
polythermal reaction path that spans the temperature range in the basin.
The React run must trace the equilibrium state of a closed system, and
hence include neither reactants nor kinetic reactions. Do not invoke options such as flow-through that imply an open system. Note that there is no provision in React for assuring that the reaction path traced is suitable for linking to Basin2.

Setting the basin2 option in React will cause the program to generate a table of mineral solubilities in dataset Btab1, which will spill over into dataset Btab2, and so on, depending on the number of minerals considered. Once React has finished, you include the table dataset or datasets in the Basin2 input stream

```plaintext
include 'Btab1'
include 'Btab2'
```

Set the cementation keyword to the names of one or more of the minerals considered in the React run

```plaintext
cementation = Dolomite + K-feldspar
```

to complete the link.

In a transient run, Basin2 tracks the amount of cement that precipitates in basin strata, but by default does not use this information to modify porosity. You can account for the effect of cementation on sediment porosity, which in turn affects permeability and hence the flow field, by setting

```plaintext
feedback = on
```

In this case, the program will calculate porosity as described in Chapter 2 and then adjust this value to account for the net volume of cementation or dissolution. The program, of course, limits the porosity adjustment to giving values in the range from zero to one. Basin2 uses the modified value of porosity throughout its calculations, including the computation of permeability and thermal conductivity; the feedback option works best when React is used to determine mineral solubility. If you use the built-in solubility correlations, be careful that you include only one silica polymorph in the calculation.

**Radial flow and wedging**

The thickness of the domain in the y direction (i.e., normal to the cross section) is by default one centimeter. You can manipulate the y-thickness to simulate radial, diverging, and converging flow systems. We might say that Basin2 is two-and-a-half dimensional.

You set the y-thickness of the domain along the left and right sides of the cross section with the y_LHS and y_RHS keywords. (LHS and RHS stand for the left-hand and right-hand sides.) Setting y_LHS to 5 cm and y_RHS to 1 cm, for example, gives a domain in which flow is focused by a factor of five from left to right. You can also set the y_max keyword to restrict the maximum y-thickness of the domain, as well as y_min, which sets the least thickness. For example, the entry
y_{LHS} = 10 \text{ cm}; y_{RHS} = 0 \text{ cm}; y_{\text{max}} = 5 \text{ cm}

produces a domain that is 5 cm thick from the left side to center, and then wedges to zero thickness from the center to right side.

**Gridding**

You control how Basin2 grids the domain with the \(nx\) and \(\text{delta}_z\) keywords. Use keyword \(nx\) to set the number of columns of interior nodes in the grid. The default is 15 columns, but this number can be as small as one or as large as desired, up to the physical limit of your computer’s memory. You might set \(nx\) to one to make a one-dimensional simulation. Basin2 spaces the columns of nodal blocks evenly across the cross section, so each column has the same width \(\Delta x\).

Keyword \(\text{delta}_z\), which you can set globally or by individual stratigraphic unit, is the target thickness \(\Delta z\) of the nodal blocks. Basin2 uses the value of this variable to decide how many rows of nodal blocks to include within a stratigraphic unit. The program converts each unit to uncompacted sediment and finds the unit’s maximum thickness. It then divides this thickness by \(\text{delta}_z\) to get the number of rows.

You can set the minimum number of rows of nodes per strat unit with the \(\text{min}_nodos\) keyword; by default, this number is one. You can further set a limiting number of rows in the grid with the \(nz_{\text{max}}\) keyword. Basin2 stops executing if this number is exceeded during a run.

Finally, keyword \(dz_0\) sets the initial thickness of nodal blocks. This variable comes into play when, as it models sediment deposition, the program adds a new row of nodal blocks along the basin surface. The program requires that the nodal blocks have a finite thickness \(\Delta z\) to initiate the time stepping algorithm and evaluate the finite difference equations. For this reason, it assigns a nominal thickness \(dz_0\) to each new block.

The value of \(dz_0\) is meant to be negligible compared to the eventual thickness of the nodal block. Setting it too large might result in instability or inaccuracy in the program results. If you set this value to be especially small, however, you may cause the program to take too many time steps. The default value is 1 cm.

**Running the programs**

You can run Basin2 from your MS Windows desktop, from the MS Windows “Command Prompt” (a “DOS Window”), or from a Unix workstation. The following sections describe the procedure in each of these cases.
To start a Basin2 session under MS Windows, click on “Start” and then “Programs” on your desktop. Under “Basin2 5.0”, select “Basin2”. The Basin2 control panel will appear on your desktop, as shown in Figure 6.2. From this panel, you can prepare input, run simulations, and render calculation results.

Specifically, the control panel lets you:

- Select a Basin2 input file for your simulation. To locate an input file, click on “Browse”. Note that Basin2 writes its output files into the directory from which the input file is taken.
- Set a suffix for the Basin2 output file names. A suffix set in the input file with the \texttt{suffix} command, however, will override any suffix specified on the control panel.
- Define any variables set in the input file (see “Input conventions”, \textit{Chapter 1}). The control panel scans the input file for variables to be defined. You set a value for each variable by clicking the “Define” button.
- Execute a Basin2 simulation, by clicking on “Run”. A window will appear in which you can watch the simulation run.
Edit your input file, by clicking “Edit Input”. This option invokes the Windows “Notepad” text editor.


Quit the Basin2 control panel application.

From the command prompt

You can also run Basin2 and B2plot from the “Command Prompt”, also known as the “DOS Window”. In this case, you launch the programs by typing commands that specify the input file and so on. The text commands for starting the programs also let you write scripts (.bat files) for running series of simulations.

To run the programs from the command line, your PATH environmental variable must be set to point to the directory where the Basin2 and B2plot executables were installed. If you do not know how to set this variable, check with your system administrator.

You start Basin2 with the b2 command. The command can take several types of arguments, each identified by a flag:

- `-i file_name` Name of input file.
- `-s suffix` Suffix for names of output files.
- `-d variable=value` Definition of a variable.

If you enter an argument without a preceding flag (e.g., `b2 My_input.txt`), the program takes the argument as the name of the input file.

By default, the program expects input from a file named `B2in.txt`, but you can specify an alternative input file with the `-i` flag. For example,

```
b2 -i My_input.txt
```

causes Basin2 to read from file `My_input.txt`.

You can set a suffix to the output files with the `-s` flag. The suffix is appended to the name of each file produced by the program. For example, the command

```
b2 -s _run1
```

causes Basin2 to write into output files named `B2_output_run1.txt`, `B2_plot_run1.txt`, and so on. This feature is useful when you want to make a series of runs without overwriting the results of previous calculations. Note that you can also set a suffix from within the input file, using the `suffix` command. A suffix set in this way overrides any value set on the command line.

Basin2 allows you to set variables in your input file which you can define from the DOS command line. You might, for example, include in your input file the entry
Here, the dollar sign marks an argument that serves as a variable. Variables can have numeric or string values; if you leave a variable undefined, Basin2 gives an error message and stops.

You use the `-d` flag to define from the command line any variables in the input file. You might, for example, include in your input file the entry

```
A_perm = $AP, B_perm = $BP
```

Here, the dollar sign marks an argument that serves as a variable. Variables can have numeric or literal values; if you leave a variable undefined, Basin2 gives an error message and stops. To set values for variables $AP$ and $BP$ in the above example, you could type

```
b2 -d AP=-7 -d BP=12
```

Note that unless enclosed in quotes (e.g., `$AP = -7$`), the definition must appear as a continuous string without blank spaces.

You invoke B2plot from the command line in a similar way. The command `b2plot` reads the calculation results in file `B2_plot.dat` of the current directory and allows you to plot them. You can use the `-i` flag

```
b2plot -i B2_plot_run1.txt
```

to specify that the program take input from an alternative file, which can reside anywhere in the file system. As with Basin2, B2plot takes an argument not preceded by a flag to be the input file, so you can shorten the command above to

```
b2plot B2_plot_run1.txt
```

The B2plot command line can include several options. The complete syntax is

```
b2plot [-i plot_file] [-c config_file] [-n]
```

The flag `-i` precedes the name of the input file, while `-c` signals the name of the configuration file to be used. Default values are `B2_plot.dat` and `b2plot_conf.dat` respectively. The option `-n`, where $n$ is an integer, indicates the time slice to be plotted (by default, the program plots the first time slice, $n=1$). For example, set `-3` to choose the third time slice in the `B2_plot.dat` file. Set $n$ very large (e.g., set a flag `-999`) to select the final time slice. Chapter 15 gives complete instructions for using B2plot.

**On a Unix workstation**

The command syntax for running Basin2 on a Unix workstation (there is currently no Unix version of B2plot) is exactly the same as under the MS Windows Command Prompt, as described in the previous section. Working under Unix, you may wish to take advantage of some of the features of the operating system.
Unix supports program execution in foreground and background. You will find it convenient to run large Basin2 jobs unattended in background while you work on something else. To launch a background job, type the Unix command

```
b2 -i My_input.txt >&! B2.log &
```

Basin2, in this example, takes input from file `My_input.txt` and sends the messages that would normally be directed to the workstation screen to a file `B2.log`. The string “>&!” serves in the Unix C-shell to redirect Basin2’s output stream (specifically, “>” redirects the normal output, the “&” redirects error messages, and the “!” allows the program to overwrite file `B2.log` if the file is not empty); the trailing “&” sends the entire process to run in the background.

You can use the Unix `nohup` command

```
nohup b2 >&! B2.log &
```

to leave the program running after you log off. This feature is convenient when you leave Basin2 running long jobs.

The Unix `tail` command allows you to monitor progress of the program by scanning what it writes into the `B2_output.txt` file. To do so, launch the program in background, as described above, and type

```
tail -f B2_output.txt
```

The `-f` flag tells `tail` to follow the end of the file as Basin2 writes into it. You can kill `tail` with `^C` (control C), and perhaps reissue the command later, without affecting the Basin2 run.

### Output tables

In addition to producing the `B2_plot.dat` dataset, Basin2 can write results in tabular form. The program produces up to five datasets named `B2_tab1.txt` through `B2_tab7.txt` into which it writes tables showing results at each nodal point in the domain. Each dataset contains tables for a family of related variables, classified as follows:

- `B2_tab3.txt`: Temperature and heat transfer.
- `B2_tab4.txt`: Salinity and mass transfer.
- `B2_tab5.txt`: Cementation by groundwaters.

By default, Basin2 does not produce any output tables. To activate the tables, enter
In this case, the program will write tables for each of the variables in Table 6.1 at each print step, as set by print_step. You can tell Basin2 to produce tables for only certain variables. The entry

\texttt{tables = porosity + permeability + pressure}

causes the program to write tables for these three variables. The tables will appear in datasets \texttt{B2_tab1.txt} and \texttt{B2_tab2.txt}, leaving the \texttt{B2_tab3.txt} through \texttt{B2_tab7.txt} empty.

### Table 6.1 Variables that can be included in each output table.

<table>
<thead>
<tr>
<th><strong>B2_tab1.txt</strong></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>depth</td>
<td>Depth below sea level (km)</td>
</tr>
<tr>
<td>porosity</td>
<td>Sediment porosity (fraction)</td>
</tr>
<tr>
<td>vzm</td>
<td>Subsidence velocity of medium (cm/yr)</td>
</tr>
<tr>
<td>vzg</td>
<td>Subsidence velocity of nodal grid (cm/yr)</td>
</tr>
<tr>
<td>delta</td>
<td>Width Δx and height Δz of nodal blocks (km)</td>
</tr>
<tr>
<td>code</td>
<td>Internal code identifying node types</td>
</tr>
<tr>
<td>rock</td>
<td>Fractions of each rock type in formation</td>
</tr>
<tr>
<td>stress</td>
<td>Effective and total stress (atm)</td>
</tr>
<tr>
<td>bulk_density</td>
<td>Bulk density of saturated sediment (g/cm³)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>B2_tab2.txt</strong></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>potential</td>
<td>Hydraulic potential of groundwater (atm)</td>
</tr>
<tr>
<td>pressure</td>
<td>Fluid pressure (atm)</td>
</tr>
<tr>
<td>overpressure</td>
<td>Overpressure relative to hydrostatic (atm)</td>
</tr>
<tr>
<td>pgrad</td>
<td>Pressure gradient ( P / Z ) (atm/km)</td>
</tr>
<tr>
<td>density</td>
<td>Fluid density (g/cm³)</td>
</tr>
<tr>
<td>viscosity</td>
<td>Fluid viscosity (cp)</td>
</tr>
<tr>
<td>velocity</td>
<td>Fluid true velocity along ( x ) and ( z ) (cm/yr)</td>
</tr>
<tr>
<td>discharge</td>
<td>Fluid specific discharge along ( x ) and ( z ) (cm/yr)</td>
</tr>
<tr>
<td>fluxes</td>
<td>Net fluid fluxes (cm³/yr)</td>
</tr>
<tr>
<td>permeability</td>
<td>Sediment permeability along ( x ) and ( z ) (log darcy)</td>
</tr>
<tr>
<td>h_tran</td>
<td>Hydraulic transmissivity along ( x ) and ( z )</td>
</tr>
<tr>
<td>oh_tran</td>
<td>Hydraulic transmissivity at the previous time level</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>B2_tab3.txt</strong></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>temperature</td>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>cpw</td>
<td>Heat capacity of groundwater (cal/g°C)</td>
</tr>
<tr>
<td>enw</td>
<td>Enthalpy of groundwater (cal/g)</td>
</tr>
<tr>
<td>cpm</td>
<td>Heat capacity of mineral grains (cal/g°C)</td>
</tr>
<tr>
<td>enm</td>
<td>Enthalpy of mineral grains (cal/g)</td>
</tr>
<tr>
<td>tcon</td>
<td>Thermal conductivity (cal/cm sec°C)</td>
</tr>
<tr>
<td>t_tran</td>
<td>Thermal transmissivity along ( x ) and ( z )</td>
</tr>
<tr>
<td>ot_tran</td>
<td>Thermal transmissivity at previous time level</td>
</tr>
<tr>
<td>TTI</td>
<td>Organic maturity (time-temperature index)</td>
</tr>
<tr>
<td>X_oil</td>
<td>Oil generated (fraction of capacity)</td>
</tr>
<tr>
<td>reflectance</td>
<td>Vitrinite reflectance (% in oil)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>B2_tab4.txt</strong></th>
<th>Description</th>
</tr>
</thead>
</table>
Several of the variables in Table 6.1 bear further explanation. Variables vzm and vzg give the rates at which the medium and the nodal points subside relative to fixed elevation. These values are the same except along the top row of nodes, where the nodal blocks expand as they accept sedimentation. Since the nodal point remains at the center of the expanding block, its motion differs from that of the sediment grains.

Variable code is an internal flag used to categorize nodal points. The categories carried internally in Basin2 are

-2 Node is not defined.
-1 A hiatus node (i.e., a node of zero thickness).
0 An interior node.
2 A boundary node.

Basin2 uses variables known as transmissivities to calculate the net fluxes of fluid, heat, and solute mass between pairs of neighboring nodal blocks. You can include hydraulic, thermal, and solute transmissivities along x and z in the output tables. The corresponding variables at the current time level are h_tran, t_tran, and c_tran, respectively, and
those at the old time level are oh_tran, ot_tran, and oc_tran. Appendix 4 shows how the transmissivities are defined, and how you can use them to recalculate fluxes.

Dataset B2_tab5.txt contains cement volumes or cementation rates. You specify as arguments the names of the minerals that you want to include in the table. The entry

```
table = cements
```

causes the program to output data for each mineral considered in the calculation.

---

**Plot interface**

Basin2 can write formatted or unformatted data into the B2_plot.dat plot interface dataset, and B2plot can read either type of data. To produce formatted data, the computer converts numbers from binary values into their character representations. You can read, edit, and print files of formatted data.

An unformatted dataset, on the other hand, is composed of numbers and characters represented by binary digits, exactly as they are held internally in the computer; we sometimes refer to these data as bitstream. Unformatted datasets are unintelligible to us but offer a convenient way for the computer to store data for itself. Files of unformatted data are compact and can be quickly written out and read back in by the computer, since there is no need to translate numbers into their character representations and then back into binary.

By default, Basin2 writes unformatted data into B2_plot.dat. Unformatted datasets, however, are not suited to manipulation by the user or to passing data among computers that represent numbers internally in different ways. In particular, PCs represent numbers differently than Unix workstations. You must, therefore, use formatted data to pass results from Basin2 between these two types of computers.

Use the plot keyword to control the dataset format. Setting the keyword to character

```
plot = character
```

causes the program to produce a formatted interface file, whereas the value bitstream sets unformatted output. The assignment

```
plot = skip
```

causes the program to skip producing the interface dataset altogether.

Finally, you can tell Basin2 to make an entry into B2_plot.dat only for the final time step in the simulation. Setting plot = final produces a single entry at the last time level in a transient run. You can also set plot = iteration to cause the program to write an entry for each iteration in a steady-state run. This feature can be useful in determining why a run fails to converge.
Debugging variables

There are several options that may be useful in debugging and troubleshooting. The first is the `residual` keyword. By setting this option on, you cause Basin2 to check the residual imbalances to the finite-difference equations describing groundwater flow, heat transfer, and mass transport. Use this test to assure that the solution method you have chosen (see `solution` keyword, Chapter 5) provides accurate results.

You can also tell Basin2 to check the energy balance and mass balances on fluid and solute. Invoke this option by setting the keyword `balance` to on. Finite difference solutions by nature seldom give exact balances, but large imbalances are cause for concern. You may be able to reduce mass or energy imbalances by better controlling the time marching algorithm, as described in Chapter 5. The balance option, however, works only with very simple basin models; its use is not recommended at this time.

Finally, you may wish to look at results for each time step over part of the simulation. By setting variables `dump_start` and `dump_end`, you direct Basin2 to write, after each time step, its calculation results into `B2_plot.dat` as well as the output tables if you have set `tables = all`. The program begins to dump results in this way, beginning with step `dump_start` and continuing through step number `dump_end`. 
7 Compaction, Pressure, and Groundwater Flow

About compaction-driven flow

As sediment is deposited in a basin, it adds to the load on underlying sediments, causing them to compact. Compaction increases pressure on the pore fluid, driving it stratigraphically upward and toward basin margins. In various studies (see reviews by Bethke, 1985, 1986; Harrison and Summa, 1991), geologists have inferred that groundwater flow regimes resulting from sediment compaction play roles in processes of petroleum migration, ore genesis, sediment diagenesis, and the origin of sedimentary brines.

The effect of compaction on fluid pressure is in many cases small. Where compaction is rapid and sediment permeability is low, however, pressure considerably in excess of hydrostatic develops in response to sediment loading. Such pressures, known as overpressures and geopressures, are of interest because of the practical difficulty and danger they pose during drilling and because of their inferred roles in geologic processes such as faulting, structural deformation, and localizing petroleum reservoirs. As discussed in Chapter 2, overpressured sediments tend to be less compacted than sediments at normal pressure because the pore fluid relieves the sediment framework of much of the weight of overlying sediments.

Two other processes affect fluid pressure in compacting basins. As sediments accumulate, underlying sediments are buried more deeply. Temperature increases along the geothermal gradient, causing the pore fluid to expand thermally. This thermal contribution, which can also arise when heat flow varies in time, has been termed aquathermal pressuring. Second, the sedimentation surface is a moving boundary. Since we judge pressure relative to a hydrostatic gradient extending downward from the surface, the moving boundary operating in the absence of compaction and thermal expansion works to produce subnormal pressure. This chapter shows how to use Basin2 to model compaction, fluid pressure, and groundwater flow as sediments accumulate in sedimentary basins.
Rate of groundwater flow

Basin2 calculates the rate at which groundwater flows through the subsurface using Darcy’s law, written for a fluid of varying density. Darcy’s law gives the fluid’s specific discharge, which is the volume of fluid crossing a unit area per unit time. Typical units of discharge are cm³/cm² yr, or simply cm/yr.

At any point, the components $q_x$ and $q_z$ of specific discharge along the $x$ and $z$ directions are given

$$q_x = -\frac{k_x}{\mu} \left( \frac{\partial P}{\partial x} - \rho g \frac{\partial z}{\partial x} \right)$$

and

$$q_z = -\frac{k_z}{\mu} \left( \frac{\partial P}{\partial z} - \rho g \right)$$  \hspace{1cm} (7.1)

Here, $k_x$ and $k_z$ are permeability in each direction, $\mu$ is fluid viscosity, $P$ is pressure, $\rho$ is fluid density, and $g$ is the acceleration of gravity.

The derivative $\partial z/\partial x$ in 7.1 is the stratigraphic slope. This term arises because, as discussed in Chapter 1, the $x$ direction in Basin2 follows stratigraphic time lines rather than the horizontal. The program carries out its calculations in this curvilinear system but reports discharge and velocity in Cartesian coordinates so the user need not be concerned about details of the internal coordinates.

The terms within brackets in 7.1, carried with the negative sign, are the driving forces for groundwater flow along $x$ and $z$. In the study of petroleum migration, these terms are known as the hydrodynamic forces. The driving forces can be expressed in traditional units (e.g., dynes) or in units of pressure over distance (e.g., atm/km or Pa/km).

Even though discharge can carry units of velocity, this variable is in fact a volume flux. The groundwater velocity, which represents the average rate of displacement of water molecules along a flow path, differs in value from the discharge. To understand why, consider groundwater discharging at a rate of 1 cm³/cm² yr through a sediment with 20% porosity. The fluid can travel only within the pore space of the rock, so the first water to cross a cm² plane in the sediment must move forward 5 cm by the end of the year to make room for the remaining discharge. The general relationship between discharge and components of the average velocity $v_x$ and $v_z$ is

$$v_x = \frac{q_x}{\phi} \quad \text{and} \quad v_z = \frac{q_z}{\phi}$$  \hspace{1cm} (7.2)

where $\phi$ is the sediment porosity. From these equations, it is clear that at a given discharge groundwater moves most rapidly through rocks of small porosity.
Hydraulic potential

Written in the form of Equation 7.1, Darcy’s law correctly accounts for convective forces that arise from lateral variations in fluid density. When fluid density remains about constant, as is the case when temperature and salinity vary little over the domain or when you set density to a constant value, Darcy’s law can be written more simply in terms of hydraulic potential. Hydraulic potential, defined by Hubbert (1940), is the mechanical energy content of a unit volume of groundwater. The potential $\Phi$ is given

$$\Phi = P - \rho g z$$  \hspace{1cm} (7.3)

where $z$ is depth below sea level. The potential function can be thought of as pressure less the hydrostatic contribution of a column of water extending downward from sea level.

Darcy’s law is written in terms of hydraulic potential as

$$-k \frac{\partial \Phi}{\partial x}$$

and

$$-k \frac{\partial \Phi}{\partial z}$$  \hspace{1cm} (7.4)

By these equations, groundwater moves from areas of high to low potential. The rate at which it moves depends on the potential gradient, permeability, and fluid viscosity.

It is convenient to represent the drive for flow by contouring the hydraulic potential function, as can easily be accomplished with B2plot (see Chapter 15). Such contours are known as equipotentials (or isopotentials). Fluid crosses equipotentials in the direction of decreasing $\Phi$; the driving force for groundwater flow in any direction is the contour interval divided by the distance between contours.

In the study of petroleum migration, you can compare this force, the hydrodynamic drive $E_{H_d}$, to the buoyant force $E_B$ arising from the lesser density of oil compared to water (Hubbert, 1953). Taking the density of water and oil to be constant, the hydrodynamic force

$$E_{H_d} = -\frac{\partial \Phi}{\partial x}$$

and

$$E_{H_d} = -\frac{\partial \Phi}{\partial z}$$  \hspace{1cm} (7.5)

is the negative gradient in hydraulic potential. You calculate the buoyant force from
\[ E_{b_t} = - (\rho - \rho_o) g \frac{\partial \zeta}{\partial x} \]

and

\[ E_{b_x} = - (\rho - \rho_o) g \]

(7.6)

where \( \rho_o \) is the oil density and \( \partial \zeta/\partial x \) is the stratigraphic slope.

Many users expect to see groundwater flow at right angles to equipotentials, as is the case in simple flow problems found in textbooks. This is seldom the case with Basin2 results, because permeability is not likely to be isotropic and, in any event, the results are almost always plotted to a vertical exaggeration. The “right angle rule” applies only to isotropic systems drawn without exaggeration.

When fluid density varies, the drive for flow unfortunately cannot be represented in terms of a scalar function like \( \Phi \); however, because equipotentials are so useful in visualizing the drive for flow, Basin2 calculates an approximate potential function during runs in which fluid density varies. The program determines potential as the difference between the calculated pressure \( P \) and pressure falling along a hydrostatic gradient passing through \( P = 0 \) at sea level. If fluid density is constant, this definition reverts to the original definition in Equation 7.3.

When drawing equipotentials in cases of varying fluid density, keep in mind that the equipotentials only approximately represent the drive for flow. You may note in such cases that fluid at some places in the domain migrates along a direction of increasing potential.

**Compaction in one dimension**

First we consider the compaction of a sediment column, assuming that only vertical flow takes place. **Input 7.1** shows the Basin2 input file we will use. The first line sets a single column of nodal blocks and tells the program to output results only at the end of the simulation. For simplicity, we assume constant values for the fluid density \( \rho \) and the density \( \rho_{sm} \) of the saturated medium. Next, the input defines the permeability correlation for rock type \( sh \) in terms of two variables \( AP \) and \( BP \). We define these values from the command line when we start the simulation. Variable \( p_{kxkz} \) sets the anisotropy in permeability, so that the vertical component \( k_z \) is one tenth of the lateral value \( k_x \).
Input 7.1  Shale compaction in one dimension.

```
x = 1;  flow = vertical;  plot = final
density = 1 g/cm^3;  bulk_density = 2.3 g/cm^3

rock sh
  A_perm = $AP;  B_perm = $BP log_darcy;  p_kxkz = 10
end_rock

X(sh) = 1;  reference = uncompacted;  heat_flow = 1 HFU

strat 'Basal unit'
  t_dep = $TIME0 m.y.
  thickness = 100 m

strat 'Shale deposited over run'
  t_dep = 0 yrs
  thickness = 10 km
```

The final lines define two stratigraphic units, each composed entirely of rock type sh. Stratigraphic thicknesses are to be entered in terms of uncompacted sediment, and the basal heat flow throughout the simulation is 1 HFU. The first stratigraphic unit is a thin layer present at the start of the simulation; the program requires that at least one unit be present at startup. The second unit is composed of a ten-kilometer pile of uncompacted sediment, which is to be deposited at a uniform rate from \( \text{TIME0} \) m.y. ago to the present.

We begin by considering the effect of permeability on pressure and porosity. Invoke the program by typing

```
b2 Input_7.1 -d AP=0 -d BP=-4 -d TIME0=-10
```

(or start Basin2 from the control panel, setting the variables as shown). This command sets the coefficients \( A \) and \( B \) in the permeability correlation (Equation 2.9) to zero and \(-4\). Since the anisotropy \( k_h/k_z \) in permeability is 10, the program will set the horizontal permeability \( k_h \) to a constant value of 100 \( \mu \)darcy, and the vertical value \( k_z \) to 10 \( \mu \)darcy. Variable \( \text{TIME0} \), set to \(-10\), is the starting time for the simulation.

Over the course of the simulation, the program added 25 nodes to the column in order to accept sediment, and took about 500 time steps. The model executed on a 400 MHz Pentium II PC in about 15 seconds. We can quickly repeat the calculation using other values for permeability on the command line. In doing so, it is convenient to use the suffix option (\(-s\)) on the command line to give unique names to the output files, as discussed in Chapter 6.

Figure 7.1, plotted with B2plot, shows the results of calculations that assumed various values for permeability. Moderate permeability values predict pressures along a hydrostatic gradient of about 100 atm/km. As we decrease permeability, pressures develop significantly in excess of hydrostatic and converge toward the lithostatic gradient of about 230 atm/km. In these runs, the sediments are too impermeable to allow fluid to be expelled rapidly enough to allow normal compaction.
Figure 7.1 Profiles versus depth for fluid pressure and porosity after deposition of 10 km of uncompacted shale over 10 m.y. (Input 7.1), as predicted by Basin2. Various lines show results of runs assuming differing values for vertical permeability \( k_z \). Fine lines show pressure gradients of 100 atm/km and 230 atm/km, for reference.

The differing amounts of compaction observed in these runs explains why the curves in Figure 7.1 extend from the surface to varying depths. In runs in which compaction proceeds normally, the 10 km pile of uncompacted sediment assumes a thickness of less than 6 km after compaction. When the pile expresses fluid too slowly to compact normally, however, the same amount of sediment assumes thickness greater than 6 km.

These calculations are unrealistic in several ways: the sedimentation rate of 1 mm/yr remains constant over 10 m.y.; the sediment is homogeneous, so there are no facies changes; and permeability does not change as the sediment compacts. To address the latter concern, we repeat the calculation for various sedimentation rates, assuming that the horizontal permeability of the shale follows the trend

\[
\log k_z \text{ (darcy)} = 8\phi - 8 \tag{7.7}
\]

taken from the data of Neglia (1979).

We invoke the program with the command

```
h2 Input_7.1 -d AP=8 -d BP=-8 -d TIME0=-10
```

and then repeat the calculation, varying the sedimentation rate by changing the value of variable \( \text{TIME0} \). The calculation results (Figure 7.2) show that as we increase the sedimentation rate, fluid pressure increases and approaches the lithostatic gradient. As before, porosity is preferentially preserved in overpressured sediments.
Figure 7.2 Profiles for fluid pressure and porosity at the end of Basin2 simulations in which 10 km of shale was deposited at differing rates. Sedimentation rates are expressed in terms of uncompacted sediment. The calculations assume that permeability follows the correlation $\log k_x = 8\phi - 8$ and that the permeability anisotropy $k_x/k_z$ is 10.

An interesting further exercise is to have Basin2 calculate the bulk density $\rho_{sm}$ from the sediment porosity, instead of assigning the variable a constant value. To accomplish this, set

```
bulk_density = variable
```

in the second line of Input 7.1. In this case, the program predicts that, as permeability and sedimentation rates increase, the fluid pressure converges to values greater than hydrostatic but somewhat less than the 230 atm/km gradient seen in the previous results.

This result occurs because the program calculates a value for the bulk density of overpressured sediments (which are undercompacted) that is considerably less than 2.3 g/cm$^3$. As such, lithostatic pressures in these runs fall to the left of the 230 atm/km gradient commonly taken to define lithostatic. Interestingly, fluid pressures measured in compacting shale basins seldom plot above a gradient of about 200 atm/km.

Compaction of the Niger Delta

In this section, we show how Basin2 can be used to model the compaction of an actual basin, the Niger Delta. Input 7.2 was compiled by Charles Norris from references listed in Appendix 5. The input describes a cross section running 432 km landward from left to right. We set the finite difference grid to contain 30 columns of nodal blocks, each with a target thickness of 800 m of uncompacted sediment. The $y$-thickness of the cross section, set by variables $y_{LHS}$ and $y_{RHS}$, increases from right to left to account for the seaward increase in the delta’s width. Distributed across the cross section are 14 wells, the first 6 km from the left, and the last 426 km from the left.
**Input 7.2** Niger Delta basin.

<table>
<thead>
<tr>
<th>x_well(km)</th>
<th>6</th>
<th>56</th>
<th>76</th>
<th>121</th>
<th>161</th>
<th>186</th>
<th>216</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>251</td>
<td>276</td>
<td>306</td>
<td>336</td>
<td>366</td>
<td>396</td>
<td>426</td>
</tr>
</tbody>
</table>

heat_flow = 1.5 HFU; relief = off

X_average = geometric, Z_average = harmonic

<table>
<thead>
<tr>
<th>strat 'pre-Eocene'</th>
</tr>
</thead>
<tbody>
<tr>
<td>t_dep = -55 m.y.</td>
</tr>
<tr>
<td>thickness = 10 m; X(sh) = 1.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>column</th>
<th>water_depth(km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1:8)</td>
<td>2.60</td>
</tr>
<tr>
<td>w(9)</td>
<td>2.56</td>
</tr>
<tr>
<td>w(10)</td>
<td>2.37</td>
</tr>
<tr>
<td>w(11)</td>
<td>2.04</td>
</tr>
<tr>
<td>w(12)</td>
<td>1.61</td>
</tr>
<tr>
<td>w(13)</td>
<td>1.14</td>
</tr>
<tr>
<td>w(14)</td>
<td>0.70</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>strat 'Early Eocene'</th>
</tr>
</thead>
<tbody>
<tr>
<td>t_dep = -49.5 m.y.</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>column</th>
<th>thickness(km)</th>
<th>water_depth(km)</th>
<th>X(ss)</th>
<th>X(sh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1:4)</td>
<td>0.0</td>
<td>2.600</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(5)</td>
<td>0.064</td>
<td>2.536</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(6)</td>
<td>0.239</td>
<td>2.361</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(7)</td>
<td>0.574</td>
<td>2.026</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(8)</td>
<td>1.081</td>
<td>1.519</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(9)</td>
<td>1.435</td>
<td>1.128</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(10)</td>
<td>1.688</td>
<td>0.682</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(11)</td>
<td>1.722</td>
<td>0.317</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(12)</td>
<td>1.722</td>
<td>0.079</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(13)</td>
<td>1.700</td>
<td>0.0</td>
<td>0.10</td>
<td>0.90</td>
</tr>
<tr>
<td>w(14)</td>
<td>0.800</td>
<td>-0.009</td>
<td>0.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>strat 'Lower Middle Eocene'</th>
</tr>
</thead>
<tbody>
<tr>
<td>t_dep = -46.5 m.y.</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>column</th>
<th>thickness(km)</th>
<th>water_depth(km)</th>
<th>X(ss)</th>
<th>X(sh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1:3)</td>
<td>0.0</td>
<td>2.600</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(4)</td>
<td>0.010</td>
<td>2.590</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(5)</td>
<td>0.171</td>
<td>2.365</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(6)</td>
<td>0.265</td>
<td>2.096</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(7)</td>
<td>0.346</td>
<td>1.679</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(8)</td>
<td>0.383</td>
<td>1.136</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(9)</td>
<td>0.400</td>
<td>0.759</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(10)</td>
<td>0.450</td>
<td>0.375</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(11)</td>
<td>0.550</td>
<td>0.111</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(12)</td>
<td>0.800</td>
<td>0.002</td>
<td>0.10</td>
<td>0.90</td>
</tr>
<tr>
<td>w(13)</td>
<td>1.000</td>
<td>-0.007</td>
<td>0.82</td>
<td>0.18</td>
</tr>
<tr>
<td>w(14)</td>
<td>0.284</td>
<td>-0.022</td>
<td>0.22</td>
<td>0.78</td>
</tr>
</tbody>
</table>

**strat 'Upper Middle Eocene'**

| w(1:2) | 0.0 | 2.600 | 0.0 | 1.0 |
| w(3) | 0.002 | 2.598 | " | * |
| w(4) | 0.135 | 2.455 | " | * |
| w(5) | 0.320 | 2.045 | " | * |
| w(6) | 0.401 | 1.694 | " | * |
| w(7) | 0.450 | 1.229 | " | * |
| w(8) | 0.475 | 0.703 | " | * |
| w(9) | 0.550 | 0.386 | " | * |
| w(10) | 0.700 | 0.118 | " | * |
| w(11) | 1.400 | 0.003 | 0.05 | 0.95 |
| w(12) | 1.200 | -0.007 | 0.72 | 0.28 |
| w(13) | 0.491 | -0.021 | 1.0 | 0.0 |
| w(14) | 0.113 | -0.049 | 0.50 | 0.50 |

**strat 'Late Eocene'**

| w(1:2) | 0.0 | 2.600 | 0.0 | 1.0 |
| w(3) | 0.044 | 2.554 | " | * |
| w(4) | 0.151 | 2.304 | " | * |
| w(5) | 0.240 | 1.805 | " | * |
| w(6) | 0.269 | 1.425 | " | * |
| w(7) | 0.271 | 0.958 | " | * |
| w(8) | 0.305 | 0.474 | " | * |
| w(9) | 0.425 | 0.213 | " | * |
| w(10) | 0.850 | 0.031 | " | * |
| w(11) | 1.400 | -0.003 | 0.5 | 0.5 |
| w(12) | 0.620 | -0.014 | 1.0 | 0.0 |
| w(13) | 0.254 | -0.035 | " | * |
| w(14) | 0.027 | -0.075 | " | * |

**strat 'Early Oligocene'**

| w(1) | 0.0 | 2.600 | 0.0 | 1.0 |
| w(2) | 0.005 | 2.595 | " | * |
| w(3) | 0.082 | 2.472 | " | * |
| w(4) | 0.165 | 2.138 | " | * |
| w(5) | 0.224 | 1.581 | " | * |
| w(6) | 0.235 | 1.190 | " | * |
| w(7) | 0.250 | 0.738 | " | * |
| w(8) | 0.500 | 0.306 | " | * |
| w(9) | 1.000 | 0.102 | " | * |
| w(10) | 2.300 | 0.001 | 0.02 | 0.98 |
| w(11) | 1.300 | -0.008 | 0.95 | 0.05 |
| w(12) | 0.526 | -0.023 | 1.0 | 0.0 |
| w(13) | 0.077 | -0.052 | " | * |
| w(14) | 0.026 | -0.100 | " | * |

**strat 'Late Oligocene'**

| w(1) | 0.0 | 2.600 | 0.0 | 1.0 |
| w(2) | 0.033 | 2.562 | " | * |
| w(3) | 0.102 | 2.370 | " | * |
| w(4) | 0.166 | 1.973 | " | * |
| w(5) | 0.202 | 1.378 | " | * |
### Early Miocene

<table>
<thead>
<tr>
<th>Column</th>
<th>Thickness (km)</th>
<th>Water Depth (km)</th>
<th>X(ss)</th>
<th>X(sh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1)</td>
<td>0.0</td>
<td>2.600</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(2)</td>
<td>0.171</td>
<td>2.392</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(3)</td>
<td>0.299</td>
<td>2.070</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(4)</td>
<td>0.400</td>
<td>1.573</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(5)</td>
<td>0.428</td>
<td>0.951</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(6)</td>
<td>0.700</td>
<td>0.253</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(8)</td>
<td>1.600</td>
<td>0.029</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(9)</td>
<td>1.921</td>
<td>-0.002</td>
<td>0.47</td>
<td>0.53</td>
</tr>
<tr>
<td>w(10)</td>
<td>1.304</td>
<td>-0.012</td>
<td>0.80</td>
<td>0.20</td>
</tr>
<tr>
<td>w(11)</td>
<td>0.500</td>
<td>-0.031</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>w(12)</td>
<td>0.140</td>
<td>-0.068</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(13)</td>
<td>0.028</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(14)</td>
<td>0.0</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
</tbody>
</table>

### Lower Middle Miocene

<table>
<thead>
<tr>
<th>Column</th>
<th>Thickness (km)</th>
<th>Water Depth (km)</th>
<th>X(ss)</th>
<th>X(sh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1)</td>
<td>0.061</td>
<td>2.539</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(2)</td>
<td>0.296</td>
<td>2.096</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(3)</td>
<td>0.391</td>
<td>1.679</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(4)</td>
<td>0.437</td>
<td>1.136</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(5)</td>
<td>0.396</td>
<td>0.555</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(6)</td>
<td>0.800</td>
<td>0.272</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(7)</td>
<td>1.600</td>
<td>0.057</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(8)</td>
<td>2.507</td>
<td>-0.002</td>
<td>0.55</td>
<td>0.45</td>
</tr>
<tr>
<td>w(9)</td>
<td>1.520</td>
<td>-0.011</td>
<td>0.80</td>
<td>0.20</td>
</tr>
<tr>
<td>w(10)</td>
<td>0.760</td>
<td>-0.030</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>w(11)</td>
<td>0.213</td>
<td>-0.064</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(12)</td>
<td>0.032</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(13:14)</td>
<td>0.0</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
</tbody>
</table>

### Upper Middle Miocene

<table>
<thead>
<tr>
<th>Column</th>
<th>Thickness (km)</th>
<th>Water Depth (km)</th>
<th>X(ss)</th>
<th>X(sh)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(1)</td>
<td>0.118</td>
<td>2.421</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(2)</td>
<td>0.248</td>
<td>1.848</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(3)</td>
<td>0.285</td>
<td>1.394</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(4)</td>
<td>0.282</td>
<td>0.854</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(5)</td>
<td>0.500</td>
<td>0.337</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(6)</td>
<td>1.060</td>
<td>0.121</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(7)</td>
<td>1.500</td>
<td>0.003</td>
<td>0.19</td>
<td>0.81</td>
</tr>
<tr>
<td>w(8)</td>
<td>1.500</td>
<td>-0.008</td>
<td>0.80</td>
<td>0.20</td>
</tr>
<tr>
<td>w(9)</td>
<td>0.740</td>
<td>-0.021</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>w(10)</td>
<td>0.550</td>
<td>-0.048</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(11)</td>
<td>0.035</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>w(12:14)</td>
<td>0.0</td>
<td>-0.100</td>
<td>&quot;</td>
<td>&quot;</td>
</tr>
<tr>
<td>Column</td>
<td>Thickness (km)</td>
<td>Water Depth (km)</td>
<td>X (ss)</td>
<td>X (sh)</td>
</tr>
<tr>
<td>--------</td>
<td>----------------</td>
<td>-----------------</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>w(1)</td>
<td>0.147</td>
<td>2.273</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>w(2)</td>
<td>0.237</td>
<td>1.611</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(3)</td>
<td>0.251</td>
<td>1.143</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(4)</td>
<td>0.600</td>
<td>0.627</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(5)</td>
<td>1.200</td>
<td>0.187</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(6)</td>
<td>1.900</td>
<td>0.038</td>
<td>0.31</td>
<td>0.69</td>
</tr>
<tr>
<td>w(7)</td>
<td>1.400</td>
<td>-0.002</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>w(8)</td>
<td>0.700</td>
<td>-0.016</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>w(9)</td>
<td>0.550</td>
<td>-0.034</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(10)</td>
<td>0.180</td>
<td>-0.072</td>
<td></td>
<td></td>
</tr>
<tr>
<td>w(11:14)</td>
<td>0.0</td>
<td>-0.100</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stratigraphic Unit: Lower Late Miocene

The model accounts for two types of basin sediments, a sandstone \( ss \) and a shale \( sh \). Except for the basal unit which is pure shale, the 14 stratigraphic units grade from sandstone landward to shale seaward.
Moving upward through the stratigraphic column, the sandstone progrades seaward across the cross section. Thus, the distribution of rock types ($x$ values) reflects in a general way the typical distribution of sedimentary facies in a delta.

Since we are mainly interested in compaction, the input suppresses topographic relief, eliminating the groundwater flow that would arise from the elevation of the subaerial portion of the cross section. Overall permeability for each unit, as discussed in Chapter 4, is determined in the $x$ direction by geometric averaging, and by harmonic averaging along $z$.

The model takes about 900 times steps and runs in about 90 seconds on a 400-MHz Pentium II PC. Figure 7.3 shows at three points in geologic time the distribution of sandy facies in the basin along with the calculated pressure distribution and flow regime.

**Figure 7.3** Distribution of overpressure (contour lines, in atm) and distribution of sandy facies (shaded areas) at three points in geologic time in the Niger Delta basin, as calculated by Basin2 and rendered using B2plot. Arrows represent velocities $v_x$, $v_z$ (see scales) of fluid expelled by sediment compaction.
8 Groundwater Flow due to Topographic Relief

About topography-driven flow

Chapter 7 introduced the mathematical model that Basin2 uses to solve for the pressure distribution in a sedimentary basin and presented examples of groundwater flow driven by sediment compaction. In this chapter we consider the role of topographic relief in driving fluid flow through the subsurface.

As discussed in Chapter 7, gradients in hydraulic potential (or, when fluid density varies, gradients in pressure and elevation) drive groundwater flow. To see why flow occurs when the surface of a basin is exposed to topographic relief, consider the definition of hydraulic potential (Equation 7.3). Basin2 assumes that sediment is saturated with fluid everywhere in the basin, so the water table lies at the land surface. Since pressure $P$ along the water table is atmospheric, term $\rho g z$ in Equation 7.3 requires that hydraulic potential increase with increasing elevation above sea level (i.e., with decreasing depth $z$ below sea level). Here, $\rho$ is fluid density, $g$ is the acceleration of gravity, and $z$ is depth below sea level.

A topographic slope, therefore, causes hydraulic potential to vary across the basin surface, giving rise to groundwater flow. No such effect occurs where the basin surface lies below sea level. Hydraulic potential is the same everywhere in a standing body of water because $\rho g z$ balances hydrostatic pressure. A subsea portion of the basin surface, therefore, defines an equipotential along which there is no drive for fluid flow.

In this chapter we present a few examples to illustrate how Basin2 can be used to model the role of topography in driving fluid flow. You set topographic relief with the keyword `water_depth`. Negative values of `water_depth` represent the elevation of the basin surface above sea level. By assigning values of `water_depth` well by well, you can specify topographic relief in any configuration along the basin cross section. As noted in Chapter 4, you can adjust the position of sea level, and hence the amount of topographic relief, with the `eustat` keyword.
Flow in homogeneous basins

We start with a simple case: a homogeneous basin in which elevation varies linearly from left to right. Input 8.1 shows the Basin2 input file used for this run. We set the program in steady-state mode, and by default leave both the left and right boundaries closed to flow. Since temperature is assumed constant and porosity does not change, topographic relief is the only force driving flow. Densities of fluid and rock (bulk density) are assumed constant for simplicity.

Input 8.1 Two-layer basin.

<table>
<thead>
<tr>
<th>run</th>
<th>steady; start = 0 yrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>nx</td>
<td>20; delta_z = 200 m</td>
</tr>
<tr>
<td>temperature</td>
<td>20 C</td>
</tr>
<tr>
<td>fluid_density</td>
<td>1 g/cm3; bulk_density</td>
</tr>
<tr>
<td>x_well(km)</td>
<td>0 50</td>
</tr>
<tr>
<td>strat 'Unit 1'</td>
<td></td>
</tr>
<tr>
<td>t_dep = -1 m.y.; X(rk1) = 100%</td>
<td></td>
</tr>
<tr>
<td>thickness = 1 km; water_depth = 0</td>
<td></td>
</tr>
<tr>
<td>strat 'Unit 2'</td>
<td></td>
</tr>
<tr>
<td>t_dep = 0 yrs; X(rk2) = 100%</td>
<td></td>
</tr>
<tr>
<td>column thickness(km) water_depth(km)</td>
<td></td>
</tr>
<tr>
<td>w(1) 2 -1</td>
<td></td>
</tr>
<tr>
<td>w(2) 1 0</td>
<td></td>
</tr>
<tr>
<td>rock rk1</td>
<td></td>
</tr>
<tr>
<td>bpor = 0; A_perm = 0; B_perm = $BP1 log_darcy; p_kxkz = 10</td>
<td></td>
</tr>
<tr>
<td>rock rk2</td>
<td></td>
</tr>
<tr>
<td>bpor = 0; A_perm = 0; B_perm = $BP2 log_darcy; p_kxkz = 10</td>
<td></td>
</tr>
<tr>
<td>end_rock</td>
<td></td>
</tr>
</tbody>
</table>

There are two stratigraphic formations. The bottom formation has a constant thickness, but in the top formation we set different values of water_depth and thickness at the left and right of the section. The water_depth values are negative or zero, so the whole basin surface lies above sea level.

Each formation is made up of a single rock type, either rk1 or rk2. Porosity and permeability for each rock type are constant (bpor = 0 and A_perm = 0); p_kxkz is set so that vertical permeability is one-tenth of the lateral value. The parameter B_perm is defined for rocks rk1 and rk2, respectively, in terms of the variables BP1 and BP2. Permeability in this two-layer basin can then be defined as either homogeneous or heterogeneous, depending on the values you set on the command line for these variables.

We begin by calculating the flow pattern when permeability is the same in both layers. Start Basin2 by typing
Figure 8.1 shows the calculated potential distribution and flow pattern. Water recharges across the basin surface at high elevations and discharges at low elevations. Except near the left and right bounds, the equipotentials are almost vertical, and flow paths indicated by the velocity vectors follow lines almost parallel to the basin’s stratigraphy. Velocities are slightly larger along the shortest pathlines (those near the basin surface).

Next we consider the more interesting case (Input 8.2) in which topography is uneven instead of linear. This case differs from the previous example in that there is a single stratigraphic unit for which the values of water_depth and thickness at a number of wells across the basin define an irregular land surface. The drop in elevation between the left and right boundaries is the same as in Input 8.1, but now there are two valleys perched on the main slope. As before, the whole basin is above sea level.

<table>
<thead>
<tr>
<th>x_well(km)</th>
<th>0 1.5 3 4.5 6 7.5 9 10.5 12 13.5 15 16.5 18 19 21 23 25 26 27 28 30 34 38 42 46 50</th>
</tr>
</thead>
</table>

Input 8.2 Homogeneous basin with uneven topographic relief.

run = steady_state; start = 0 yrs
nx = 40; delta_z = 100 m
temperature = 20 C
fluid_density = 1 g/cm3; bulk_density = 2.3 g/cm3

Figure 8.1 Basin cross section showing equipotentials and flow velocities in a homogeneous basin (Input 8.1 with BP1 = −3 and BP2 = −3), as predicted by Basin2 at steady state.
Figure 8.2 shows the steady-state flow pattern calculated by Basin2. The potential distribution differs considerably from that in the first example. The upper half of the basin is divided into three sub-basins, and the two points of high elevation act as groundwater divides. A regional flow system, in which all water flows from left to right, appears only at depth. The influence of the water table configuration on the upper half of the basin is felt also in the lower half, where equipotentials are not spaced as evenly as those in the previous example. Tóth (1963) and Freeze and Witherspoon (1967) show further examples of how the water table configuration and permeability distribution affect basin flow regimes.

<table>
<thead>
<tr>
<th>column</th>
<th>thickness (km)</th>
<th>water_depth (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>w(3)</td>
<td>3.00</td>
<td>-1.00</td>
</tr>
<tr>
<td>w(2)</td>
<td>2.90</td>
<td>-0.90</td>
</tr>
<tr>
<td>w(3)</td>
<td>2.84</td>
<td>-0.84</td>
</tr>
<tr>
<td>w(4)</td>
<td>2.80</td>
<td>-0.80</td>
</tr>
<tr>
<td>w(5)</td>
<td>2.78</td>
<td>-0.78</td>
</tr>
<tr>
<td>w(6)</td>
<td>2.74</td>
<td>-0.74</td>
</tr>
<tr>
<td>w(7)</td>
<td>2.71</td>
<td>-0.71</td>
</tr>
<tr>
<td>w(8)</td>
<td>2.72</td>
<td>-0.72</td>
</tr>
<tr>
<td>w(9)</td>
<td>2.75</td>
<td>-0.75</td>
</tr>
<tr>
<td>w(10)</td>
<td>2.78</td>
<td>-0.78</td>
</tr>
<tr>
<td>w(11)</td>
<td>2.79</td>
<td>-0.79</td>
</tr>
<tr>
<td>w(12)</td>
<td>2.80</td>
<td>-0.80</td>
</tr>
<tr>
<td>w(13)</td>
<td>2.78</td>
<td>-0.78</td>
</tr>
<tr>
<td>w(14)</td>
<td>2.72</td>
<td>-0.72</td>
</tr>
<tr>
<td>w(15)</td>
<td>2.64</td>
<td>-0.64</td>
</tr>
<tr>
<td>w(16)</td>
<td>2.62</td>
<td>-0.62</td>
</tr>
<tr>
<td>w(17)</td>
<td>2.63</td>
<td>-0.63</td>
</tr>
<tr>
<td>w(18)</td>
<td>2.64</td>
<td>-0.64</td>
</tr>
<tr>
<td>w(19)</td>
<td>2.66</td>
<td>-0.66</td>
</tr>
<tr>
<td>w(20)</td>
<td>2.68</td>
<td>-0.68</td>
</tr>
<tr>
<td>w(21)</td>
<td>2.69</td>
<td>-0.69</td>
</tr>
<tr>
<td>w(22)</td>
<td>2.64</td>
<td>-0.64</td>
</tr>
<tr>
<td>w(23)</td>
<td>2.55</td>
<td>-0.55</td>
</tr>
<tr>
<td>w(24)</td>
<td>2.30</td>
<td>-0.30</td>
</tr>
<tr>
<td>w(25)</td>
<td>2.13</td>
<td>-0.13</td>
</tr>
<tr>
<td>w(26)</td>
<td>2.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
**Flow in heterogeneous basins**

We now consider flow in basins composed of stratigraphic layers of differing permeability. In the first example, we take a two-layer basin in which an aquitard overlies an aquifer. In the input (**Input 8.1**), we set the aquifer to be an order of magnitude more permeable than the aquitard. Invoke Basin2 by typing

```
b2 Input_8.1 -d BP1=-2 -d BP2=-3
```

Here, the values of **BP1** and **BP2** are the log permeabilities (in log darcys), respectively, of the aquifer (type `rk1`) and aquitard (type `rk2`). Figure 8.3 shows the equipotentials and fluid velocities calculated by Basin2.

The results displayed in Figure 8.3 differ from those shown in Figure 8.1. Flow in the top layer is now mainly vertical, whereas in the more permeable bottom layer it is mostly horizontal. Equipotentials are far from vertical in the top layer, in agreement with the direction of flow indicated by the flow velocity vectors. Note that if the approximately 10:1 vertical distortion of the plot were eliminated, equipotentials near the left and right boundaries in the top layer would be almost horizontal. Most water in the basin flows through the aquifer from left to right; it is only because the left and right boundaries are closed that water migrates vertically through the aquitard.
With Basin2 you can predict the flow pattern in a basin having a rock composition that varies not only with depth but also from well to well. Consider the data in Input 8.3. The basin is composed of four layers. The lowermost layer is a sandstone aquifer that runs through the basin. The second layer from the bottom and the uppermost layer are homogeneous aquitards made up of shale and carbonate, respectively. The third layer from the bottom is heterogeneous: the left half is composed of sandstone and the right half of shale. The left half of this layer is therefore a second aquifer. Figure 8.4 shows equipotentials and velocity vectors calculated by Basin2.

Input 8.3 Four-layer basin.

```
run = steady_state; start = 0 yrs
nx = 20; delta_z = 100 m
temperature = 20 C
fluid_density = 1 g/cm³; bulk_density = 2.3 g/cm³
width = 50 km
x_well(km) 0 25 30 50
strat 'Unit 1'
t_dep = -3 m.y.; X(ss) = 100%
thickness = 500 m
strat 'Unit 2'
t_dep = -2 m.y.; X(cn) = 100%
thickness = 700 m
strat 'Unit 3'
t_dep = -1 m.y.
thickness = 300 m
column X(ss) X(sh)
w(1:2) 1 0
w(3:4) 0 1
strat 'Unit 4'
t_dep = 0 yrs; X(sh) = 100%
column thickness(km) water_depth(km)
w(1) 1.5 -1.0
w(2) 1.0 -0.5
w(3) 0.9 -0.4
w(4) 0.5 0.0
```
The equipotentials in Figure 8.4 are spaced most closely together near the left and right boundaries, indicating that potential gradients are greatest there. The vertical gradients drive water into the top aquifer in the left half of the basin and out of the bottom aquifer near the right boundary. Flow is channeled along a path of high permeability, following the sandstone aquifers. Although water is drawn into the top aquifer, significant horizontal flow does not develop within it because the permeable part of the layer spans only part of the basin; therefore, water has to travel vertically downward to the bottom aquifer. In the top layer, hydraulic potential has a more constant gradient, and flow paths near the surface are similar to those of the homogeneous basin of the first example. Because of the different permeabilities in underlying formations, however, a smaller fraction of the total discharge in this example passes near the surface.
9 Erosion and Groundwater Flow

About the effect of erosion on flow

The effect of erosion on fluid pressure and groundwater flow within sedimentary basins is quite unlike that of sedimentation. Whereas overpressures characteristically develop in compacting basins where sedimentation is rapid and permeability low, subnormal pressures tend to develop within aquitards in basins undergoing surficial erosion.

Several processes are believed to be significant in accounting for such effects on fluid pressure. Erosion of the land surface reduces the total stress on the underlying sediment, allowing it to expand and thus regain some of the porosity it lost during burial. Sediments cool along the geothermal gradient as they are uncovered and move closer to the land surface. Expansion of the rock and the thermal contraction of the pore fluid work to decrease fluid pressure. The erosional surface, however, is a moving boundary. Since pressure is judged relative to a hydrostatic gradient extending from the land surface, the moving boundary works to create overpressures by shifting the hydrostatic gradient.

According to a study by Corbet and Bethke (1992), sediment expansion in response to unloading has a greater effect on fluid pressure than does the moving boundary or the thermal contraction of the fluid. For this reason, the net effect of erosion is to create underpressure. In this chapter, we show how to use Basin2 to model the effects of erosion on subsurface pressure and groundwater flow.

One-dimensional model

We start by modeling in one dimension the effect of erosion on pressure within a shale aquitard. In the model (Input 9.1), the aquitard is sandwiched between two sandstone aquifers. These three formations, each containing 1 km of uncompacted sediment, have already been deposited when the simulation starts at −1 m.y. We set a single column of nodes and a nodal block height of 100 m in the aquifers and 50 m in the aquitard; the program will make a single pass through the transient solution cycle at each time step.
Input 9.1  *Effect of erosion on fluid pressure in a shale layer.*

\[
\begin{align*}
\text{start} &= -1 \text{ m.y.; } \text{end} = 0 \text{ yrs; } \text{print}_\text{step} = 1/2 \text{ m.y.} \\
nx &= 1; \ \text{delta}_z = 100 \text{ m; } \text{passes} = 1 \\
\text{compaction} &= \text{irreversible} \\
\text{rock sh} \\
\quad \text{bpor}_\text{ul} &= .1 /\text{km} \\
\quad A_{\text{perm}} &= 0; \ B_{\text{perm}} = -8 \log_{\text{darcy}}; \ p_{\text{kzx}} = 1 \\
\text{end_rock} \\
\text{width} &= 10 \text{ km} \\
x_{\text{well}}(\text{km}) &= 5 \\
X(\text{ss}) &= 1; \ \text{reference} = \text{uncompacted} \\
\text{left} &= \text{open}; \ \text{right} = \text{open} \\
\text{strat 'basal sand'} \\
\quad t_{\text{dep}} &= -3 \text{ m.y.} \\
\quad \text{thickness} &= 1 \text{ km} \\
\text{strat 'shale aquitard'} \\
\quad t_{\text{dep}} &= -2 \text{ m.y.} \\
\quad \text{thickness} &= 1 \text{ km} \\
\quad X(\text{ss}) &= 0; \ X(\text{sh}) = 1 \\
\quad \text{left} &= \text{closed}; \ \text{right} = \text{closed} \\
\quad \text{delta}_z &= 50 \text{ m} \\
\text{strat 'upper sand'} \\
\quad t_{\text{dep}} &= -1 \text{ m.y.} \\
\quad \text{thickness} &= 1 \text{ km} \\
\text{strat 'interval of erosion'} \\
\quad t_{\text{dep}} &= 0 \text{ yrs} \\
\quad \text{thickness} &= -.5 \text{ km}
\end{align*}
\]

We assume that the two aquifers are well enough connected hydraulically to the land surface to remain at hydrostatic pressure; to reflect this assumption in our one-dimensional simulation, we leave open the left and right boundaries of the upper and lower formations. As the aquitard expands, fluid migrates inward from the aquifers. To model this vertical flow, we set closed boundaries for the aquitard.

To trace a realistic model of the aquitard as it rebounds, we set the option for irreversible compaction (Chapter 2) and set a value for the unloading coefficient \(\text{bpor}_\text{ul}\) of 0.1, which is considerably smaller than the default compaction coefficient \(\text{bpor}\) of .85. At these settings, the shale will regain during unloading only a fraction of the porosity it lost during burial and compaction. Using keywords \(A_{\text{perm}}, B_{\text{perm}},\) and \(p_{\text{kzx}}\), we set permeability in the aquitard to \(10^{-8}\) darcy.

Over the one million years of the simulation, Basin2 erodes 500 m of sediment from the uppermost unit. Figure 9.1 shows how hydraulic potential within the aquitard changes over time. The initial condition is hydrostatic pressure, so hydraulic potential at 1 m.y. is 1 atm, or atmospheric pressure. With time, hydraulic potential within the aquitard decreases, permitting fluid to migrate inward from the surrounding aquifers.
Figure 9.1 Effect over time of surficial erosion on hydraulic potential in an aquitard (center unit) sandwiched between aquifers. Squares show positions of nodal blocks across the aquitard; horizontal lines delimit stratigraphic units.

The shape of the potential profile (Figure 9.1) is roughly parabolic; it would be even more nearly parabolic if we had set fluid density and viscosity to be constant. When we repeat the run assuming different thicknesses for the aquitard, we find that the magnitude of the potential decrease at the center of the formation varies with the square of thickness. Experiments in which we vary the assumed permeability show that permeability and the potential decrease are inversely related.

Western Canada Sedimentary basin

As a second example, we consider a cross section through the Western Canada Sedimentary basin, studied by Corbet and Bethke (1992). The Alberta section of the basin is of interest because maps of pressure, expressed as hydraulic potential, show that the aquitards there contain local minima in hydraulic potential that are closed in three dimensions.

This closure, and the fact that hydraulic potential in the section reaches values smaller at depth than anywhere along the basin surface, indicate clearly that fluid movement in the basin has yet to adjust to an equilibrium with the relief of the land surface. Several hypotheses have been proposed to explain low fluid pressures in this and other basins.

Corbet and Bethke (1992) used Basin2 to calculate a regional model of groundwater flow in the basin. Their model, which includes the effects of erosion over the past 5 million years, reproduces the general features of the regional pressure distribution. Results of the modeling suggest that unloading by erosion has played the dominant role in creating the underpressures observed in the basin.

Input 9.2 is a simplified version of the data Corbet and Bethke (1992) used in their calculations. The simulation begins at –5 m.y., following deposition of seven Paleozoic and Mesozoic formations and a subsequent hiatus in deposition from –65 m.y. to –5 m.y. The run spans
an initial period of erosion followed by a hiatus and a second interval of erosion.

**Figure 9.2** shows the simulation results at two points in geologic time. Hydraulic potential in the results reaches a minimum within the Colorado Shale aquitard. Because of the minimum, fluid migrates vertically from underlying and overlying aquifers into the aquitard. In the present day, hydraulic potential at the left side of the aquitard is almost 20 atm less than at the land surface there, and about 4 atm less than where the basin’s surface lies at its topographically lowest point.

**Input 9.2 Western Canada Sedimentary basin.**

```
start = -5 m.y.
fx = 20; delta_z = 80 m; passes = 1; min_nodes = 2
initial = steady; compaction = irreversible

rock ss
  phi0 = .40; phi1 = .05; bpor = .50 /km; bpor_ul = .10 /km
rock sh
  phi0 = .55; phi1 = .05; bpor = .85 /km; bpor_ul = .17 /km
  A_perm= 8; B_perm = -9 log_darcy; p_kxxz = 10
rock cn
  phi0 = .40; phi1 = .05; bpor = .55 /km; bpor_ul = .11 /km
end_rock
bulk_density = 2.3 g/cm3

xwell(km) 0 25 29 38 50 65 69

surface_temp = 5 C; heat_flow = 1.15 HFU
X_average = geometric; Z_average = harmonic
reference = compacted

left = open; right = open

strat 'Paleozoic carbonates'
  t_dep = -230 m.y.
  thickness = 300 m; X(cn) = 1

strat 'Lower Cretaceous aquifer'
  t_dep = -120 m.y.
  thickness = 150 m; X(ss) = 80%; X(sh) = 20%
end_strat

left = closed; right = closed

strat 'Colorado shale (lower part)'
  t_dep = -90 m.y.
  thickness = 145 m; X(sh) = 1

strat 'Bow Island formation'
  t_dep = -89 m.y.
  thickness = 50 m; X(ss) = 50%; X(sh) = 50%

strat 'Colorado shale (upper part)'
  t_dep = -88 m.y.
  thickness = 305 m; X(sh) = 1
```
strat 'Milk River aquifer'
  t_dep = -80 m.y.
  thickness = 120 m; X(ss) = 60%; X(sh) = 40%
end_strat

Z_average = geometric

strat 'Upper Cretaceous aquitard'
  t_dep = -65 m.y.
  X(ss) = 20%; X(sh) = 80%
  delta_z = 160 m
  left_table = 0 m; right_table = 0 m
  column thickness(m)
  w(1) 1220
  w(2)  805
  w(3)  720
  w(4)  780
  w(5)  865
  w(6)  925
  w(7)  920

strat 'Hiatus in deposition'
  t_dep = -5 m.y.
  thickness = 0 m
  left_table = -1450 m; right_table = -1450 m
  column water_depth(m)
  w(1) -1860
  w(2) -1420
  w(3) -1340
  w(4) -1380
  w(5) -1420
  w(6) -1470
  w(7) -1485

strat 'First interval of erosion'
  t_dep = -4 m.y.
  left_table = -1250 m; right_table = -1250 m
  column thickness(m) water_depth(m)
  w(1) -655 -1260
  w(2) -240 -1210
  w(3) -155 -1180
  w(4) -155 -1220
  w(5) -150 -1280
  w(6) -155 -1340
  w(7)  0  -1465

strat 'Hiatus in erosion'
  t_dep = -2 m.y.
  thickness = 0
  left_table = -1250 m; right_table = -1250 m
  column water_depth(m)
  w(1) -1260
  w(2) -1210
  w(3) -1180
  w(4) -1220
  w(5) -1280
  w(6) -1340
  w(7) -1465
Figure 9.2 Effect of erosion on hydraulic potential and groundwater flow in the Western Canada Sedimentary basin at –4 m.y. and the present day, as calculated by Basin2. Contours are equipotentials labeled in atm.
10 Heat Transfer and Thermal Convection

About heat transfer

Basin2 can calculate basin thermal regimes accounting for groundwater flow, variation in thermal conductivity of basin sediments, and changing heat flows and surface temperature. Determining the effects of these factors on the subsurface temperature regime and on the thermal history of a basin are essential steps in attempting to model the thermal maturation of organic matter in basin strata (see Chapter 11).

Basin2 can also calculate the effect of buoyant forces in driving fluid convection. Buoyant forces arise whenever fluid density, and hence temperature, vary laterally. For this reason, variation in heat flow, surface temperature, or thermal conductivity along the cross section can cause fluid convection. Convection can also arise spontaneously in an aquifer heated from below, even if initially there is no lateral temperature gradient, depending on the aquifer’s permeability, thickness, and thermal conductivity, and the thermal gradient across it. Combarnous and Bories (1975) give a thorough description of the origin and nature of thermal convection.

Rate of heat transfer

Basin2 calculates heat transfer by conduction through sediments and pore fluid and, if specified (see Chapter 6), by fluid advection. The program does not account for radiative heat transfer, because at submetamorphic temperatures sediments and rocks are opaque to infrared radiation.

Fourier’s law gives the rate of heat conduction $q_H$

$$ q_{H_x} = -K_x \frac{\partial T}{\partial x} \tag{10.1} $$

and

$$ q_{H_z} = -K_z \frac{\partial T}{\partial z} $$
from the thermal conductivity $K_x$ and $K_z$ and the temperature gradient along $x$ and $z$. Here, $q_H$ might be given in cal/cm$^2$ sec or J/cm$^2$ sec, and the thermal conductivity in cal/cm$^2$ sec °C or J/cm$^2$ sec °C.

The rate of advective transport $q_A$, in cal/cm$^2$ sec or J/cm$^2$ sec, is the rate at which migrating fluid carries thermal energy across a unit plane. This quantity is the product of the mass flux and the fluid’s enthalpy $h_w$

$$q_A = \rho q_x h_w$$

and

$$q_A = \rho q_z h_w$$

where $\rho$ is fluid density, $q_x$ and $q_z$ are specific discharge along $x$ and $z$, and $h_w$ is fluid enthalpy, as discussed in Chapter 3.

### Thermal convection

To illustrate how we use Basin2 to model heat transfer, we calculate at steady state the effect of topographic relief on thermal convection. We set up a cross section 20 km wide and about 2 km deep (see Input 10.1). The section is composed of a basal formation overlain by a wedge of sediment that extends from the left to the center of the section. We set heat flow to be 4 HFU at the left of the cross section, 2 HFU at its center, and 1 HFU along the right side. The variation in heat flow creates a lateral temperature gradient that drives convection.

### Input 10.1 Effect of topography on thermal convection.

```
run = steady; start = 0 yrs
nx = 30; delta_z = 100 m
temperature = full; surface_temp = 20 C

rock ss
   A_perm = 0; B_perm = -2 log_darcy; p_kxkz = 10
   phi0 = 30%; phi1 = 0; bpor = 0
end_rock

X(ss) = 1
x_well(km) 0 10 20

strat 'Basal unit'
   t_dep = -1 m.y.
   thickness = 2 km

strat 'Topography'
   t_dep = 0 yrs
   column water_depth(m) thickness(m) heat_flow
   w(1) $TOPO $THICK 4
   w(2) 0 0 2
   w(3) 0 0 1
```

The wedge and underlying formation are composed of a single rock type. We set porosity to a constant value of 30%, and lateral and vertical permeability, respectively, to $10^{-2}$ and $10^{-3}$ darcy.
Variables TOPO and THICK control the elevation and thickness of the wedge. We set TOPO to a negative value and THICK to a positive number of the same magnitude. For example, we might initialize a run with the command

```
b2 -i B2in_convect.txt -d TOPO=-50 -d THICK=50
```

In this way, the base of the wedge and the top of the underlying formation lie along the horizontal.

We set a steady-state run, and in doing so implicitly assume that with time the flow regime becomes invariant. This assumption is not necessarily valid, because natural flow regimes in which fluids convect actively sometimes will oscillate rather than assuming a steady flow pattern. For this reason, Basin2 may have difficulty converging to solutions for certain problems posed at steady-state.

Figure 10.1 shows the results of the calculation made by setting zero, 50 m, and 100 m of topographic relief. When no relief is set, a plume of upwelling fluid develops along the left side of the section, above the point of highest heat flow. The effect of 50 m of relief is to diminish the plume and produce a second plume toward the right side of the section, where water driven by the topography discharges. With 100 m of relief, a single plume develops in the right half of the cross section, even though the basal heat flow is smaller there than along the left half.
Figure 10.1 Effects of topography on thermal convection, calculated assuming (top) no relief, and (middle) 50 m and (bottom) 100 m of relief from left side to center of cross section. Contours are isotherms labeled in °C. Arrows show velocities $v_x$, $v_z$ (see scale) of fluid migration driven by topographic relief and buoyant forces.
11 Organic Maturation

About modeling organic maturation

One useful function of Basin2 is to predict the depth interval in which oil is now being generated and the time in the geologic past when source beds became thermally mature. Because the program can account for variations in thermal conductivity, heat flow, and surface temperature, and for advective heat transport, it is well suited for this purpose.

Three models are available in Basin2 for calculating the degree of organic maturity and the extent of petroleum generation. First, the program uses the Lopatin model, either in a discrete or continuous form, to calculate the time-temperature index \((TTI)\) of thermal maturity. The Lopatin model is based on the simple assumption that the rate of maturation doubles with each 10°C increase in temperature.

Second, Basin2 can use the Arrhenius model to evaluate the oil generated as a fraction of the source bed’s capacity. This model predicts oil generation from a single type of kerogen from a pre-exponential factor \(A_o\) and activation energy \(E_A\). These parameters are commonly obtained from hydrous pyrolysis experiments on samples of kerogen found in source beds.

The third method, the LLNL vitrinite model, is a parallel reaction model, which uses a set of Arrhenius reaction rates to calculate vitrinite reflectance. LLNL is an acronym for Lawrence Livermore National Laboratory, where the model was developed. This model is more comprehensive than the Arrhenius model because it accounts for a diversity of reactions with a range of activation energies.

Lopatin model

Time and temperature are the two most important factors in generating and destroying oil in sedimentary basins. Lopatin (1971) developed the time-temperature index \((TTI)\) of maturity to estimate the thermal maturation of kerogen from a basin’s thermal history. The \(TTI\) of a sediment is given as the sum of maturities developed in each temperature interval

\[
TTI = \sum_{n} \left(\Delta t_n\right) \left(2^n\right)
\]

(11.1)
Here \( n \) serves to index the temperature intervals encountered by the sediment. A value of zero represents temperatures in the interval 100°C to 110°C. For each 10°C increase in temperature, index \( n \) increases by one; for each 10°C decrease in temperature, the value decreases by one. \( \Delta t_o \) is the length of time (in million years) the sediment spends within each temperature interval. The temperature factor \( 2^n \) reflects the dependence of the maturation rate on temperature.

The degree of thermal maturity is related to \( TTI \) values as follows (Waples, 1980):

<table>
<thead>
<tr>
<th>( TTI )</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>Onset of oil generation.</td>
</tr>
<tr>
<td>75</td>
<td>Peak oil generation.</td>
</tr>
<tr>
<td>160</td>
<td>End of oil generation.</td>
</tr>
<tr>
<td>(~500 \sim 1000)</td>
<td>Deadline for preserving oil.</td>
</tr>
<tr>
<td>(~1,500)</td>
<td>Deadline for preserving wet gas.</td>
</tr>
<tr>
<td>(&gt;65,000)</td>
<td>Deadline for preserving dry gas.</td>
</tr>
</tbody>
</table>

According to this interpretation, oil forms when \( TTI \) falls in the range of 15 to 160. \( TTI \) values given by the Lopatin model can be correlated to other maturity parameters (Waples, 1980), such as the \( TAI \) (thermal alteration index) and \( R_o \) (vitrinite reflectance). For example, the corresponding vitrinite reflectance values (in percent reflectance in oil) correlated to the \( TTI \) oil window range from 0.65 to 1.3.

The Lopatin model treats temperature in discrete blocks of 10°C instead of continuously. As a result, the calculated \( TTI \) curves against time show small kinks, and its contour plots tend to be jagged. In reality, sediment temperature varies continuously through geologic time. To accurately account for gradual temperature change, Wood (1988) presented a version of the Lopatin model that employs a continuous function of temperature \( T_K \) (in Kelvins)

\[
TTI = \int \frac{2^{(T_o / 10 - 37.815)}}{T_T} dt
\]

(11.2)

to calculate \( TTI \). This function produces smooth \( TTI \) contours and curves.

**Arrhenius model**

Basin2 can trace the fraction of oil generated by a source rock using the Arrhenius method of Lewan (1985). In this method, the Arrhenius equation gives the rate constant \( k \)

\[
k = A_o e^{-E_o / R T_K}
\]

(11.3)
in hr\(^{-1}\). Here \( A_o \) is the pre-exponential factor (hr\(^{-1}\)), \( E_o \) is the activation energy (kJ/mol), \( R \) is the gas constant (8.31432 J K\(^{-1}\) mol\(^{-1}\)), and \( T_K \) is absolute temperature (K).
In this model, the extent of oil generation is expressed as a fraction $X_o$ of the rock’s capacity for generating oil. Integrating the first-order rate law
\[
\frac{dX_o}{dt} = k(1 - X_o)
\]
(11.4)
where the rate constant $k$ is given by the Arrhenius equation (Equation 11.3), gives $X_o$ as a function of time. Basin2 integrates Equation 11.4 numerically.

According to the Arrhenius equation, the extent of oil generation depends on the activation energy $E_a$ and pre-exponential factor $A_o$, and on the basin’s thermal history. You obtain the activation energy and pre-exponential factor on a plot of $\ln k$ versus $1/T_k$ for a series of hydrous pyrolysis experiments. Typically, such plots show linear relations so the rates can be extrapolated to the lower temperatures found in the natural system. Hydrous pyrolysis experiments are commonly performed at high temperatures (260°C-365°C) to achieve oil generation within days or weeks, rather than the much longer time periods (1 million–100 million years) characteristic of sedimentary basins.

In Basin2, kinetic parameters determined for the Woodford Shale ($E_a = 218.25$ kJ mol$^{-1}$, $A_o = 6.51 \times 10^{16}$ hr$^{-1}$) serve as default values. The Devonian-Mississippian Woodford Shale of Oklahoma and some of its age-equivalent units are significant sources of oil in several basins within North America. However, as Lewan (1985) points out, kinetic parameters differ among the various types of kerogen found in source rocks. For example, the Woodford Shale has a larger activation energy and pre-exponential factor than does the Phosphoria Retort Shale. Such differences serve to remind us that the timing of oil generation is not the same for all source rocks.

**LLNL vitrinite model**

Basin2 can predict the evolution of vitrinite reflectance, a commonly employed measure of thermal maturity, using the parallel reaction model of Sweeney and Burnham (1990), also known as the LLNL vitrinite model. Sweeney and Burnham break down kerogen into various components, each of which has its own activation energy. They treat vitrinite maturation as a set of parallel reactions of these components.

The LLNL vitrinite model calculates the reaction rate $k_m$ of component $m$ from the Arrhenius equation (Equation 11.3). The pre-exponential factor $A_o$ in the equation is taken for each component as a constant value of $10^{13}$ sec$^{-1}$. The activation energies of components in the model range widely from 34 to 72 kcal/mol. In the model, each component is weighted by a stoichiometric coefficient $f_m$. The weighting, or stoichiometric coefficients, of components evolved in reaction vary from 0.01 to 0.07 (Table 11.1). Some vitrinite components are unreactive, so the sum of the stoichiometric coefficients is 0.85, instead of 1.
Table 11.1 Weighting coefficients and activation energies in the LLNL model.

<table>
<thead>
<tr>
<th>( f_m )</th>
<th>( E_A ) (kcal/mol)</th>
<th>( f_m )</th>
<th>( E_A ) (kcal/mol)</th>
<th>( f_m )</th>
<th>( E_A ) (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>.03</td>
<td>34</td>
<td>.04</td>
<td>48</td>
<td>.05</td>
<td>62</td>
</tr>
<tr>
<td>.03</td>
<td>36</td>
<td>.04</td>
<td>50</td>
<td>.04</td>
<td>64</td>
</tr>
<tr>
<td>.04</td>
<td>38</td>
<td>.07</td>
<td>52</td>
<td>.03</td>
<td>66</td>
</tr>
<tr>
<td>.04</td>
<td>40</td>
<td>.06</td>
<td>54</td>
<td>.02</td>
<td>68</td>
</tr>
<tr>
<td>.05</td>
<td>42</td>
<td>.06</td>
<td>56</td>
<td>.02</td>
<td>70</td>
</tr>
<tr>
<td>.05</td>
<td>44</td>
<td>.06</td>
<td>58</td>
<td>.01</td>
<td>72</td>
</tr>
<tr>
<td>.06</td>
<td>46</td>
<td>.05</td>
<td>60</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The compositional components considered in the LLNL vitrinite model have different reaction kinetics, so we calculate the rate of vitrinite maturation as the sum of the contributions of each component. According to the first-order rate law, the mass of an unreacted component \( m \) is given by

\[
\frac{dC_m}{dt} = -k_m C_w
\]  (11.5)

This equation is integrated to yield the fraction \( C_m/C_m^o \) of unreacted component \( m \) remaining in the system, where \( C_m^o \) is the component’s initial concentration. The extent of reaction \( F \)

\[
F = \sum f_m \left(1 - \frac{C_m}{C_m^o}\right)
\]  (11.6)

is the sum of the contribution from each component. After computing \( F \) by Equation 11.6, the program calculates vitrinite reflectance (in %) directly by the relation

\[
R_o = e^{(-1.6+3.7F)}
\]  (11.7)

In the vitrinite model, \( F \) ranges from 0 to 0.85, so values of \( R_o \) calculated using Equation 11.7 can vary from 0.2% to about 4.7%.

Effect of heat flow

In this section we consider how basal heat flow affects thermal maturation during sedimentation in a subsiding basin. Input 11.1 is the input file for the simulations. The first stratigraphic unit is a thin layer already deposited at the beginning of the simulation (–60 m.y). Two stratigraphic units, each composed of 2 km of uncompacted shale, are deposited at an uniform rate over the course of simulation. The bottom layer is deposited from –60 m.y. to –30 m.y. The top layer is deposited from –29 m.y. to the present. We define a short hiatus in deposition from –30 m.y. to –29 m.y. that separates the bottom layer and top layer.
Input 11.1  Organic maturation during sedimentation and burial.

\[
\begin{align*}
\text{start} & = -60 \text{ m.y.}; \quad \text{end} = 0 \text{ m.y.}; \quad \text{print\_step} = 1 \text{ m.y.} \\
\text{nx} & = 1; \quad \text{delta\_z} = 250 \text{ m} \\
\text{tti} & = \$\text{TTI}; \quad \text{vitrinite} = \text{on}; \quad \text{arrhenius} = \text{on} \\
X(\text{sh}) & = 1 \\
\text{strat 'Basal unit'} & \\
& \quad \text{t\_dep} = -60 \text{ m.y.} \\
& \quad \text{heat\_flow} = \$\text{HFLOW1} \\
& \quad \text{thickness} = 50 \text{ m} \\
\text{strat 'Bottom layer'} & \\
& \quad \text{t\_dep} = -30 \text{ m.y.} \\
& \quad \text{heat\_flow} = \$\text{HFLOW1} \\
& \quad \text{thickness} = 2 \text{ km} \\
\text{strat 'Hiatus (change in heat flow)'} & \\
& \quad \text{t\_dep} = -29 \text{ m.y.} \\
& \quad \text{heat\_flow} = \$\text{HFLOW2} \\
& \quad \text{thickness} = 0 \text{ km} \\
\text{strat 'Top layer'} & \\
& \quad \text{t\_dep} = 0 \text{ m.y.} \\
& \quad \text{heat\_flow} = \$\text{HFLOW2} \\
& \quad \text{thickness} = 2 \text{ km}
\end{align*}
\]

In the calculation, we vary the basal heat flow during the deposition of each unit by setting from the command line the variables $\text{HFLOW1}$ and $\text{HFLOW2}$ to either 1.5 or 2 HFU. By setting a hiatus in deposition with heat flow $\text{HFLOW2}$, we cause Basin2 to maintain a constant heat flow while the uppermost unit is deposited. If we were to omit the hiatus, the program would vary heat flow linearly from $\text{HFLOW1}$ to $\text{HFLOW2}$ (see Figure 6.1) as the upper unit is deposited.

A series of four simulations illustrates the effects of heat flow on the thermal maturity. We consider four scenarios: (1) a constant heat flow of 1.5 HFU, (2) a constant heat flow of 2.0 HFU, (3) a low heat flow (1.5 HFU) in the first 30 m.y. followed by high heat flow (2.0 HFU) in the second 30 m.y., and (4) a high heat flow in the first 30 m.y. followed by low heat flow in the second 30 m.y. We use keywords $\text{tti}$, $\text{arrhenius}$, and $\text{vitrinite}$ to set the maturation models considered in calculation; variable $\text{TTI}$ is set from the command line to either $\text{continuous}$ or $\text{discrete}$.

Figure 11.1 shows how the calculated maturation indices ($\text{TTI}$, fraction of oil generation, and vitrinite reflectance) at the deepest nodal point in the basin evolve through time, assuming various basal heat flow scenarios. The results show that, depending on the basal heat flow, the sediment reaches peak generation at different points in geologic time. A basin experiencing a high heat flow throughout the burial history reaches peak generation first. The effect of high heat flow on thermal maturity is more pronounced when the source beds are more deeply buried, because the rate of organic maturation increases exponentially with temperature (or burial depth). In basins undergoing continuous burial, an episode of
low heat flow followed by high heat flow yields higher levels of thermal maturity than an episode of high heat flow followed by low heat flow.

**Figure 11.1** Calculated evolution of thermal maturity at the deepest nodal point in a basin accepting continuous sedimentation (Input 11.1). Plots show versus time (a) continuous TTI model, (b) discrete TTI model, (c) fraction $X_o$ of oil generation, and (d) vitrinite reflectance $R_o$. Various lines show results of runs assuming differing values for heat flow over time. The discrete model (b) calculates TTI assuming temperature in discrete blocks of 10°C, which causes the small kinks on the curves.

**Organic maturation of Niger basin**

In a second example, we use Basin2 to model the thermal history and organic maturation of the Niger delta. We use the input file from Chapter 7 (Input 7.2) for the simulation. To activate the maturation calculation, we set the `tti` keyword to `continuous` and the `vitrinite` keyword to `on`.

**Figure 11.2** shows the calculated position of the oil window in the present day, as determined by TTI in the range 15 to 160 and vitrinite reflectance values in the range 0.65% to 1.30%. The results shown in this figure are based on the assumption that the basin has had a constant heat flow of 1.5 HFU. The predicted interval of oil generation could vary with the choice of thermal conductivity, basal heat flow, and burial history assumed in the model; these values represent the greatest uncertainties in estimating thermal maturity.
Figure 11.2 Calculated distribution of thermal maturity (shaded, in TTI and vitrinite reflectance) and pressure gradient (contours of P/Z, in atm/km) in the present-day Niger basin. Shaded areas map the oil window, which shows the depth interval where oil generation can be expected according to the models if source beds are present.

In the calculation results, the oil window over much of the section is found near the transition zone between the overpressured shales and the normally pressured sandstone facies. This result suggests that the oil generated within the source beds could migrate upward into shallower reservoirs because of its buoyancy and the large gradients in hydraulic potential found in the transition zone.
12 Mass Transport and Salinity

About modeling salt transport

Basin2 can calculate the salinity distribution in a basin, accounting for diffusion and dispersion of dissolved salt as well as salt transport by advection in a groundwater flow regime, from boundary conditions you supply. The program can also account for the effects on groundwater flow of buoyant forces arising from variations in salinity.

You should note, however, that even basic questions such as the origin of solutes in sedimentary basins are vigorously debated in the scientific literature. Hence, you do not always have a clear choice for setting boundary conditions when you calculate salinity distributions. In addition, few guidelines exist for estimating, at basin scale, values for critical hydrologic properties, such as dispersivity, that control mass transport. For these reasons, constructing models of mass transport and salinity distributions in basins is less straightforward than, for example, computing models of heat transfer (Chapter 10).

Rate of mass transport

Basin2 accounts for molecular diffusion, hydrodynamic dispersion, and advection as transport processes. Diffusion differs from dispersion in that the former is a molecular process, whereas the latter is a process of mechanical mixing operating both on microscopic and macroscopic scales due to the irregular nature of flow through porous media. Texts on groundwater hydrology such as Freeze and Cherry (1979) give further information on hydrodynamic dispersion.

The coefficient of hydrodynamic dispersion is a tensor quantity with entries $D_{xx}$, $D_{xz}$, $D_{zx}$, and $D_{zz}$; it represents the combined processes of diffusion and dispersion along the $x$ and $z$ directions. Basin2 calculates the coefficient at each point in the basin from the porous medium diffusion constant $D^*$, the dispersivities $\alpha_L$ and $\alpha_T$ along and across the direction of flow (the longitudinal and transverse directions), and the groundwater velocities $v_k'$ along curvilinear $x$ and $z$.

By default, Basin2 ignores the cross terms $D_{xz}$ and $D_{zx}$ in the tensor by setting their values to zero, which is the case if flow is primarily along or...
across stratigraphy. In this case, the coefficient of dispersion is a vector quantity with entries

\[ D_{xx} = D^* + \alpha_L v_x' + \alpha_T v_x' \]

and

\[ D_{zz} = D^* + \alpha_L v_z' + \alpha_T v_z' \] (12.1)

If you set \texttt{disp\_tensor = on}, however, the program calculates the complete tensor according to

\[ D_{xx} = D^* + \alpha_L v + (\alpha_L - \alpha_T) \frac{v_x'^2}{v} \]

\[ D_{zz} = D_{xx} = (\alpha_L - \alpha_T) \frac{v_x'^2}{v} \]

and

\[ D_{zz} = D^* + \alpha_T v + (\alpha_L - \alpha_T) \frac{v_z'^2}{v} \] (12.2)

In these equations, \( D^* \) may be expressed in cm²/sec, \( \alpha_L \) and \( \alpha_T \) in cm, and \( v_x' \) and \( v_z' \) in cm/sec. Note that in the current release, the complete tensor option is intended for models in which each stratigraphic unit is composed of a single rock type.

By Equations 12.1 and 12.2, the effect of dispersion varies with the velocity of fluid flow. Under conditions of no flow, diffusion operates alone. Because the diffusion coefficient is very small (about \( 10^{-6} \) cm²/sec) and dispersivity coefficients relatively large, the effects of dispersion dominate those of diffusion at all but the slowest rates of fluid flow.

Basin2 calculates, along \( x \) and \( z \), the solute flux \( q_D \) due to diffusion and dispersion from concentration gradients, according to Fick’s law:

\[ q_{D_x} = -\phi \left( D_{xx} \frac{\partial C}{\partial x} + D_{xz} \frac{\partial C}{\partial z} \right) \]

and

\[ q_{D_z} = -\phi \left( D_{xz} \frac{\partial C}{\partial x} + D_{zz} \frac{\partial C}{\partial z} \right) \] (12.3)

In these equations, \( q_{D_x} \) and \( q_{D_z} \) are the rates at which salt crosses a unit plane normal to \( x \) and \( z \), in mol/cm² sec, and \( C \) is the volumetric salt concentration in mol/cm³.

The advective salt flux \( q_A \) is the product of volumetric concentration \( C \) and specific discharge \( q \):

\[ q_{A_x} = q_x C \]

and
Here, the advective fluxes are in mol/cm² sec, concentration in mol/cm³, and specific discharge in cm/sec.

\[ q_{Az} = q_z C \]  (12.4)

Infiltration of a surface brine

In our first example, we consider the infiltration of a surface brine due to the buoyant forces exerted by its high density. We set up a 10-km long cross section (Input 12.1) in which a carbonate platform overlies a basal aquifer of interbedded sandstone and shale. We treat the upper veneer of the carbonate as a separate unit and use it to vary water depth or elevation above sea level along the section. The left and right boundaries are open to flow. We specify a steady-state solution and, to aid the program in converging, set the under-relaxation variable to a value considerably less than 1 (see Chapter 5).
Input 12.1 Infiltration of a surface brine.

run = steady; start = 0 yrs; nx = 40; delta_z = 20 m
mtemperature = vertical; heat_flow = 1 HFUs; salinity = full;
salt_flux = 0; under_relax = 0.04
rock
   B_perm = -1; A_perm = 0
   B_perm = -5; A_perm = 0
   B_perm = -3; A_perm = 0
end_rock

x_well(km)  0  1.5  1.6  2  2.4  2.5  4  5  5.1  10
left = open; right = open
strat 'Basal sand'
   t_dep = -2 m.y.
   thickness = 100 m
   X(ss) = 80%; X(sh) = 20%
strat 'Carbonate beds'
   t_dep = -1 m.y.
   thickness = 200 m
   X(cn) = 100%
strat 'Upper beds'
   t_dep = 0 yrs
   X(cn) = 100%
column water_depth(m) thickness(m) surface_conc(molal)
   w(1)  -10  30  0
   w(2)   0  20  "
   w(3)   "  3
   w(4)   10  10  "
   w(5)   0  20  "
   w(6)   "  0
   w(7)  -5  25  "
   w(8)   0  20  "
   w(9)   "  1/2
   w(10)  10  10  "

A lagoon extending from well 3 to well 5, near the left of the section, reaches 10 m in water depth. The section rises 10 m above sea level to the left of the lagoon and 5 m above sea level to the right. The right half of the cross section falls below sea level to a maximum of 10 m in water depth. Using the surface_conc keyword within a column block, we set salinity to 3 molal in the lagoon, one-half molal for seawater, and zero where the section emerges above sea level and is exposed to rain water. Note the close spacing of wells 2 and 3, wells 5 and 6, and wells 8 and 9, which serves to fix the positions of the lagoon and the exposed and subsea segments of the section.

The calculation results (Figure 12.1) show the interaction of flow regimes driven by topography and the negative buoyancy of the brine. Brine migrates downward from the lagoon, mixes by dispersion with surrounding groundwater, and then flows offshore along the sandstone aquifer under the regional hydraulic gradient. Topography to the sides of
the lagoon drives small flow regimes by which lenses of fresh water extend downward into the platform.

Figure 12.1 The infiltration of a surface brine (salinity contours in molal), as calculated by Basin2. A lagoon near the left of the section contains seawater concentrated to 3 molal, which infiltrates due to its high density. The basin surface is exposed to rainfall (zero molal) to the left and right of the lagoon, and to seawater along the right half of the section.

Buried halite layer

As a second example, we calculate how a buried halite layer might affect salinity in a groundwater flow regime. In Input 12.2, we seek a steady-state solution that accounts for vertical heat conduction and salt transport by diffusion, dispersion, and advection. We set salinity along the basin surface to zero and provide for no flux of salt across the basin’s basal boundary.

Input 12.2 Effect of a buried halite layer.

run = steady; start = 0 yrs
nx = 30; delta_z = 50 m
temperature = vertical; heat_flow = 1 HFU
salinity = full; salt_flux = 0; surface_conc = 0
under_relax = 0.1

rock ss
   A_perm = 0;  B_perm = -2 log_darcy;  p_kxkz = 10 
   phi0 = 25%;  phi1 = 0;  bpor = 0
rock sh
   A_perm = 0;  B_perm = -5 log_darcy;  p_kxkz = 10 
   phi0 = 25%;  phi1 = 0;  bpor = 0
rock hal
   A_perm = 0;  B_perm = -4 log_darcy;  p_kxkz = 10 
   phi0 = 25%;  phi1 = 0;  bpor = 0
end_rock

x_well(km)  0 30 35 50 65 70 100
halite_sat = hal
strat 'Basal layer'
  t_dep = -2 m.y.
  thickness = 100 m
  X(ss) = 90%; X(sh) = 10%

strat 'Middle layer'
  t_dep = -1 m.y.
  thickness = 100 m
  column    X(ss)  X(hal)
  w(1:2)     100%     0
  w(3:5)       0    100%
  w(6:7)     100%     0

strat 'Upper layer'
  t_dep = 0 yrs
  X(ss) = 90%; X(sh) = 10%
  column    water_depth(m) thickness(m)
  w(1)           -100          600
  w(2:6)            &            &
  w(7)              0          500

The basin, 100 km long, is composed of a halite layer (rock type hal) sandwiched between layers of sandstone with shale interbeds. Halite in the middle layer extends from well 3 (35 km from the left) to well 5 (65 km from the left). By setting keyword halite_sat to rock type hal, we require that groundwater along the halite bed maintain a salinity corresponding to saturation with respect to this mineral.

We specify a porosity of 25% for each rock type, and set permeability for the sandstone, halite bed, and shale, respectively, to 10, 0.1, and 0.01 m/darcy; 100 m of topographic relief across the basin provides the drive for a regional flow regime. Note the use of the ampersand (&) to command the program to interpolate the relief and layer thicknesses for wells 2 through 6 from the values at wells 1 and 7, saving effort in configuring the input.

The calculation results (Figure 12.2) show that the halite layer has a significant influence on the salinity of the flow system. Salinity is small in the recharge area but large in the discharge area, especially at depth, where a layer of saline, nearly motionless fluid has accumulated. The high density of groundwater along the halite beds causes fluid to sink into the underlying layer and then flow toward the basin margins. The effect of this density flow is to carry salt back toward the recharge area, causing an increase in fluid salinity upstream from the halite bed.
Figure 12.2 The effect of a buried halite layer on salinity in a groundwater flow regime, as calculated by Basin2. Arrows show fluid velocity (see scale) and contours give salinity in molal. Shaded area shows the extent of the halite layer.
13 Groundwater Flow and Cementation

About modeling cementation

Basin2 can trace the volume of minerals that precipitate or dissolve in basin strata as groundwaters migrate along temperature and pressure gradients. The model predicts cumulative volume changes of minerals considered in a transient simulation and, in a steady-state run, instantaneous rates of precipitation and dissolution. The calculation is based on the assumption that minerals maintain local equilibrium with migrating groundwaters and their solubilities depend only on temperature or temperature and pressure. The model does not account for other factors that might control mineral precipitation or dissolution such as reaction kinetics or mixing fluids of differing composition.

Basin2 uses built-in solubility correlations to calculate solubilities of five minerals — quartz, chalcedony, cristobalite, amorphous silica, and anhydrite. The program assumes their solubilities depend on temperature or, in the case of anhydrite, on temperature and pressure. Alternatively, the model can call on the React geochemical model to calculate how mineral solubility varies with temperature; this linking accounts for the influence of pH, salinity, and chemical interactions such as common ion effects.

This chapter shows how to use Basin2 to predict the diagenetic effects of groundwater migration and how to link Basin2 to React.

Mineral solubility

In order to calculate the rates at which various minerals dissolve and cements precipitate in basin strata, we need to know how their solubilities change with temperature and pressure. In Basin2, we use one of two ways to determine these derivatives of mineral solubility.

First, Basin2 has built-in correlations for the solubilities of silica minerals (quartz, chalcedony, cristobalite, amorphous silica) and anhydrite. For silica, we assume that the mineral is soluble as SiO$_2$(aq), as is generally the case except under alkaline conditions, and that the species has an activity coefficient of 1. In this case, the correlations of
Rimstidt and Barnes (1980) give the molal solubility (mol/kg H₂O) of silica minerals as a function of absolute temperature \( T_K \) (Table 13.1). By these correlations, the solubility of silica minerals increases with increasing temperature (Figure 13.1). Over the temperature range considered in sedimentary basins, the solubility of silica minerals depends only weakly on pressure and fluid salinity.

### Table 13.1 Solubility correlations versus absolute temperature for silica minerals.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Equilibrium solubility (mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>( \log m = 1.881 - 2.028 \times 10^{-3} T_K - 1560 T_K^{-1} )</td>
</tr>
<tr>
<td>Chalcedony</td>
<td>( \log m = 2.219 - 2.323 \times 10^{-3} T_K - 1547.8 T_K^{-1} )</td>
</tr>
<tr>
<td>( \alpha )-Cristobalite</td>
<td>( \log m = -0.0321 - 988.2 T_K^{-1} )</td>
</tr>
<tr>
<td>Amorphous silica</td>
<td>( \log m = 0.338 - 7.889 \times 10^{-4} T_K - 840.1 T_K^{-1} )</td>
</tr>
</tbody>
</table>

Figure 13.1 Dissolved volumes \( V_k \) (cm³ solid/cm³ solution) of silica minerals as a function of temperature (upper diagram), calculated from the correlations of Rimstidt and Barnes (1980). The bottom diagram shows the derivatives of these solubilities with respect to temperature.

Anhydrite solubility depends on temperature, pressure, and fluid salinity. We correlate solubility to values measured by Blount and Dickson (1969) for a 2 molal NaCl solution. Blount and Dickson’s measurements span the range of about 100°C to 250°C and 5 to 1350 bars, so the correlation serves to extrapolate the data to temperatures found in shallow strata. The regression

\[
\ln m_{\text{sol}} = -2.33 - 1.59 \times 10^{-3} T + 6.1 \times 10^{-4} P \\
+ 1.82 \times 10^{-7} T^2 - 7.05 \times 10^{-8} P^2 + 3.14 \times 10^{-7} T \cdot P
\]  

(13.1)
gives molal solubility as a function of temperature $T$ (°C) and pressure $P$ (bars). By this correlation, anhydrite solubility decreases with increasing temperature but increases with increasing pressure, especially at lower temperatures.

In diagenetic problems, it is more useful to know the change in a mineral’s volume than its mass change because the volume change gives information regarding how porosity evolves in reaction. We can calculate the dimensionless solubility $V_k$, or the dissolved volume of mineral $k$ per unit volume of groundwater, from the mineral’s molal solubility $m_k$ by

$$V_k = \frac{m_k \cdot M_v \cdot \rho \left(1 - \frac{TDS}{10^6}\right)}{1000}$$

(13.2)

Here $M_v$ is the molar volume of the mineral (cm$^3$/mol), $\rho$ is fluid density (g/cm$^3$), and $TDS$ is the total dissolved solutes (mg/kg) in the fluid. Because the greatest uncertainty in evaluating the cementation model comes from estimating groundwater flow rates, it is sufficient for our purposes to take $TDS$ to be zero and $\rho$ to be 1 in this equation.

Second, Basin2 can incorporate the React geochemical model to calculate dissolved mineral volumes in a chemical system of interest over a range of temperatures. The React calculation accounts for chemical interactions such as the common ion effect, as well as many other factors that might affect a mineral’s solubility. For example, calcite solubility varies with temperature, CO$_2$ fugacity, and salinity of the fluid. By linking React to Basin2, you can account for these factors.

### Mathematical model

Basin2 calculates the cementation or dissolution rate of mineral $k$ in basin strata by solving a mass balance equation that describes transport of the dissolved mineral by diffusion, dispersion, and advection. The equation is

$$\frac{1}{\phi} \frac{dY_k}{dt} = \left(\frac{\partial V_k}{\partial T} \frac{dT}{dt} + \frac{\partial V_k}{\partial P} \frac{dP}{dt}\right)$$

$$+ \left[ D_T \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial x} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial x} \right) + D_x \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial z} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial z} \right) \right]$$

$$+ \left[ D_T \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial z} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial z} \right) + D_z \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial x} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial x} \right) \right]$$

$$- v'_x \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial x} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial x} \right) - v'_z \left( \frac{\partial V_k}{\partial T} \frac{\partial T}{\partial z} + \frac{\partial V_k}{\partial P} \frac{\partial P}{\partial z} \right)$$

(13.3)

where $Y_k$ is the volume of mineral $k$ precipitated or dissolved per unit volume of the formation, $T$ and $P$ are temperature and pressure, $\phi$ is porosity, and $v'_x$ and $v'_z$ are lateral and vertical groundwater velocities
(cm/yr) in curvilinear coordinates. $D_x$ and $D_z$ are coefficients of hydrodynamic dispersion (cm$^2$/yr), which account for diffusion of the solute as well as dispersion (i.e., the mechanical mixing that occurs when groundwater flows through a porous medium; see Chapter 12).

The first term on the right hand side of Equation 13.3 describes the effects of temperature and pressure changes, as might occur in response to burial and exhumation or changes in heat flow, on cementation. In a steady-state flow regime there are no such effects, because $T$ and $P$ do not change. In this case, cementation is caused only by hydrologic mass transport and chemical diffusion. The second and the third terms describe cementation by chemical diffusion and hydrodynamic dispersion. The last two terms account for cementation by groundwater advection.

Basin2 evaluates Equation 13.3 explicitly by a finite difference approach. Basin2 first calculates the flow velocities and $T$ and $P$ distribution in basin strata, as discussed in previous chapters. To evaluate the derivatives $\partial V_k / \partial T$ or $\partial V_k / \partial P$, Basin2 uses either built-in correlations or the interface tables passed from React. The program then calculates the reaction rate $dY_k / dt$ of a mineral $k$ directly by evaluating the right hand side of the equation.

**Linkage to React**

Basin2 communicates with React through interface tables that React generates. First, you select a geochemical system that contains an aqueous fluid and the minerals of interest. You then use React to trace the precipitation and dissolution of minerals in the system over a polythermal reaction path. To cause React to produce the interface tables, you enter the command

```
basin2
```

This command causes React to create tables that contain temperatures and corresponding mineral volumes in dataset Btab1 through Btab5. The number of tables generated depends on the number of minerals considered in simulation; up to 4 minerals appear in each table and 20 minerals is the overall limit.

The volume listed in the interface tables is that of a mineral phase, not the dissolved volume. Therefore, a mineral whose volume increases with temperature shows a decrease in solubility, and vice versa. The total volume of a mineral considered is not important as long as the mineral remains saturated over the reaction path. Instead, Basin2 works with the changes in mineral volume.

In setting up your reaction path in React, it is important to make sure that the path is suitable for linking to Basin2. You should not link the model to a React run that considers an open system. Paths that include reactants, kinetics of mineral precipitation or dissolution, or the flow-through or flush options, for example, are not suitable. It is also
important to make sure that each mineral you wish to consider remains saturated over the reaction path. The volume of any mineral that becomes undersaturated appears as a value of 0 in the dataset.

After tracing a reaction path and creating the interface tables, you establish communication with commands of the form

```
include 'Btab1'
```

in your Basin2 input file. You use one `include` command for each interface table that React produces. Basin2 reads the file and determines solubility derivatives for minerals by interpolating or extrapolating the tabulated data.

---

**Cementation in a sloping aquifer**

In this section, we use Basin2 to calculate the diagenetic patterns and instantaneous cementation rates of quartz produced within a sloping aquifer by a convective flow system. In **Input 13.1**, a 500 m-thick sloping sandstone is sandwiched between two shale aquitards. For simplicity, we set porosity in the sandstone and aquitards to constant values with the keywords `bpor`, `phi0`, and `phi1`. With keywords `A_perm`, `B_perm` and `p_kzz`, we set permeability in the sandstone and aquitards to 0.1 darcy and $10^{-5}$ darcy, respectively. With the command

```
cementation = quartz
```

we set the program to calculate the rate of quartz cementation.

**Input 13.1** *Quartz cementation in a sloping aquifer.*

```
run = steady; start = 0 yrs
nx = 20; delta_z = 100 m
temperature = full; cementation = quartz

rock ss
  phi0=0; phi1 = 30%; b_por = 0
  A_perm = 0; B_perm = -1 log_darcy; p_kzz = 1
rock sh
  phi0=0; phi1 = 15%; b_por = 0
  A_perm = 0; B_perm = -5 log_darcy; p_kzz = 1
end_rock

x_well(km)   0  1  2
strat 'basal shale'
  t_dep = -1 m.y.
  X(sh) = 100%
  column thickness(m)
  w(1)  100
  w(2)  700
  w(3)  100
strat 'sloping aquifer'
  t_dep = -.5 m.y.
  thickness = 500 m
  X(ss) = 100%
```
The contrast in thermal conductivity between the aquifer and the surrounding shales creates lateral temperature gradients. The temperature variation, in turn, causes fluid density to vary laterally and fluid within the aquifer to convect. The migrating fluid drives diagenesis because it encounters variation in temperature along the flow path. Quartz, which has a prograde solubility, is removed from the sandstone where fluid travels from cooler regions to hotter regions, and precipitates where fluid moves from hotter regions toward cooler regions (Figure 13.2). The most extensive precipitation or dissolution occurs where the fluid crosses the isotherms at a sharp angle.

The greatest rates of quartz cementation predicted by the calculation are about 0.05% per m.y. At rates of this magnitude, it will take many millions of years for cementation to significantly alter porosity in the formation.

**Cementation near a fault zone**

As a second example, we examine quartz cementation in a steady-state flow system near a fault zone. Our basin (Input 13.2) contains two sandstone aquifers separated by a shale aquitard. We set the porosity and permeability of each rock type to constant values, as in the previous example.
Input 13.2 Quartz cementation near a fault zone.

run = steady; start = 0 yrs
nx = 40; delta_z = 100 m
cementation = quartz; under_relax = 1/2; temperature = full

rock ss
  phi0=0; phi1 = 30%; b_por= 0
  A_perm = 0; B_perm = -1 log_darcy; p_kxkz = 1

rock sh
  phi0=0; phi1 = 15%; b_por= 0
  A_perm = 0; B_perm = -5 log_darcy; p_kxkz = 1
end_rock

x_well(km)    0   10   20   30   40   50
left = open; right = open

strat 'basal shale'
  t_dep = -4 m.y.; thickness = 1 km; X(sh) = 100%

strat 'lower ss'
  t_dep = -3 m.y.; thickness = 500 m
  column X(ss)  X(sh)
  w(1:4)    1    0
  w(5:6)    0    1

strat 'middle sh'
  t_dep = -2 m.y.; thickness = 350 m; X(sh) = 100%

strat 'upper ss'
  t_dep = -1 m.y.; thickness = 500 m
  column X(ss)  X(sh)
  w(1:3)    0    1
  w(4:6)    1    0

strat 'top sh'
  t_dep = 0 yrs; X(sh) = 100%
  column thickness(m)  water_depth(m)
  w(1)        680          -200
  w(2)        530           -50
  w(3)        450            0
  w(4)        400            *
  w(5)        340            *
  w(6)        280            *

fault 'one'
  fault_position = 30 km; fault_bottom = 2; fault_top = 4
  fault_xperm = 1 darcy; fault_zperm = 1 darcy
end_fault

In the input file, we use a fault block (see Chapter 4) to define a fault that cuts through the two sandstones. We set the keyword fault_bottom

In the input file, we use a fault block (see Chapter 4) to define a fault that cuts through the two sandstones. We set the keyword fault_bottom to 2 and fault_top to 4, so that the fault penetrates from the second unit deposited, the lower sandstone, to the fourth unit deposited, the upper sandstone. We use the keyword fault_position to place the fault 30 km from the left side of the cross section, where the two sandstones grade into less permeable shales. With the keywords fault_xperm and fault_zperm, we set permeability in the fault zone to 1 darcy.

Figure 13.3 shows the predicted flow field, temperature distribution, and pattern of quartz cementation predicted by Basin2. Fluid flows from
left to right because of the relief across the basin’s surface. As the fluid in
the lower sandstone encounters the low-permeability shales near the fault
zone, it migrates upward through the fault zone into the upper sand body
and continues eastward. The isotherms are disturbed near the fault zone
where warm groundwaters from the lower sand discharge upward into
the upper sand.

**Figure 13.3** Calculated temperature distribution (contours) and rate of
quartz cementation (shading; see scale bar) near a fault zone.
Arrows represent fluid velocity (see scale).

The model predicts that the most intensive precipitation occurs along
the fault zone where the fluid cools as it moves upward. As the fluid
flows through the fault zone, it precipitates quartz at a maximum rate of
about 0.07% per m.y.
14 Isotope Transport

About modeling isotope transport

Basin2 can consider the transport of the isotopes $^3$He, $^4$He, $^{36}$Cl, and $^{40}$Ar. These isotopes are radiogenic and, in the case of $^{36}$Cl, radioactive. Since the isotopes are produced very slowly (and $^{36}$Cl decays slowly), they are useful in interpreting the residence times of very old groundwater and the nature of flow regimes deep in the Earth’s crust.

The model can consider up to two isotopes in a simulation. One of the “isotopes” can be total chlorinity, which allows the model to output the $^{36}$Cl/Cl ratio. In this case, the Cl “isotope” concentration is simply set to the groundwater chlorinity, as determined by solving the salinity equation (keyword salinity; see “Salinity distributions” in Chapter 6, and Chapter 12).

Basin2 can also carry $^{36}$Ar as an isotope. This isotope in groundwater is of predominantly atmospheric origin; little is produced in the subsurface, and hence its distribution in a Basin2 simulation simply reflects the boundary conditions specified. Nonetheless, carrying $^{36}$Ar as an isotope can be useful because it allows the $^{40}$Ar/$^{36}$Ar isotope ratio to be calculated.

Basin2 models isotope transport just as it computes the salinity distribution in a basin. As with modeling salinity, you specify transport parameters (see “Diffusion and dispersion”, Chapter 2) and set boundary conditions (see “Isotope transport”, Chapter 6). In addition, you tell Basin2 how to determine the rates of in-situ isotope production and decay, as described in the following section.

Source rates of the isotopes

This section summarizes how Basin2 calculates production and decay rates for the various isotopes it considers. Production rates $J_i$ for an isotope $i$ are given in units of mol released per g of rock per yr. The rates may be converted to units of mol/cm$^3$ medium • yr using the relation

$$R_i = \rho_{rk} J_i (1-\phi)$$

(14.1)
Here, \( R_i \) is the production rate per volume of saturated sediment per year, \( \rho_s \) is the density of the rock grains, and \( \phi \) is sediment porosity, expressed as a fraction.

**Neutron production**

To calculate the rates at which isotopes \(^3\text{He}\) and \(^{36}\text{Cl}\) are produced by neutron activation, we need to determine the rate at which free neutrons are produced within basin sediments. Neutrons are liberated by the spontaneous fission of \(^{238}\text{U}\), as well as when various elements in the rock (especially Na, Mg, Al, Si, and Ca) are bombarded with \( \alpha \) particles given off by the series decay of U and Th.

The neutron production rate (neutrons/g of rock • yr) is given by

\[
P_n = A_{1,\text{nflux}}[U] + A_{2,\text{nflux}}[Th]
\]

Here [U] and [Th] are the U and Th concentrations in the sediment (ppm), and the coefficients \( A_{1,\text{nflux}} \) and \( A_{2,\text{nflux}} \) give the numbers of neutrons produced per \( \mu \)g of U and Th, per year. The user sets values for the U and Th concentrations with the Basin2 keywords \texttt{ppm}_\texttt{U} and \texttt{ppm}_\texttt{Th}, and for the neutron production coefficients with keywords \texttt{A1}_\texttt{nflux} and \texttt{A2}_\texttt{nflux}.

The neutron production coefficients depend on the decay rates of U and Th as well as the concentrations in the rock of the various neutron-emitting elements that emit neutrons when bombarded with \( \alpha \) particles. The coefficients can be calculated from rock composition using the correlations

\[
A_{1,\text{nflux}} = \frac{\sum_i S_i F_i Y_i^{U}}{\sum_i S_i F_i} + 0.4764
\]

and

\[
A_{2,\text{nflux}} = \frac{\sum_i S_i F_i Y_i^{Th}}{\sum_i S_i F_i}
\]

(see Andrews et al., 1989; Fritzel, 1996). In these equations, \( S_i \) is the mass stopping power of element \( i \) (in MeV g\(^{-1}\) cm\(^{-2}\), \( F_i \) is each element’s mass fraction in the rock, and \( Y_i^{U} \) and \( Y_i^{Th} \) are the neutron yields of each element, expressed per ppm of U and Th per year; the constant 0.4764 represents neutron production by the spontaneous fission of \(^{238}\text{U}\).

Suitable values for \( S_i \) and \( Y_i \) for most elements may be found in Andrews et al. (1989; their Table 2). Feige et al. (1968; their Table 1) give values of \( S_i \) for C and Ca; \( Y_i \) for C may be taken as twice that for O, and this coefficient for Ca can be taken as zero. Parker (1967) gives general values of \( F_i \) for crustal rocks, which can be used where specific data are not available.
lacking. Since the values of coefficients $A_{1, \text{nflux}}$ and $A_{2, \text{nflux}}$ vary with rock composition, they are set independently in Basin2 for each rock type.

Basin2 converts the neutron production rate $P_n$ to a neutron flux, $\Phi_n$ (neutrons/cm$^2$ yr), by dividing $P_n$ by the neutron absorption cross-section of the rock

$$\Phi_n = \frac{P_n}{\sum_i N_i \sigma_i}$$

(14.4)

where $N_i$ is the number of atoms of each element $i$ per gram of rock, and $\sigma_i$ is the corresponding neutron absorption cross-section (cm$^2$). The summation represents the neutron absorption cross-section per gram of rock; the user sets this value using the $\text{Axsect}$ keyword.

Production of $^3\text{He}$

$^3\text{He}$ is produced in the subsurface by neutron capture reactions involving $^6\text{Li}$. Neutrons are released within basin sediments when elements in the rock grains are bombarded with alpha particles, as described in the previous section. For each $^6\text{Li}$ atom that captures a neutron, one $^3\text{He}$ atom is formed

$$^6\text{Li} + n \rightarrow \alpha + ^3\text{He} \quad (\beta \text{ decay to } ^3\text{He})$$

(14.5)

The production rate of $^3\text{He}$ released from the rock grains, in mol/g rock $\cdot$ yr, is calculated as

$$J_{^3\text{He}} = \Lambda_{^3\text{He}} \frac{\Phi_n \sigma_6 [\text{Li}]}{10^6 M_w \chi_6}$$

(14.6)

Here $\Lambda_{^3\text{He}}$ is the release factor, $\sigma_6$ is the neutron absorption cross-section of $^6\text{Li}$, $[\text{Li}]$ is the concentration (ppm) of Li in the rock, $\chi_6$ is the fraction of $^6\text{Li}$ in Li, and $M_w$ is the atomic weight of Li. The user sets the value of $\Lambda_{^3\text{He}}$ with keyword $\text{reelfac} _{^3\text{He}}$, $\sigma_6$ with $\text{Axsect} _{^6\text{Li}}$, and [Li] with ppm_Li.

Production of $^4\text{He}$

$^4\text{He}$ is produced in the subsurface largely through the radioactive decay of U and Th, according to

$$^{238}\text{U} \rightarrow ^{206}\text{Pb} + 8 \quad ^4\text{He}$$

$$^{235}\text{U} \rightarrow ^{207}\text{Pb} + 7 \quad ^4\text{He}$$

$$^{232}\text{Th} \rightarrow ^{208}\text{Pb} + 6 \quad ^4\text{He}$$

(14.7)

(Andrews et al., 1985). Basin2 determines the net rate of $^4\text{He}$ production ($J_{^4\text{He}}$, in mol/g rock $\cdot$ yr) from the linear approximation

$$J_{^4\text{He}} = \Lambda_{^4\text{He}} \left( A_{1, ^4\text{He}} [\text{U}] + A_{2, ^4\text{He}} [\text{Th}] \right)$$

(14.8)
(e.g., Ballantine et al., 1991). Here, $\Lambda_{4\text{He}}$ is the isotope's release factor, $A_{1, 4\text{He}}$ and $A_{2, 4\text{He}}$ are linear coefficients (mol/μg yr) for the rate law (which represent the number of moles of $^4\text{He}$ produced per μg of U and Th per year), and $[\text{U}]$ and $[\text{Th}]$ are the concentrations (ppm) of U and Th in the rock grains. The user sets these variables with keywords `realfac_4He`, `A1_4He`, `A2_4He`, `ppm_U`, and `ppm_Th`. Suitable values for $A_{1, 4\text{He}}$ and $A_{2, 4\text{He}}$ are $0.5336 \times 10^{-17}$ and $0.1333 \times 10^{-17}$ mol/μg yr (Torgersen, 1980); these are the default settings in Basin2.

**Decay and production of $^{36}\text{Cl}$**

The radioactive isotope $^{36}\text{Cl}$ is produced naturally in the atmosphere through spallation and neutron activation by cosmic rays, and dissolves in rainwater. When rainwater recharges the subsurface, it is isolated from the atmospheric source and its $^{36}\text{Cl}$ content decreases as the isotope decays. Since the half-life $T_{1/2}$ of $^{36}\text{Cl}$ is about 301,000 years, the residual $^{36}\text{Cl}$ content provides a means of estimating the residence time of very old groundwater.

$^{36}\text{Cl}$ forms $^{36}\text{S}$ and $^{36}\text{Ar}$ by branched decay at a rate given by

$$ \frac{dN_{36}}{dt} = \lambda_{36} N_{36} $$

(14.9)

Here $N_{36}$ is the number of $^{36}\text{Cl}$ atoms in a volume of groundwater and $\lambda_{36}$ is the isotope's decay constant ($\lambda = \ln 2 / T_{1/2}$, where $T_{1/2}$ is half life). Basin2 uses equation (14.9) and a value for $\lambda_{36}$ of $2.31 \times 10^{-6}$ yr$^{-1}$ (equivalent to a half life of $301 \times 10^6$ yr) to calculate the rate at which $^{36}\text{Cl}$ decays.

In addition to decaying, $^{36}\text{Cl}$ is produced in the subsurface, mainly by neutron activation of $^{35}\text{Cl}$

$$ ^{35}\text{Cl} + \frac{1}{2}n \rightarrow ^{36}\text{Cl} $$

(14.10)

Neutrons released by the decay of U and Th collide with $^{35}\text{Cl}$ atoms present in solution or contained in evaporite minerals. The subsurface production rate is commonly small compared to the rate of decay, but under certain circumstances may be significant. Where the residence time is large, sediments are rich in U and Th, or the presence of brines or evaporites provide large numbers of target $^{35}\text{Cl}$ atoms, for example, the production of $^{36}\text{Cl}$ may be important.

Basin2 calculates $^{36}\text{Cl}$ production rates from the neutron flux and the neutron absorption cross-section of $^{35}\text{Cl}$. The rate $J_{^{36}\text{Cl}}$ (mol/g rock • yr) resulting from activation of Cl found within the rock grains is calculated as

$$ J_{^{36}\text{Cl}} = \frac{\Lambda_{^{36}\text{Cl}} \Phi_n \sigma_{^{35}\text{Cl}} [\text{Cl}] \chi_{^{35}\text{Cl}}}{10^5 M_w} $$

(14.11)

Here, $\Lambda_{^{36}\text{Cl}}$ is the isotope’s release factor, $\sigma_{^{35}\text{Cl}}$ is its neutron absorption cross-section, $[\text{Cl}]$ is the concentration (ppm) of Cl in the rock, $\chi_{^{35}\text{Cl}}$ is the
fraction of $^{35}$Cl in Cl (about 0.758), and $M_a$ is the atomic weight of Cl. The program converts the result of evaluating this equation to a value for $R_{^{36}Cl}$ (mol/cm$^3$ medium • yr) according to Equation (14.1).

Basin2 also calculates the rate $R_{^{36}Cl}^w$ (mol/cm$^3$ medium • yr) of $^{36}$Cl production resulting from neutron activation of Cl dissolved in the fluid (water) phase, according to

$$R_{^{36}Cl}^w = \Phi C_{\text{Cl}} \sigma_{^{35}} \phi \chi_{^{35}} \rho_{\text{w}} \times 10^{-3}$$

(14.12)

where $C_{\text{Cl}}$ is the molal concentration of Cl in the fluid. The $^{36}$Cl production rate $R_{^{36}Cl}$ is the sum of $R_{^{36}Cl}^r$ and $R_{^{36}Cl}^w$. The user sets values for $\Lambda_{^{36}Cl}$, $\sigma_{^{35}}$, and [Cl] with keywords relfac_36Cl, Axsect_35Cl, and ppm_Cl.

**Production of $^{40}$Ar**

$^{40}$Ar is produced in the subsurface primarily by radioactive decay of $^{40}$K contained in potassium-bearing minerals (Zaikowski et al., 1987; Torgersen et al., 1989; Andrews et al., 1991; Castro and Marty, 1993). The rate of $^{40}$Ar production ($J_{^{40}Ar}$, in mol/g rock • yr) is set in Basin2 by the linear approximation

$$J_{^{40}Ar} = \Lambda_{^{40}Ar} A_{^{40}Ar} [K]$$

(14.13)

(e.g., Ballantine et al., 1991). Here, $\Lambda_{^{40}Ar}$ is the isotope’s release factor, $A_{^{40}Ar}$ is the linear coefficient (mol/μg yr) for the rate law (which represents the number of moles of $^{40}$Ar produced per μg of K per year), and [K] is the concentration (ppm) of K in the rock grains. The user sets these values with keywords relfac_40Ar, A1_40Ar, and ppm_K. The default value for $A_{^{40}Ar}$ is .1733×10$^{-21}$.

**Helium distribution in a basin**

As an example of modeling isotope transport, we consider the distribution at steady state of the helium isotopes $^3$He and $^4$He in groundwater flow within a hypothetical basin, loosely following the calculations of Zhao et al. (1998). In the input file (Input 14.1), we specify a steady-state model calculated assuming for simplicity invariant fluid density and viscosity, temperature and salinity.

**Input 14.1 Distribution of helium isotopes.**

```
run            = steady
density        = constant
viscosity      = constant
temperature    = 20 C
salinity       = 0
isot_type      = He3
isot_equation  = full
csurf_isot     = 2.8e-15 molal
isot_flux      = 7e-26
```
conv_isol = 1e-30

iso2_type = He4
iso2_equation = full
csurf_iso2 = 2.0e-9 molal
iso2_flux = 2e-18
conv_iso2 = 1e-20

nx = 40; delta_z = 100 m

rock ss
phi0 = .2
beta_por = 0
A_perm = 0
B_perm = 0  # k = 1 darcy
p_kxkz = 1
diff_con = 1e-4
alpha_l = 1000 cm
alpha_t = 100 cm
Ppm_rck_U = 2
Ppm_rck_Th = 6
Ppm_rck_Li = 30
end_rock

rock sh
phi0 = .25
beta_por = 0
A_perm = 0
B_perm = -4.3  # k = 5x10^-5 darcy
p_kxkz = 1
diff_con = 1e-4
alpha_l = 1000 cm
alpha_t = 100 cm
Ppm_rck_U = 8
Ppm_rck_Th = 14
Ppm_rck_Li = 40
end_rock

left = open; right = open
reference = uncompacted
x_well(km) 0 100 200 300 400 500 600 700 800 \\
900 1000

strat 'Basal sandstone'
X(ss) = 1; thickness = 1000 m; t_dep = -2 my

strat 'Confining shale'
X(sh) = 1; t_dep = 0 yrs

column water_depth(m) thickness(m)
w(1) -700 0
w(2) & 1000
w(3) & 1400
w(4) & 1700
w(5) & 1900
w(6) & 2000
w(7) & 1900
w(8) & 1700
w(9) & 1400
w(10) & 1000
w(11) 0 0
end_strat
In the input, we set isotope 1 to be $^3$He, and isotope 2 to be $^4$He; for each we specify a “full” model accounting for transport by advection, diffusion, and dispersion. We set surface boundary conditions reflecting equilibrium with helium isotopes in the atmosphere, and a basal boundary equivalent to the degasing rate of the Earth’s crust (see Zhao et al., 1998). We also set appropriate convergence criteria.

The basin is composed of two rock types, sandstone that makes up a basal aquifer, and shale that forms a confining layer. The sandstone and shale have permeabilities of one darcy and $5 \times 10^{-5}$ darcy, respectively. We set a diffusion constant appropriate for helium (which diffuses readily), longitudinal and transverse dispersivities, and the amount of U, Th, and Li in the rock.

The basal aquifer is 1000 m thick and overlain by a confining layer of varying thickness. There is 700 m of topographic relief across the basin, which drives a groundwater flow regime through basin strata.

Figure 14.1 shows the calculation results. Helium concentration is controlled primarily by the basal flux and secondarily by in-situ production within basin strata; it increases generally along the direction of flow and with depth in the basin. The isotopic composition, as reflected by the $^3$He/$^4$He ratio, reflects the different helium sources, as discussed by Zhao et al. (1998). The ratio is highest near the recharge area, where atmospheric helium is important, and lowest in the confining layers, where the helium produced in-situ is richer in $^4$He than either atmospheric helium or helium produced in the crystalline crust.

**Figure 14.1** Calculated distribution of helium (He concentration = concentration of $^4$He, the dominant isotope; above) in a hypothetical groundwater flow regime, and the predicted $^3$He/$^4$He ratio (below).
15 Using B2plot

About B2plot

B2plot, a graphics program designed to display output from Basin2, lets you draw four types of plots. You can generate a basin cross section displaying several variables at once. Alternatively, you can plot one or more variables versus distance across the basin, variables versus depth, or variables versus time. The program features a point-and-click interface that presents options in pull-down menus and dialog boxes.

The best way to learn how B2plot works is to use it! Once you have run Basin2 to create a `b2_plot.dat` file, you start B2plot, as discussed in Chapter 6. The program opens a window, which looks like the one shown in Figure 15.1. You can change the window size by dragging any corner with the left mouse button and releasing it when the window reaches the size you want.

![Figure 15.1 The B2plot window, as displayed on the computer screen.](image-url)
You can leave B2plot active when you run further Basin2 simulations. Each time Basin2 completes a run and writes the results to the current B2_plot.dat file, it signals B2plot. B2plot then updates its display to reflect the new results.

The window is labeled in the upper left corner with the name of the current datafile. Below the window label is a horizontal menu bar that has a number of buttons. Each button activates a pull-down menu that lets you control aspects of the plot.

### “File” menu

You use the “File” menu, located at the left side of the B2plot menubar, to control input to and output from the program. From this menu, you can
- Open a new B2_plot.dat data file containing the results of a Basin2 simulation, or re-open the current data file.
- Load a new configuration file describing the current settings for your plot, or save the current settings to a file.
- Import “scatter data,” data points to overlay on your plots.
- Reset the plot configuration or axis ranges, or refresh the display of the current plot.
- Print the current plot, or save it as an image in a variety of graphics formats.
- Quit the program, either saving the current configuration as the starting point for the next B2plot session, or discarding it.

### “Plot” menu

The “Plot” menu, located on the menubar to the right of the “File” menu, lets you select the type of plot to use to render the results of your Basin2 simulation. There are two general types of plots: cross-section and x-y.

In a cross-section plot, you can represent field variables at any point in time in your Basin2 results using contours, a color map, or a color mask. You can also represent fluid velocity as a vector field. In addition, you can use the B2plot animation feature to show how the Basin2 results vary over the course of the simulation.

X-y plots show how variables in the simulation results change across the basin, with depth in the basin, or with time. You may plot a single line on such plots, or several related lines.

For example, in a plot versus depth, you can choose to plot:
- Several variables with the same units (such as hydraulic potential, pressure, and overpressure) at a position along the cross section and at a single point in time.
One variable at a position along the cross section, at several points in time.

Or, one variable at a single point in time, at several positions along the cross section.

The sections below describe cross-section and x-y plots in more detail.

Cross-section plots

You initiate a cross-section plot by choosing “Basin Cross Section” under “Plot” on the menubar. Several additional menus on the menubar let you configure the plot.

Under the “Edit” menu, you control the color map, color mask, and contour features. A dialog for each of these features defines how a field variable is mapped to the plot. In the “Contour...” dialog, for example, you set the range of values to be contoured, and the interval between contour lines. In the “Color Map...” dialog, you choose a color for the maximum and minimum values to be mapped, and optionally a midpoint value and color. You can also set various options in these dialogs, such as whether the variable is mapped in linear or logarithmic coordinates.

Also under the “Edit” menu are buttons to let you control details of the plot, such as colors, line widths, character sizes, and so on. Each of these buttons launch a dialog or pulldown menu. You use the “Velocity Arrows...” dialog to define how the groundwater velocity field is rendered. As well, you can set the units of time, distance, and velocity to be used in rendering the plot, and (under MS Windows) copy the plot to the clipboard.

The “View” menu lets you select the features to be included in the plot. Selecting “Contour Line Labels”, for example, toggles whether contour lines are labeled with their numerical values.

Finally, the “Time Level” menu lets you select the time level in the Basin2 simulation to represent. You can move forward or backward in time, or move to a specific time level. You can also select “Animate...” to set up an animation of the simulation results. You can also record the frames in the animation for use in producing a videotape (see “Animation and video”, below).

Plots versus distance, depth, or time

When you select (under the “Plot” menu) to plot “Variable vs. Distance”, “Variable vs. Depth”, or “Variable vs. Time”, menus labeled “Edit”, “X Axis”, and “Y Axis” are available on the menubar. Options under these menus let you control the appearance and content of your plot.

The “Edit” menu provides options for controlling the appearance of the plot, such as setting line color and thickness, character sizes, and so
on. You can also set the units for distance and time variables, and copy
the plot to the clipboard.

Under the “X Axis” menu, you set coordinate mapping for the
horizontal axis. Options include whether the axis is linear or logarithmic,
the units to use, and the axis range. You can also reset the axis range to
span the data range.

The “Y Axis” menu similarly lets you set mapping for the vertical
axis. In addition to the options available for the x axis, you can choose
the variable (or variables) to be plotted, position in the basin, and the
time level of interest.

Global keystroke commands

Once you become familiar with the program, you will find that issuing
commands with the keyboard is easier than reaching for the mouse to
open a menu or a dialog box. The options in the File menu have a
keystroke equivalent listed next to it. For example, next to the Print
option you can read Ctrl+P, which directs you to press the Ctrl and the
P keys simultaneously. You will quickly become familiar with the
keystrokes corresponding to the commands you use most frequently.

You can also interact with B2plot without using the mouse. The
arrow keys move the cursor from one menu to the next on the top bar and
from one button to the next on the side bar. Once a menu or a dialog box
is open, the arrows move the cursor from one option to the next and the
Enter key activates the selected option. The Tab key moves the cursor
from one group of buttons to the next, for example, from the plotting
options to the commands arranged in the bottom row of each dialog box
(OK, Apply, Cancel, and Reset).

Overlaying “scatter data”

B2plot can overlay data points (scatter data) on any of the diagrams it
produces, including cross-section and x-y plots. To add scatter data,
prepare a dataset containing the data in table form, then load the dataset
by selecting the “Get Scatter Data...” option from the “File” menu.

The scatter dataset contains the data in columns; each column
contains values for one of the variables B2plot can render. Columns in
the table are separated by “white space” (one or more blank or tab
characters).

The variables include may include time, distance along the cross
section, depth, or any of the variables available for plotting by B2plot
(pressure, temperature, and so on). The latter variables are those that
appear, for example, in the “Contour...” dialog under the “Edit” menu, or
the “Variable...” dialog under the “Y Axis” menu.
You enter values for time in years, and depth and distance in km; the other variables are entered in their native units, which are shown in Table 1.2. (You may, however, render the data in the various units B2plot recognizes.) The entries are set as linear, as opposed to logarithmic, values.

The first line in the table is a header that names each column. The column name is the name of a variable (e.g., Time, Depth, Distance, Temperature). You spell the column name in upper and lower case characters, exactly as it appears in B2plot menus, and enclose multiword names in quotes (e.g., "Vitrinite reflectance").

Subsequent lines contain the numeric values. Where no value exists, enter a non-numeric string such as n/d or -- as a place holder to preserve alignment in the table. To add error bars to the data points, enter a triplet of values separated by vertical bars (|). The values represent the minimum extreme of the error bar, the data point, and the maximum extreme. Exclude blank spaces from the triplet, or enclose it in quotes. The entry 0.5|2.0|3.5, for example, signifies a data point at 2.0 with an error bar extending from 0.5 to 3.5. The entry 0.5||3.5 prescribes the same error bar, omitting the symbol representing the data point.

You may include comments within the table. Comments extend from the number sign (#) to the end of the line. You may also include, as separators in the table, blank lines and lines of dashes (-) underscores (_), or equal signs (=). Your table might look like:

<table>
<thead>
<tr>
<th>Depth</th>
<th>Temperature</th>
<th>&quot;Vitrinite reflectance&quot;</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>58</td>
<td>0.45</td>
</tr>
<tr>
<td>1.8</td>
<td>70</td>
<td>0.52</td>
</tr>
<tr>
<td>2.3</td>
<td>78</td>
<td>0.75</td>
</tr>
</tbody>
</table>

To render these data, run Basin2 on a problem in which it calculates temperature and vitrinite reflectance, producing a B2_plot.dat file. Then start B2plot, load the dataset with the “Get Scatter Data...” option, and choose a plot of temperature or vitrinite reflectance versus depth. If scatter values lie outside the plot axis ranges, touch control-Z.

By default, B2plot renders data points as 16-point black squares. You can choose to represent the variable in each column with any of the following symbols:

- ■ square
- ● blot
- ▲ triangle
- ▼ yield
- ◆ diamond
- ● bullet
- ★ star
- ✗ hourglass
- + plus
- □ box
- ○ circle
- △ delta
- ▽ del
- ◇ caution
- ◯ degree
- ★ pentagram
- ☆ mobius
- × cross
To choose symbols, add a line to the table with symbol names (or a place holder such as “--”). Adding the line

```
--   box   cross
```

to the scatter dataset shown above, for example, causes temperature to be represented by boxes, and vitrinite reflectance by crosses.

You set symbol color and point size in a similar manner. Choose from among colors shown on the “Colors ...” dialog, enclosing multiword colors in quotes (e.g., "Cornflower blue"). To set marker point size, use fields like 15pt, 30pt, and so on.

**Configuration file**

When you exit the program with the “Quit (Save Configuration)” option, B2plot writes the choices you have made in configuring your plot into a file named `b2plot_conf.dat` in your current directory. When you run the program again from within the same directory, it automatically adopts the settings saved into the configuration file.

You can save your plot configuration into a file of your choice. Later, you can reread the file to return B2plot to that configuration. To do this you use the options “Save Configuration...” and “Load Configuration...” in the “File” menu. The same menu has the option to “Reset Plot Configuration”, which brings all settings back to their default values.

**Clipboard**

Under MS Windows, you can copy the current plot to the clipboard as an “Enhanced Metafile”. To do so, select “Copy” from the “Edit” pulldown on the menubar, or touch `control-C`. You can then paste the plot image directly into a variety of word processing and presentation graphics programs.

**Saving and exporting images**

In many cases you will want to adjust label positions or change the annotation or coloring on your plot. Such changes can be made quickly using an illustration program such as Canvas or Powerpoint. You can, furthermore, save images and import them into your reports or documents prepared with a word processor such as MS Word.

To save an image, you select “Save image...” from the “File” pulldown on the menubar, or then choose one of the file formats supported:

- Pict (.pct)
- PostScript (.ps)
- Black-and-white PostScript (.ps)
- Encapsulated PostScript (.eps)
• Binary CGM (.cgm)
• Enhanced metafile (MS Windows only) (.emf)

Note that since each of these graphics formats has its own limitations, the plot once imported to another program may appear somewhat different than on your computer screen. Using your illustration program or word processor, however, you can quickly alter the diagram’s appearance to suit your needs.

**Animation and video**

When you make a cross-section plot for a transient simulation, you can animate the results to show how the basin evolved through time. To do so, select “Animate...” under “Time Level”, choose the starting and ending times of the animation, and whether you want it to run continuously, and click on “Run”. The animation will appear in the B2plot window; touch any key to stop it.

You can also make a video rendering of the animation. To do so, you record the individual frames of the animation to your disk by selecting this option on the animation dialog. You then import the frames to a video mastering program, many of which are available commercially or in the public domain. Because so many high-quality video mastering programs are available, we no longer maintain program B2video, which you may have encountered in previous Basin2 releases.
Appendix 1  Glossary of Basin2 Keywords

About Basin2 keywords

This Appendix describes the use of each of the keywords that Basin2 recognizes. The keywords are listed alphabetically. Keywords and arguments may appear in any combination of upper and lower case; embedded underscores are ignored.
Keyword glossary

**A1_3He, A1_36Cl**

**arguments:** real values

**previous defaults:**

- $A_1^1$-He = 858.9 (ss and other), 1314.0 (sh), and 523.5 (cn)
- $A_1^{36}$Cl = 10,230 (ss and other), 15,940 (sh), and 6059 (cn)

**units:** ppm

**set:** by rock type

**description:** These keywords are obsolete and provided for compatibility with previous releases of Basin2; the preferred method for describing neutron capture is with keywords $Axsect$, $Axsect_{6Li}$ and $Axsect_{35Cl}$. To reproduce results from past releases, set these keywords to the previous default values, listed above; in this case, any values set for $Axsect$, $Axsect_{6Li}$ or $Axsect_{35Cl}$ will be ignored.

$A_1^1$-He and $A_1^{36}$Cl are constants used to calculate the production rates of the isotopes $^3$He and $^{36}$Cl, which are produced in-situ by neutron activation of $^6$Li and $^{35}$Cl, respectively. The isotope production rate is calculated from the neutron production rate (see keywords $A1_nflux$ and $A2_nflux$), the concentration (ppm) of Li or Cl in the rock, and the value set for $A_1$ using these keywords. The rock concentrations are set using the keywords $ppm_{Cl}$ and $ppm_{Li}$.

**discussion:** Chapter 14

**A1_4He, A2_4He, A1_40Ar**

**arguments:** real values

**default:**

- $A_1^4$He = $5.336 \times 10^{-17}$
- $A_2^4$He = $1.333 \times 10^{-17}$
- $A_1^{40}$Ar = $1.733 \times 10^{-21}$

**units:** mol/μg yr

**set:** globally

**description:** Use these keywords to set the constants used to calculate production rates for the isotopes $^4$He and $^{40}$Ar, which are formed in-situ in the basin by radioactive decay. Coefficients $A_1^4$He and $A_2^4$He are multiplied by the concentrations of U and Th in the rock; $A_1^{40}$Ar by the K concentration. The elemental concentrations (ppm) are set using the keywords $ppm_K$, $ppm_{Th}$, and $ppm_{U}$.

**discussion:** Chapter 14
\textbf{A1\_nflux, A2\_nflux}

arguments: real values
default: $A_1\_nflux = 1.042$ (ss and other), $1.390$ (sh), and $0.9612$ (cn)
$A_2\_nflux = 0.2458$ (ss and other), $0.4091$ (sh), and $0.1892$ (cn)
units: neutrons/μg yr
set: by rock type
description: $A_1\_nflux$ and $A_2\_nflux$ are empirical constants used to calculate the neutron production rate within a rock from the rock’s U and Th concentrations (ppm), respectively. The neutron production rate is then used to determine the rates at which the isotopes produced by neutron activation ($^3\text{He}$ and $^{36}\text{Cl}$) are produced \textit{in-situ}, for runs in which these isotopes are considered.
discussion: Chapter 14

\textbf{A\_mk, B\_mk, C\_mk, D\_mk, E\_mk}

arguments: real values
default: $0.2198$, $123.3 \times 10^{-6}$, $2.652 \times 10^{-9}$, $-0.7218$, and $-3.292 \times 10^{-3}$ (except built-in rock types)
units of: heat capacity
default unit: cal/g°C
set: by rock type
description: These coefficients of the Maier-Kelley equation give heat capacity $C_p$ of the rock framework as a function of absolute temperature $T_K$.
discussion: Chapter 2

\textbf{A\_perm}

argument: real value
default: 15
units: none
set: by rock type
description: Use this keyword to set the slope $A$ of the correlation of permeability $k_x$ with porosity $\phi$.
discussion: Chapter 2
**A tc**

- **argument:** real value
- **default:** \(-0.0044\) cal/cm sec °C
- **units of:** thermal conductivity
- **default unit:** cal/cm sec°C
- **set:** by rock type
- **description:** Use this keyword to set the slope \(A\) of the correlation of thermal conductivity \(K\) with porosity \(\phi\).
- **discussion:** Chapter 2

**act_eng**

- **a.k.a.:** activation_energy
- **argument:** real value, positive
- **default:** 218.25 kJ/mol
- **units of:** energy/mole
- **default units:** kJ/mol
- **set:** globally or by strat unit
- **description:** The activation energy used in the Arrhenius model of organic maturation.
- **discussion:** Chapter 6

**alpha_L**

- **argument:** real value, zero or positive
- **default:** 1000 cm
- **units of:** length
- **default unit:** cm
- **set:** by rock type
- **description:** Use this keyword to set the longitudinal dispersivity \(\alpha_L\) of a rock type.
- **discussion:** Chapter 2

**alpha_T**

- **argument:** real value, zero or positive
- **default:** 100 cm
- **units of:** length
- **default unit:** cm
- **set:** by rock type
- **description:** Use this keyword to set the transverse dispersivity \(\alpha_T\) of a rock type.
- **discussion:** Chapter 2
**arrhenius**

- **argument**: on or off
- **default**: off
- **set**: globally
- **description**: Set this option on during transient simulations to use the Arrhenius method to calculate the thermal maturity of oil source beds in the basin.
- **discussion**: Chapter 6

---

**Axsect**

- **argument**: real value
- **default**: $5.665 \times 10^{-3}$ (ss and other), $10.992 \times 10^{-3}$ (sh), and $3.824 \times 10^{-3}$ (cm)
- **units**: cm$^2$/g rock
- **set**: by rock type
- **description**: $Axsect$ is the macroscopic neutron absorption cross-section per gram for the rock grains. Use keyword $Axsect$ to set this value in cm$^2$/g.
- **discussion**: Chapter 14

---

**Axsect_6Li, Axsect_35Cl**

- **arguments**: real values
- **default**: $Axsect_6Li = 941, Axsect_35Cl = 43.74$
- **units**: barns (1 barn = $10^{-24}$ cm$^2$)
- **set**: globally
- **description**: $Axsect_6Li$ and $Axsect_35Cl$ are the neutron absorption cross-sections for $^6$Li and $^{35}$Cl. Use keywords $Axsect_6Li$ and $Axsect_35Cl$ to set these values in barns, where 1 barn = $10^{-24}$ cm$^2$.
- **discussion**: Chapter 14

---

**B_perm**

- **argument**: real value
- **default**: $-3$ log darcy
- **units**: log permeability
- **default unit**: log darcy
- **set**: by rock type
- **description**: Use this keyword to set the intercept $B$ of the correlation of permeability $k_x$ with porosity $\phi$.
- **discussion**: Chapter 2
**B tc**
- **argument:** real value, positive
- **default:** 0.00535 cal/cm sec °C
- **units of:** thermal conductivity
- **default unit:** cal/cm sec °C
- **set:** by rock type
- **description:** This keyword controls the intercept $B$ of the correlation of thermal conductivity $K_x$ with porosity $\phi$.
- **discussion:** Chapter 2

**balance**
- **argument:** on or off
- **default:** off
- **set:** globally
- **description:** Set this option on to calculate mass and energy balances during the numerical solution, as a check on accuracy. This option is not yet fully implemented.
- **discussion:** Chapter 6

**beta_por**
- **argument:** real value, zero or positive
- **default:** not set
- **units of:** reciprocal stress
- **default unit:** atm$^{-1}$
- **set:** by rock type
- **description:** Set this keyword if you wish to describe compaction in terms of the compressibility $\beta$ of the reducible pore volume instead of a compaction coefficient $b$ (bpor). A value set for beta_por overrides any setting for bpor.
- **discussion:** Chapter 2
**beta_ul**

- **argument:** real value, zero or positive
- **default:** not set
- **units of:** reciprocal stress
- **default unit:** atm–1
- **set:** by rock type
- **description:** Set this keyword if you wish to describe sediment rebound during unloading in terms of the compressibility $\beta_u$ of the reducible pore volume instead of a compaction coefficient $b_{ul} (bpor_{ul})$. A value set for beta_ul overrides any setting for bpor_{ul}.
- **discussion:** Chapter 2

**bottom_conc**

- **a.k.a.:** chasew
- **argument:** halite, or a real value
- **default:** 0.5 molal
- **units of:** concentration
- **default unit:** molality
- **set:** globally or by strat unit and/or well
- **description:** Use this keyword to specify the salinity along the basin’s bottom surface. Argument halite sets the salinity to the solubility of halite at the basement temperature. This boundary condition, when set within a strat block, applies at the unit’s $t_{dep}$ rather than over its entire interval of deposition. You may set either salt_flux (see below) or bottom_conc, but not both.
- **discussion:** Chapter 6

**bpor**

- **argument:** real value, zero or positive
- **default:** 0.5 km–1 (except built-in rock types)
- **units of:** reciprocal length
- **default unit:** km–1
- **set:** by rock type
- **description:** Use this keyword to set the exponential coefficient $b$ describing sediment compaction with burial, according to the compaction model selected.
- **discussion:** Chapter 2
**bpor Ul**

**argument:** real value, zero or positive

**default:** $0.1\,\text{km}^{-1}$ (except built-in rock types)

**units of:** reciprocal length

**default unit:** $\text{km}^{-1}$

**set:** by rock type

**description:** Use this keyword to set the exponential coefficient $b_{ul}$ describing sediment compaction under conditions of unloading, when compaction is set to irreversible.

**discussion:** Chapter 2

---

**bulk_density**

**argument:** variable, constant, or a real value

**default:** variable

**units of:** density

**default units:** $\text{g/cm}^3$

**set:** globally

**description:** Use this option to set the sediment bulk density to a constant value, or to let the program calculate bulk density from the sediment’s porosity and the densities of fluid and rock grains (the variable option). The argument constant implies a bulk density of 2.3 $\text{g/cm}^3$.

**discussion:** Chapter 2

---

**cbase_iso1, cbase_iso2**

**a.k.a.:** cbasew_iso1, bottom_conc_iso1, cbasew_iso2, bottom_conc_iso2

**arguments:** real values

**default:** not set

**units of:** concentration

**default units:** molality

**set:** globally or by strat unit and/or well

**description:** Use these keywords to set the concentrations of isotope-1 and isotope-2 along the basin’s basal boundary. When set within a strat block, the boundary value applies at the unit’s $t_{dep}$ rather than over the unit’s interval of deposition. For either isotope, you may set the basal concentration using one of these keywords, or a basal flux using keyword $\text{isol_flux}$ or $\text{iso2_flux}$, but not both. By default, the program assumes a zero flux for the basal boundary condition. This boundary condition is ignored for an isotope set to $Cl$.

**discussion:** Chapter 6
**cementation**

*argument:* off, all, or mineral name(s)

*default:* off

*set:* globally

*description:* Use this keyword to command the program to calculate the effects of migrating groundwaters on cementation in basin strata. You may specify one or more minerals individually by name, or include all minerals with the argument all. The minerals available are either those built in to the program (quartz, chalcedony, cristobalite, amorphous silica, and anhydrite) or those passed to Basin2 from React. 

*discussion:* Chapter 6

**column**

*arguments:* column heading, optionally with units

*description:* Use a column statement to initialize a block in which you set stratigraphic properties and boundary conditions at wells across the cross section. The arguments are the keywords corresponding to the columns in the block. You may set units for each keyword by following the keyword with an appropriate unit name in parentheses. You then set values for the keywords with \( w() \) statements. 

*discussion:* Chapter 4

**compaction**

*argument:* reversible or irreversible

*default:* reversible

*set:* globally

*description:* This option controls whether or not sediment compaction is considered as a reversible process by which porosity is lost during loading and fully regained during unloading. Select the irreversible argument to allow sediment to regain during unloading only some of the porosity lost during loading. 

*discussion:* Chapter 2
**conc_increase**

**a.k.a.:** eps4  
**argument:** real value, greater than zero  
**default:** .05 molal  
**units of:** concentration  
**default units:** molality  
**set:** globally or by strat unit  
**description:** This keyword sets the greatest increase in salinity the program will attempt to allow over a time step, as calculated by the rate of increase in this variable over the previous step. Decreasing this setting results in shorter time steps if the rate of salinity increase controls the step size.  
**discussion:** Chapter 5

**conv_conc**

**argument:** real value, greater than zero  
**default:** $10^{-4}$ molal  
**units of:** concentration  
**default units:** molality  
**set:** globally  
**description:** Use this keyword to set the convergence criterion for salinity values when seeking a steady-state solution or initial condition.  
**discussion:** Chapter 5

**conv_iso1, conv_iso2**

**a.k.a.:** conv_conc_iso1, conv_conc_iso2  
**arguments:** real values, greater than zero.  
**default:** $10^{-4}$ molal  
**units of:** concentration  
**default units:** molality  
**set:** globally  
**description:** Use these keywords to set the convergence criterion for the concentrations of isotope-1 and isotope-2, when seeking a steady state solution or initial condition. Note that the default value is not especially useful for isotopes present in small concentrations.  
**discussion:** Chapter 5
\texttt{conv\_press}

- \textit{argument:} real value, greater than zero
- \textit{default:} $10^{-4}$ atm
- \textit{units of:} pressure
- \textit{default units:} atm
- \textit{set:} globally
- \textit{description:} Set this option to specify the convergence criterion for pressure values when seeking a steady-state solution or initial condition.
- \textit{discussion:} Chapter 5

\texttt{conv\_temp}

- \textit{argument:} real value, greater than zero
- \textit{default:} $10^{-4}$ $\Delta{\degree}{C}$
- \textit{units of:} temperature change
- \textit{default units:} $\Delta{\degree}{C}$
- \textit{set:} globally
- \textit{description:} Use this option to set the convergence criterion for temperature values when seeking a steady-state solution or initial condition.
- \textit{discussion:} Chapter 5

\texttt{conv\_tres}

- \textit{argument:} real value, greater than zero.
- \textit{default:} $10^{3}$ years
- \textit{units of:} time
- \textit{default units:} years
- \textit{set:} globally
- \textit{description:} Use this keyword to set the convergence criterion for the residence time equation, when seeking a steady state solution or initial condition. Keyword applies to runs in which \texttt{residence\_time} is set to \texttt{on}.
- \textit{discussion:} Chapter 5
**csurf_isol, csurf_iso2**

*a.k.a.:* csurfw_isol, top_conc_isol, surface_conc_isol, csurfw_iso2, top_conc_iso2, surface_conc_iso2

**arguments:** real values, positive

**default:** zero

**units of:** concentration

**default units:** molality

**set:** globally or by strat unit and/or well

**description:** Use these keywords set the concentrations of isotope-1 and isotope-2 along the basin’s top surface. When set within a strat block, the boundary value applies at the unit’s $t_{dep}$ rather than over the unit’s interval of deposition. This boundary condition is ignored for an isotope set to Cl.

**discussion:** Chapter 6

**delta_z**

*a.k.a.:* dstarg

**argument:** real value

**default:** 400 m

**units of:** length

**default unit:** km

**set:** globally or by strat unit

**description:** Use this keyword to set the target thickness of nodal blocks within the thickest part of a strat unit. Nodal block height varies with position along the cross section and, as sediments compact, with time.

**discussion:** Chapter 6

**density**

*a.k.a.:* fluid_density

**argument:** variable, constant, batzle-wang, or a real value

**default:** variable

**units of:** density

**default units:** g/cm$^3$

**set:** globally

**description:** Use this option to set the fluid density to a constant value or to have the program calculate density from the fluid’s temperature, pressure, and salinity (the variable and batzle-wang options). The argument constant implies a density of 1 g/cm$^3$. Setting density to a constant value eliminates buoyant forces from the calculation.

**discussion:** Chapter 3
**diff_con**

*argument:* real value, positive  
*default:* $10^{-6}$ cm$^2$/sec  
*units:* cm$^2$/sec  
*set:* by rock type  
*description:* Use this keyword to set the diffusion coefficient $D^*$ for a rock type to be used in calculating the distribution of salinity (as well as cements). If you set a temperature dependence with keyword **diff_T**, keyword **diff_con** sets the diffusion coefficient at the reference temperature, 25°C.  
*discussion:* Chapter 2

**diff_iso1, diff_iso2**

*a.k.a.:* diffcon_iso1, diffcon_iso2  
*arguments:* real values  
*default:* value set for keyword **diff_con**  
*units:* cm$^2$/sec  
*set:* by rock type  
*description:* Use these keywords to set values for the diffusion coefficients for isotope-1 and isotope-2. If you set a temperature dependence with keyword **diff_tiso1** or **diff_tiso2**, keyword **diff_iso1** or **diff_iso2** sets the diffusion coefficient at the reference temperature, 25°C.  
*discussion:* Chapter 2

**diff_T**

*argument:* real value  
*default:* zero  
*units:* K  
*set:* by rock type  
*description:* Use this keyword to set for a rock type the temperature dependence of the diffusion coefficient $D^*$ for salt.  
*discussion:* Chapter 2
**diff_tres**

*a.k.a.*: diffcon_tres  
*argument*: real value  
*default*: zero  
*units*: cm²/sec  
*set*: by rock type  
*description*: Basin2 carries a coefficient for a “diffusion constant” for use when calculating hydrologic residence time. By default, this value is set to zero. Depending on how you concentrate residence time, however, you may wish to set a value for the self-diffusion coefficient of water, using the `diff_tres` keyword. If you set a temperature dependence with keyword `difft_tres`, keyword `diff_tres` sets the diffusion coefficient at the reference temperature, 25°C.  

*discussion*: Chapter 6

**difft_isol, difft_iso2**

*arguments*: real values  
*default*: zero  
*units*: K  
*set*: by rock type  
*description*: Use these keywords to set the temperature dependence of the diffusion coefficients for isotope-1 and isotope-2.  

*discussion*: Chapter 2

**difft_tres**

*arguments*: real value  
*default*: zero  
*units*: K  
*set*: by rock type  
*description*: Use this keywords to set the temperature dependence of the diffusion coefficients for hydrologic residence time.  

*discussion*: Chapter 2
**disequilibrium**

*argument:* on or off  
*default:* on  
*set:* globally  
*description:* Set this option on to consider the “disequilibrium” effects of nonhydrostatic fluid pressure on sediment porosity, or off to ignore these effects. The *equilibrium* keyword works in the opposite sense.  
*discussion:* Chapter 2

**disp_tensor**

*a.k.a.:* cross_terms, dispersivity_tensor  
*argument:* on or off  
*default:* off  
*set:* globally  
*description:* Set this option on to consider the “cross terms” $D_{xz}$ and $D_{zx}$ in the dispersivity tensor, or off to ignore these terms. The cross terms may be significant where fluid flows not along or across stratigraphy, but at an angle to it. In the current release, this option is intended for models in which each stratigraphic unit is composed of a single rock type.  
*discussion:* Chapter 12

**dt_max**

*a.k.a.:* max_step  
*argument:* real value, positive  
*default:* time span of run divided by $10^4$.  
*units of:* time  
*default units:* years  
*set:* globally or by strat unit  
*description:* Use this keyword to set the largest time step the program can take.  
*discussion:* Chapter 5

**dump_end**

*argument:* integer value, positive  
*default:* not set  
*set:* globally  
*description:* This keyword sets the final step for dumping results, if keyword *dump_start* has been set.  
*discussion:* Chapter 6
**dump_start**

- **argument:** integer value, positive
- **default:** not set
- **set:** globally
- **description:** Use this keyword in a transient run to command the program to begin writing output into B2_plot.dat and the table datasets after each time step. The program will begin dumping results at time step number dump_start and continue indefinitely or to step number dump_end, if this keyword has been set. This option is sometimes useful for debugging a run.
- **discussion:** Chapter 6

**dz0**

- **argument:** real value, $10^{-3}$ cm or greater
- **default:** 1 cm
- **units of:** length
- **default units:** cm
- **set:** globally or by strat unit
- **description:** This negligibly small value is used as the thickness of empty nodal blocks when they are added along the top of the domain to accept sedimentation.
- **discussion:** Chapter 6

**end**

- **a.k.a.:** t_end
- **argument:** real value
- **default:** time of deposition ($t_{dep}$) of uppermost strat unit
- **units of:** time
- **default unit:** years
- **set:** globally
- **description:** This option specifies the ending point in time for a transient simulation.
- **discussion:** Chapter 5

**end_fault**

- **arguments:** none
- **units:** none
- **description:** Use an end_fault statement to define the end of a fault block. If a fault statement follows immediately, you may omit the end_fault statement.
- **discussion:** Chapter 4
end_rock
arguments: none
units: none
description: An end_rock statement terminates the definition block for a rock type. You may omit an end_rock statement that is followed immediately by another rock statement.
discussion: Chapter 2

end_strat
arguments: none
units: none
description: Use an end_strat statement to define the end of a strat block. Assignments within a strat block apply to only the stratigraphic unit in question. Assignments not within a strat block (i.e., those following an end_strat statement but before a strat statement), however, apply to all stratigraphic units remaining to be defined. If a strat statement follows immediately, you may omit the end_strat statement.
discussion: Chapter 4

equilibrium
argument: on or off
default: off
set: globally
description: Set this option on to ignore the “disequilibrium” effects of nonhydrostatic fluid pressure on sediment porosity, or off to consider these effects. The disequilibrium keyword works in the opposite sense.
discussion: Chapter 2

eustat
argument: real value
default: zero
units of: distance
default units: km
set: globally or by strat unit
description: This keyword sets a eustatic shift in sea level, either upward (negative) or downward (positive). The program adds the magnitude of this shift to all values entered for water depth.
discussion: Chapter 4
explain
    argument: on or off
    default: off
    set: globally
    description: Set this option on to have the program report in the B2_output.txt dataset the factor constraining the size of each time step.
    discussion: Chapter 5

fault
    arguments: label for the hydraulic fault
    units: none
    description: Use a fault statement to initialize a fault block in which you define the properties of a hydraulic fault. All fault properties must be defined within a fault block. Enclose the label in single quotes. You terminate a fault block with an end_fault statement.
    discussion: Chapter 4

fault_begin
    a.k.a.: fault_start
    argument: real value
    default: not set
    units of: time
    default unit: years
    set: by fault
    description: Use this keyword to specify the point in time when a hydraulic fault begins to exist. This assignment must be made within a fault block.
    discussion: Chapter 4

fault_bottom
    argument: index of a strat unit, 1 or greater
    default: not set
    units: none
    set: by fault
    description: Use this keyword to specify the stratigraphically lowest unit that the fault in question penetrates. Strat units are indexed upward beginning with 1 for the first unit deposited. This assignment must be made within a fault block.
    discussion: Chapter 4
**fault_end**

<table>
<thead>
<tr>
<th>argument</th>
<th>real value</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>not set</td>
</tr>
<tr>
<td>units of</td>
<td>time</td>
</tr>
<tr>
<td>default unit</td>
<td>years</td>
</tr>
<tr>
<td>set</td>
<td>by fault</td>
</tr>
</tbody>
</table>

**description:** Use this keyword to specify the point in time when a hydraulic fault ceases to exist. This assignment must be made within a fault block.

**discussion:** Chapter 4

**fault_position**

<table>
<thead>
<tr>
<th>a.k.a.</th>
<th>x_fault</th>
</tr>
</thead>
<tbody>
<tr>
<td>argument</td>
<td>real value, zero or greater</td>
</tr>
<tr>
<td>default</td>
<td>none</td>
</tr>
<tr>
<td>units of</td>
<td>length</td>
</tr>
<tr>
<td>default unit</td>
<td>km</td>
</tr>
<tr>
<td>set</td>
<td>by fault</td>
</tr>
</tbody>
</table>

**description:** The position along the cross section of the fault in question. The program will choose the column of nodal blocks nearest this position to represent the fault. This assignment must be made within a fault block.

**discussion:** Chapter 4

**fault_top**

<table>
<thead>
<tr>
<th>argument</th>
<th>index of a strat unit, 1 or greater</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>not set</td>
</tr>
<tr>
<td>units</td>
<td>none</td>
</tr>
<tr>
<td>set</td>
<td>by fault</td>
</tr>
</tbody>
</table>

**description:** Use this keyword to specify the stratigraphically highest unit that the fault in question penetrates. Strat units are indexed upward beginning with 1 for the first unit deposited. This assignment must be made within a fault block.

**discussion:** Chapter 4
**fault_xperm**
  a.k.a.: kx_fault  
  argument: real value, greater than zero  
  default: not set  
  units of: permeability  
  default unit: Darcy  
  set: by fault  
  description: Use this keyword to set the permeability along $x$ to be assigned to the nodal blocks that make up a fault. This assignment must be made within a fault block. If no value is set for this variable, the program will assign an $x$-direction permeability to the nodal blocks in the fault in the usual manner.  
  discussion: Chapter 4

**fault_zperm**
  a.k.a.: kz_fault  
  argument: real value, greater than zero  
  default: none  
  units of: permeability  
  default unit: darcy  
  set: by fault  
  description: Use this keyword to set the vertical permeability to be assigned to the nodal blocks that make up the fault in question. This assignment must be made within a fault block.  
  discussion: Chapter 4

**feedback**
  argument: on or off  
  default: off  
  set: globally  
  description: Set this option on to account in transient runs for the effects of cementation on sediment porosity.  
  discussion: Chapter 6

**flip**
  argument: on or off  
  default: off  
  set: globally  
  description: Set this option on to reverse the orientation of the cross section. In this case, the left boundary appears to the right, and vice versa.  
  discussion: Chapter 4
flow

  a.k.a.: pressure
  argument: full (or 2-D), vertical, or hydrostatic
  default: full
  set: globally

  description: This option controls how the groundwater flow (pressure) equation is solved. By default the program considers a full model of flow in two dimensions, but you can select only vertical flow or a hydrostatic pressure profile. In the latter case, the program ignores groundwater flow.

  discussion: Chapter 6

halite_sat

  argument: the label for a rock type
  default: not set
  set: globally

  description: Use this option to specify that fluid salinity maintain saturation with halite wherever a certain rock type occurs in the basin. The label of this rock type is the argument.

  discussion: Chapter 6

halite_solubility

  a.k.a.: halite_sol
  argument: real number, positive
  default: tabulated values versus temperature
  units of: concentration
  default unit: molality
  set: globally

  description: Use this keyword to set to a specific value the NaCl concentration in equilibrium with halite. This value is used when you set a halite solubility as a basal boundary condition for the salinity equation, or when you specify halite solubility at points within the basin.

  discussion: Chapter 3
**heat_flow**

*a.k.a.*: h_flow, h_floww

*argument*: real value, positive

*default*: 1.5 HFU

*units of*: heat flow

*default unit*: HFU

*set*: globally or by strat unit and/or well

*description*: Use this keyword to specify the rate at which heat is conducted into the basin from the underlying crust. This boundary condition, when set within a strat block, applies at the unit’s t_dep rather than over its entire interval of deposition.

*discussion*: Chapter 6

**include**

*argument*: a file name in single quotes

*description*: Use an include statement to redirect input to another file. Upon reaching the end of the file, the program resumes reading the original input stream. You may nest include statements within included files. Be sure to enclose the file name within single quotes.

*discussion*: Chapter 1

**initial**

*a.k.a.*: initial_cond

*argument*: hydrostatic or steady (or steady_state)

*default*: hydrostatic

*set*: globally

*description*: This option controls how the program sets initial conditions for transient runs. By default, the initial condition is a hydrostatic pressure distribution, a vertical conduction profile for temperature, and a vertical diffusive gradient for salinity. Specifying steady gives as the initial condition the full steady-state solution corresponding to the settings of the pressure, temperature, and salinity keywords.

*discussion*: Chapter 6
**initial_step**

*a.k.a.:* dt_init

*argument:* real value, positive

*default:* time span of run divided by $10^6$

*units of:* time

*default units:* years

*set:* globally

*description:* This option controls the length of the first time step the program takes. The step should be rather small. The program will quickly increase the size of the time step to a reasonable size.

*discussion:* Chapter 5

**isol_flux, iso2_flux**

*a.k.a.:* sfluxw_isol, sflux_isol, mass_flux_isol, sfluxw_isol2, sflux_isol2, mass_flux_isol2

*arguments:* real values

*default:* zero

*units of:* mass flux

*default units:* mol/cm$^2$ sec

*set:* globally or by strat unit and/or well

*description:* Use these keywords to set the basal flux of isotope-1 and isotope-2 into basin. For either isotope, you may set the basal flux using one of these keywords, or a basal concentration using keyword `cbase_isol` or `cbase_isol2`, but not both. By default, the program assumes a zero flux for the basal boundary condition. This boundary condition is ignored for an isotope set to Cl.

*discussion:* Chapter 6
**isol\_increase, iso2\_increase**

*a.k.a.*: conc\_increase\_isol, eps\_isol, conc\_increase\_iso2, eps\_iso2  

**arguments:** real values, greater than zero  
**default:** 0.05 molal  
**units of:** concentration  
**default units:** molality  
**set:** globally or by strat unit  

**description:** These keywords set the greatest increase in the concentrations of isotope-1 and isotope-2 that the program will allow over a time step in a transient run, as calculated by the rate of increase of the previous time step. Note that the default setting is not especially useful for isotopes present at small concentration.

**discussion:** Chapter 5
**isol_equation, iso2_equation**

* a.k.a.: isotopel_eq, isotope2_eq, isotopel_equation, isotope2_equation
* arguments: full, diffusive, vertical, constant, off, or a real value;
on or off (for Cl)
* default: off
* units of: concentration
* default units: molality
* set: globally

**description:** These keywords control how the program calculates the distributions of isotope-1 and isotope-2 within the basin. By default, the program does not consider isotope transport. You can set the concentration of either (or both) isotopes to a constant value (e.g., isotopel_eq = 10^{-18} molal), or to the keyword constant, which fixes a uniform concentration of zero molal. Alternatively, you can calculate the concentration along a vertical profile (vertical), or use a solution in two dimensions that ignores (diffusive) or considers (full) mass transport by advection. The argument advective is synonymous with full, and 2-D with diffusive.

For the special case of an isotope set to Cl, when you set argument on (or any argument except off), the program will set the isotope molal concentration equal to the molal salinity, as determined by solving the salinity equation (see keyword salinity). This feature allows you to predict the ^{36}Cl/Cl ratio as the concentration ratio of isotope 1 to isotope 2. In this case, the various boundary conditions to the isotope equation (keywords csurf_isol, etc.) are ignored.

**discussion:** Chapter 6
**isol_type, iso2_type**

*a.k.a.*: isotope1_type, isotope2_type, isotope1_element, isotope2_element

**arguments:** He3, He4, Cl, Cl36, Ar36, Ar40,
3He, 4He, Cl, 36Cl, 36Ar, 40Ar,
Helium3, Helium4, Chlorine, Chlorine36, Argon36,
Argon40,

**default:** not set

**set:** globally

**description:** This keyword controls which isotopes (among 3He, 4He, 36Cl, 36Ar, and 40Ar) are to be carried as isotope-1 and isotope-2 in the simulation. You can also set one of the “isotopes” equal to Cl, to cause Basin2 to calculate the 36Cl/Cl ratio. In this case, the isotope molal concentration is set to the molal salinity of the fluid, as determined by solving the salinity equation.

**discussion:** Chapter 6

**iterations**

*a.k.a.:* n_iter

**argument:** integer, zero or greater

**default:** zero

**units:** none

**set:** globally

**description:** Use this option to specify the number of iterations the program will make in seeking a steady-state solution. A value of zero, the default, causes the program to iterate to convergence.

**discussion:** Chapter 5

**left**

**argument:** open or closed

**default:** closed

**units:** none

**set:** globally or by strat unit

**description:** This keyword sets the left boundary of the basin to be either open or closed to groundwater flow. You may set some strata open and others closed to flow over the simulation.

**discussion:** Chapter 6
**left_table**

- a.k.a.: `left_wt`
- argument: real value
- default: not set
- units of: length
- default unit: km
- set: globally or by strat unit

**description:** When you set an open side boundary, the program by default assumes that the position of the water table coincides with the land surface or, where the surface is subsea, with sea level. Use `left_table` to specify another position for the water table along the left bound. By convention, negative values lie above and positive values lie below sea level. If you set `left_table` by strat unit, the value set applies at each unit’s `t_dep` rather than over the entire interval of deposition.

**discussion:** Chapter 6

---

**max_iter**

- a.k.a.: `max_iters`
- argument: integer, one or greater
- default: 9999
- units: none
- set: globally

**description:** In steady-state runs with `iterations` set to zero, this value is the maximum number of iterations the program will take in its attempt to converge, before giving up.

**discussion:** Chapter 5

---

**max_passes**

- a.k.a.: `max_pass`
- argument: integer, one or greater
- default: 99
- units: none
- set: globally

**description:** This keyword controls the maximum number of passes the program will make at a time step while trying to converge during a transient simulation, if `passes` is set to zero. If the solution has not converged after this number of passes, the program will write a warning message to `B2_output.txt` and attempt to continue the simulation with the next time step.

**discussion:** Chapter 5
**max_steps**

* a.k.a.: nts_max, steps
* argument: integer, greater than one
* default: 99999
* units: none
* description: This keyword controls the maximum number of time steps that the program will take in a transient run before quitting.
  
  *discussion: Chapter 5*

**min_nodes**

* argument: integer, one or greater
* default: one
* units: none
* set: globally
* description: This option sets the minimum number of rows of nodes to be included within each strat unit.
  
  *discussion: Chapter 6*

**meteoric_conc**

* argument: on or off
* default: off
* set: globally
* description: Set this option on to cause the program to set the surface boundary condition for the salinity equation to zero where the basin surface rises above sea level (i.e., wherever water depth is negative). Note that this setting overrides the settings for surface_conc, where the basin is exposed above sea level.
  
  *discussion: Chapter 12*

**nx**

* argument: integer, one or greater
* default: 15
* units: none
* set: globally
* description: The option sets the number of columns of nodal blocks in the finite difference grid. Set nx to 1 to set up a vertical one-dimensional model.
  
  *discussion: Chapter 6*
**nz_max**

* a.k.a.: nz
* argument: integer, 2 or greater
* default: no limit
* units: none
* set: globally
* description: This keyword specifies the maximum number of rows of nodal blocks in the finite-difference grid.
* discussion: Chapter 6

**p_kxkz**

* argument: real value, greater than zero
* default: 2.5 (except built-in rock types)
* units: none
* set: by rock type
* description: This option sets the anisotropy $k_x/k_z$ in the permeability of a rock type.
* discussion: Chapter 2

**passes**

* a.k.a.: n_pass
* argument: integer, between zero and 10.
* default: 2
* units: none
* set: globally or by strat unit
* description: This variable controls the number of passes the program will make through the solution cycle at each time step. Setting a value of zero causes the program to iterate to convergence at each step.
* discussion: Chapter 5

**perm_max**

* argument: real value, greater than zero
* default: 1 darcy (except built-in rock types)
* units of: permeability
* default unit: darcy
* set: by rock type
* description: This option controls the maximum permeability that the program will assign to a rock type.
* discussion: Chapter 2
phi0
  argument: real value in range zero to one
  default: 0.4 (except built-in rock types)
  units: none
  set: by rock type
  description: This keyword controls the reducible porosity $\phi_0$ present at deposition.
  discussion: Chapter 2

phi1
  argument: real value in range zero to one
  default: 0.05 (except built-in rock types)
  units: none
  set: by rock type
  description: Use this option to set the irreducible porosity $\phi_1$ of a rock type.
  discussion: Chapter 2

plot
  argument: bitstream or character; also skip, final, or iteration
  default: bitstream; skip, final, and iteration options not selected
  set: globally
  description: Use the plot keyword to command Basin2 to write unformatted (bitstream) or formatted (character) data into B2_plot.dat, the dataset providing interface between Basin2 and the graphics programs. Keyword unformatted is synonymous with bitstream, and formatted with character. Use the skip argument to bypass output to B2_plot.dat. Use the keyword with the final argument to cause the program to write results only at the end of a transient simulation into B2_plot.dat and the table datasets. Use the iteration argument to have the program write the status after each iteration in a steady-state solution (these results may aid in debugging runs that fail to converge).
  discussion: Chapter 6
**ppm\_Cl, ppm\_K, ppm\_Li, ppm\_Th, ppm\_U**

*a.k.a.*: ppm\_rck\_Cl, ppm\_rck\_K, ppm\_rck\_Li, ppm\_rck\_Th, ppm\_rck\_U

**arguments:** real values

**default:**
- Cl: 10 (`ss` and other), 180 (`sh`), and 150 ppm (`cn`)
- K: 10700 (`ss` and other), 26600 (`sh`), and 2700 ppm (`cn`)
- Li: 15 (`ss` and other), 66 (`sh`), and 5 ppm (`cn`)
- Th: 3.9 ppm (`ss` and other), 11.7 ppm (`sh`), and 1.2 ppm (`cn`)
- U: 1.4 ppm (`ss` and other), 3.2 ppm (`sh`), and 1.9 ppm (`cn`)

**units:** ppm

**set:** by rock type

**description:** Use these keywords to set the concentrations (ppm) of Cl, K, Li, Th, and U within the rock grains, for each rock type. The program uses these values to calculate *in-situ* rates of isotope production.

**discussion:** Chapter 14

**pre\_fac**

**argument:** real value, positive

**default:** $6.51 \times 10^{16}$ hr$^{-1}$

**units of:** reciprocal time

**default units:** hr$^{-1}$

**set:** globally or by strat unit

**description:** The pre-exponential factor used in the Arrhenius model of organic maturation.

**discussion:** Chapter 6

**press\_increase**

*a.k.a.*: $\epsilon_{p1}$

**argument:** real value, greater than zero

**default:** 1 atm

**units of:** pressure

**default units:** atm

**set:** globally or by strat unit

**description:** Use this keyword to set the greatest increase in pressure that the program will attempt to allow over a time step, as determined by the rate of increase in this variable over the previous step. Decreasing the setting results in shorter time steps if the rate of pressure increase controls the step size.

**discussion:** Chapter 5
**print_step**

*a.k.a.:* dt_print  
**argument:** real value, final, or iteration  
**default:** print after deposition of each strat unit  
**units of:** time  
**default units:** years  
**set:** globally  
**description:** Use this keyword to specify, in transient runs, how often the program writes (“prints”) results to the B2_plot.dat and table datasets. By default, this output occurs after each strat unit has been deposited, but you can specify a constant interval. The final and iteration options are the same as for the plot keyword.  
**discussion:** Chapter 5

**reference**

*a.k.a.:* icref, comp_state  
**argument:** compacted or uncompacted  
**default:** compacted  
**units:** none  
**set:** globally or by strat unit  
**description:** This keyword specifies the state of compaction at which your input values of thickness and X_rock refer. These values may be specified either in terms of compacted or uncompacted sediment. The keyword does not apply to erosional thicknesses (negative values of thickness), which are always set in terms of the compaction state of basin sediments when erosion occurs.  
**discussion:** Chapter 4
relax

<table>
<thead>
<tr>
<th>a.k.a.:</th>
<th>relaxation</th>
</tr>
</thead>
<tbody>
<tr>
<td>argument:</td>
<td>real value, positive</td>
</tr>
<tr>
<td>default:</td>
<td>1</td>
</tr>
<tr>
<td>units:</td>
<td>none</td>
</tr>
<tr>
<td>set:</td>
<td>globally or by strat unit</td>
</tr>
<tr>
<td>description:</td>
<td>Relaxation may be applied to the velocity constraint on the size of time steps in transient solutions. This constraint requires that time steps be no longer than the time required for fluid to traverse the width or the height of any nodal block. Setting a value of 2, for example, allows time steps twice as long as the velocity constraint would allow. Setting too large a value causes the solution to become unstable.</td>
</tr>
</tbody>
</table>

discussion: Chapter 5

relfac_3He, relfac_4He, relfac_36Cl, relfac_40Ar

| arguments: | real values, from zero to one, inclusive |
| default:   | one                                      |
| units:     | none                                     |
| set:       | globally                                 |
| description: | These keywords set the release factors that describe the fractions of the isotopes $^3$He, $^4$He, $^{36}$Cl, and $^{40}$Ar generated within rock grain that are released to the pore fluid. Release factors can vary from zero (no isotopes released) to one (release occurs at the rate of generation). |

discussion: Chapter 14

relief

| argument: | on or off |
| default:  | on        |
| set:      | globally  |
| description: | This option controls whether or not topographic relief is considered in the calculation. Selecting off forces the basin surface to lie at or below sea level. This option is sometimes convenient when topography drives flow in shallow parts of the basin so quickly that the program takes very small time steps. |

discussion: Chapter 4
**residence_time**

a.k.a.: res_time, H2Oage_equation, H2Oage_eq, H2Oage

**argument:** on, off
**default:** off
**set:** globally

**description:** Use this keyword to control whether the program calculates the hydrologic residence time of groundwater in the basin. The hydrologic residence time is the average physical age of water molecules in a nodal block, calculated as time lapsed since recharge. Argument **full** is equivalent to **on**.

**discussion:** Chapter 14

**residual**

a.k.a.: residuals

**argument:** on or off
**default:** off
**set:** globally

**description:** Setting this option to **on** causes the program to report the residual imbalances to the finite-difference equations after their solution, as a test of the solution method. The imbalances should be quite small.

**discussion:** Chapter 6

**rho_rk**

**argument:** real value, greater than zero.
**default:** 2.653 g/cm³ (except built-in rock types)
**units of:** density
**default unit:** g/cm³
**set:** by rock type

**description:** Use this option to set the average density of the framework of a rock type (i.e., the density of minerals, excluding pore space).

**discussion:** Chapter 2
**right**

*argument:* open or closed  
*default:* closed  
*units:* none  
*set:* globally or by strat unit  
*description:* This keyword sets the right boundary of the basin to be either open or closed to groundwater flow. You may set some strata open and others closed to flow over the simulation.

*discussion:* Chapter 6

**right_table**

*a.k.a.:* right_wt  
*argument:* real value  
*default:* not set  
*units of:* length  
*default unit:* cm  
*set:* globally or by strat unit  
*description:* When you set an open side boundary, the program by default assumes that the position of the water table coincides with the land surface or, where the surface is subsea, with sea level. Use right_table to specify another position for the water table along the right bound. By convention, negative values lie above and positive below sea level. If you set right_table by strat unit, the value set applies at each unit’s t_dep rather than over the entire interval of deposition.

*discussion:* Chapter 6

**rock**

*argument:* a label of three or fewer characters  
*units:* none  
*description:* A rock statement signals the start of a definition block for a rock type. Such a block contains data describing the rock properties. All rock properties must be defined within a block; properties cannot be set globally. The argument is a label of three characters or fewer, which may be one of the built-in rock types (ss, sh, cn) or a type to be defined by the user. Use an end_rock statement to delimit the block.

*discussion:* Chapter 2
run
  argument: transient or steady (or steady_state)
  default: transient
  set: globally
  description: Use this option to set either a transient or steady-state model.
  discussion: Chapter 5

salinity
  a.k.a.: concentration
  argument: full, diffusive, vertical, constant, or a real value
  default: 0.5 molal
  units of: concentration
  default units: molality
  set: globally
  description: Use this keyword to control how the program calculates the salinity of basin groundwaters. By default, the program assumes a salinity of 0.5 molal, about that of seawater; this choice corresponds to the constant option. You can set another salinity directly or use a transport model. The transport models are full, which considers diffusion, dispersion, and advection in two dimensions; diffusive, which accounts for diffusion in two dimensions; and vertical, which sets salinity along a vertical diffusive profile. The argument advective is synonymous with full, and 2-D with diffusive.
  discussion: Chapter 6

salt_flux
  a.k.a.: mass_flux, s_flux, s_fluxw
  argument: real value
  default: zero
  units of: mass flux
  default unit: mol/cm² sec
  set: globally or by strat unit and/or well
  description: Use this keyword to specify the rate at which salt diffuses into the basin from the underlying crust. This boundary condition, when set within a strat block, applies at the unit’s t_dep rather than over its entire interval of deposition. You may set either salt_flux or bottom_conc (see above), but not both.
  discussion: Chapter 6
solution
  argument: L-U or sparse
  default: L-U
  set: globally
  description: This keyword sets the method to solve the matrix equations representing finite-difference equations written in two dimensions. **L-U** specifies a decomposition method for factoring band matrices that runs quickly on current generation computers. **Sparse** specifies a generally slower method that uses less memory to store matrix arrays; this option was important when computer memories were small, but is seldom used today.
  discussion: Chapter 5

start
  a.k.a.: t_start
  argument: real value
  default: time of deposition (t_dep) of lowermost strat unit in a transient run, or that of uppermost unit in a steady-state run
  units of: time
  default unit: years
  set: globally
  description: The starting point in time of a transient simulation, or the time level at which the program should calculate a steady-state model. The value must correspond to the time of deposition (t_dep) of a strat unit.
  discussion: Chapter 5

step_increase
  a.k.a.: eps3
  argument: real value, greater than one
  default: 2
  units: none
  set: globally or by strat unit
  description: Use this keyword to specify the greatest proportionate increase in step size the program will allow from one time step to the next. Setting the value smaller causes the program to increase the step size more slowly.
  discussion: Chapter 5
**strat**
- **arguments:** label for the stratigraphic unit
- **units:** none
- **description:** Use a `strat` statement to initialize a `strat` block in which you define the properties of a stratigraphic unit. Assignments within a strat block apply to the stratigraphic unit in question, whereas those outside a block apply to all units remaining to be defined. The argument is a label for the stratigraphic unit, which should appear in single quotes. You terminate a strat block with an `end_strat` statement.
- **discussion:** Chapter 4

**suffix**
- **argument:** a literal value, enclosed in single quotes
- **description:** Use a `suffix` statement to append a label to the names of output files produced by the Basin2 run. The suffix specified overrides any value set on the command line. To preserve upper case characters, be sure to enclose the label in single quotes.
- **discussion:** Chapter 6

**surface_conc**
- **a.k.a.:** `top_conc, c_surfw`
- **argument:** real number, positive
- **default:** 0.5 molal
- **units of:** concentration
- **default unit:** molality
- **set:** globally or by strat unit and/or well
- **description:** Use this keyword to set salinity along the basin’s top surface. This boundary condition, when set within a strat block, applies at the unit’s `t_dep` rather than over its entire interval of deposition. Note that this setting can be overridden where the basin surface rises above sea level by the `meteoric_conc` option.
- **discussion:** Chapter 6
**surface_temp**

* a.k.a.: t_surf, t_surfw
* argument: real value, positive
* default: 20°C
* units of: temperature
* default unit: °C
* set: globally or by strat unit and/or well
* description: Use this keyword to set temperature along the basin’s top surface. This boundary condition, when set within a strat block, applies at the unit’s t_dep rather than over its entire interval of deposition.
* discussion: Chapter 6

**sw_density**

* a.k.a.: rho_sw
* argument: variable, constant, or a real value
* default: variable
* units of: density
* default units: g/cm³
* set: globally
* description: Where the basin surface lies below sea level, the program calculates pressure along the top boundary, assuming a water column that extends upward to sea level. By default (the variable argument), the program assumes that the density of the overlying seawater is the same as the density of fluid in the top nodal block. Use this keyword to set a constant value for the density of seawater. The constant argument implies a density of 1 g/cm³.
* discussion: Chapter 6

**t_dep**

* a.k.a.: deposited
* argument: real value
* default: none
* units of: time
* default unit: years
* set: by strat unit
* description: Use this keyword to specify the point in time at which deposition of a strat unit is complete. No two strat units may have the same t_dep value.
* discussion: Chapter 4
**t_kxkz**

*argument:* real value, greater than zero  
*default:* 1.0  
*units:* none  
*set:* by rock type  
*description:* Use this keyword to set the anisotropy $K_x/K_z$ in the thermal conductivity of a rock type.  
*discussion:* Chapter 2

**tables**

*a.k.a.:* table  
*argument:* all, off, or one or more variable names  
*default:* off  
*units:* none  
*set:* globally  
*description:* You control the data written into the table dataset with the tables keyword. Set off if you want the program to skip writing tables altogether, and all if you want the program to write the complete set of variables. You may also specify the names of one or more individual variables, as listed in Chapter 6.  
*discussion:* Chapter 6

**temp_increase**

*a.k.a.:* eps2  
*argument:* real value, greater than zero  
*default:* $1 \, ^\circ \mathrm{C}$  
*units of:* temperature change  
*default units:* $^\circ \mathrm{C}$  
*set:* globally or by strat unit  
*description:* The greatest increase in temperature the program will attempt to allow over a time step, as determined by the rate of increase in this variable over the previous step. Decreasing the setting results in shorter time steps if the rate of temperature increase controls the step size.  
*discussion:* Chapter 5
**temperature**

*argument:* full, conductive, vertical, constant, or a real value  
*default:* vertical  
*units of:* temperature  
*default unit:* °C  
*set:* globally  
*description:* The temperature keyword controls how the program calculates temperature within the basin. You can set temperature to a constant value (e.g., 10 °C) or to the keyword constant, which assumes a temperature of 20°C. Alternatively, you can calculate temperature along a vertical conductive profile (vertical) or use a transient solution in two dimensions that ignores (conductive) or considers (full) heat transport by advection. The argument advective is synonymous with full, and 2-D with conductive.  
*discussion:* Chapter 6

**theta**

*argument:* real value in range zero to 1  
*default:* 0.7  
*units:* none  
*set:* globally or by strat unit  
*description:* This time weighting variable controls the method and thus the stability of the finite-difference solutions. You set a value of 1 to give the most stable method. Smaller values decrease truncation error, but values of 0.5 or less are unlikely to give stable solutions.  
*discussion:* Chapter 5

**thickness**

*a.k.a.:* thick, thickw  
*argument:* real value  
*default:* zero  
*units of:* length  
*default unit:* km  
*set:* globally or by strat unit and/or well  
*description:* Use this keyword to set the thickness of a strat unit along the cross section. A unit’s thickness varies over the simulation as it compacts during burial (see keyword reference). A value of zero indicates that the unit has pinched out and is missing from that part of the basin. Negative values denote erosion.  
*discussion:* Chapter 4
**title**

*argument:* character string within single quotes  
*units:* none  
*set:* globally  
*description:* You may set up to four title lines for a run. The program writes the titles into the `B2_output.txt` dataset; the first two titles appear at the top of the printout, and the remaining two above the stratigraphic grid.  
*discussion:* Chapter 1

**tol_conc**

*argument:* real value, greater than zero  
*default:* $10^{-2}$ molal  
*units of:* concentration  
*default units:* molality  
*set:* globally  
*description:* This keyword sets the tolerance for convergence of salinity values in a time step in a transient run, if `passes` is set to zero.  
*discussion:* Chapter 5

**tol_iso1, tol_iso2**

*a.k.a.:* `tol_conc_iso1, tol_conc_iso2`  
*arguments:* real values, greater than zero.  
*default:* .01 molal  
*units of:* concentration  
*default units:* molality  
*set:* globally  
*description:* These keywords set the tolerance for converge of the transport equation for isotope-1 and isotope-2 over a time step in a transient run, if `passes` is set to zero. Note that the default setting is not especially useful for isotopes present at small concentration.  
*discussion:* Chapter 5
**tol_press**

- **argument:** real value, greater than zero
- **default:** $10^{-2}$ atm
- **units of:** pressure
- **default units:** atm
- **set:** globally
- **description:** This keyword sets the tolerance for convergence of pressure values in a time step in a transient run, if passes is set to zero.
- **discussion:** Chapter 5

**tol_temp**

- **argument:** real value, greater than zero
- **default:** $10^{-2} \, \Delta^\circ C$
- **units of:** temperature change
- **default units:** $\Delta^\circ C$
- **set:** globally
- **description:** This keyword sets the tolerance for convergence of temperature values in a time step in a transient run, if passes is set to zero.
- **discussion:** Chapter 5

**tol_tres**

- **argument:** real value, greater than zero.
- **default:** $(end - start) / 10^6$
- **units of:** time
- **default units:** years
- **set:** globally
- **description:** This keyword sets the tolerance for convergence of the groundwater residence time equation over a time step in a transient run, if residence_time is set to on and passes is set to zero.
- **discussion:** Chapter 5
tres_increase
  a.k.a.: eps_tres
  argument: real value, greater than zero
  default: value set for keyword dt_max
  units of: time
  default units: years
  set: globally or by strat unit
  description: This keyword sets the greatest increase in groundwater residence time the program will allow over a time step, as calculated by the rate of increase in this variable over the previous step. Keyword applies to transient runs in which residence_time is set to on.
  discussion: Chapter 5

TTI
  argument: on, off, discrete, or continuous
  default: off
  set: globally
  description: Setting this option on causes the program, during transient runs, to calculate the time-temperature index for sediments in the basin. Two calculation methods are available. You choose the discrete method by default when you set on. The continuous option specifies a method which produces smoother contours and curves than generated by the discrete method.
  discussion: Chapter 6

under_relax
  a.k.a.: u_relax
  argument: real value in range zero to 1
  default: 1
  units: none
  set: globally
  description: Under-relaxation slows the rate at which temperature and salinity values change as the program seeks a steady-state solution. The program does not apply under-relaxation to equations being solved in one dimension (the vertical options for the temperature and salinity keywords). Setting small values decreases the rate of change; a value of 1 applies no under-relaxation.
  discussion: Chapter 5
**viscosity**
- argument: variable, constant, batzle-wang, or a real value
- default: variable
- units of: viscosity
- default units: cp
- set: globally
- description: Use this option to set fluid viscosity to a constant value or to let the program calculate viscosity from the fluid’s temperature and salinity (the variable or batzle-wang options). The argument constant implies a viscosity of 1 cp.
- discussion: Chapter 3

**vitrinite**
- argument: on or off
- default: off
- set: globally
- description: Set this option on, during transient simulations, to use the LLNL model for calculating the vitrinite reflectance of basin sediments.
- discussion: Chapter 6

**water_depth**
- a.k.a.: dep_wat, dep_wtw
- argument: real value
- default: zero
- units of: length
- default unit: km
- set: globally or by strat unit and/or well
- description: This keyword sets water depth along the cross section. Negative values represent emergence of the cross section above sea level; you use negative water depths to specify the nature of topographic relief. This boundary condition, when set within a strat block, applies at the unit’s $t_{dep}$ rather than over its entire interval of deposition.
- discussion: Chapter 4
well()
  a.k.a.: commonly abbreviated to \( w() \)
  arguments: well index or indices, and list of values corresponding to column headings.
  description: Use well() statements to set assignments within a column block. Wells are indexed according to the order in which positions are set on the \( x_{well} \) command(s). A well index, or a range or list of indices (e.g., \( 2:4, 1, 3, 4 \), or \( 6: \)), appears within the parentheses. The rest of the line contains values corresponding to the keywords and units set on the previous column command.
  discussion: Chapter 4

well_name
  argument: list of names, each enclosed within single quotes.
  default: none
  set: globally
  description: Use the well_name statement to set a label for each well across the cross section. The names are passed to B2plot for annotating cross-section plots. Labels are given in the same order as well positions in the \( x_{well} \) command. You may use commas or plus signs to separate names. If you have too many values to fit on a line, continue onto the next line with a backslash or use additional well_name statements.
  discussion: Chapter 4

width
  argument: real value, positive
  default: the position of the right-most well
  units of: distance
  default units: km
  set: globally
  description: Use this keyword to specify the width of the basin. The value set must be at least as large as the position \( (x_{well}) \) of the right-most well.
  discussion: Chapter 4
**X_average**

*a.k.a.:* kxmodel, kxmodl  
*argument:* arithmetic, geometric, harmonic, or special  
*default:* arithmetic  
*units:* none  
*set:* globally or by strat unit and/or well  
*description:* This keyword specifies the averaging technique to be applied along the x-direction in strat units composed of more than one rock type. Each argument is a technique used to determine the permeability, thermal conductivity, and dispersion coefficient of nodal blocks. The special option, which is outdated, sets an arithmetic average where a unit contains at least 30% sandstone (rock type ss) and sets a geometric average elsewhere. The preferred method is to vary the averaging technique along the cross section using a column block.

*discussion:* Chapter 4

**X_rock()**

*a.k.a.:* commonly abbreviated to X()  
*argument:* real value in the range zero to 1  
*default:* zero  
*units:* none  
*set:* globally or by strat unit and/or well  
*description:* This option controls the volume fraction of each rock type within a strat unit. The rock type’s label of one to three characters appears within the parenthesis (e.g., \(X(ss) = 50\%\)). The volume fractions for each strat unit must sum to 1 everywhere along the cross section. You do not need to specify \(X_{rock}\) values for strata with zero or negative thickness values (i.e., hiatuses in deposition or intervals of erosion).

*discussion:* Chapter 4
**x_well**

**argument:** unit in parentheses (optional), and list of positive real values

**default:** none

**units of:** length

**default unit:** km

**set:** globally

**description:** Use the `x_well` statement to specify the position of each well across the cross section. Position is measured from zero at the left of the cross section. Set units by placing the unit name in parentheses following the `x_well` keyword and before the position values (e.g., `x_well (mi) 10 20 30`). You may use commas or plus signs to separate the position values. If you have too many values to fit on a line, continue onto the next line with a backslash or use additional `x_well` statements.

**discussion:** Chapter 4

**y_LHS**

**argument:** real value, greater than zero

**default:** 1 cm

**units of:** length

**default units:** cm

**set:** globally

**description:** Use this option to set the \( y \)-thickness of the cross section at its left-hand side. Use `y_LHS` and `y_RHS` to make a wedge-shaped cross section.

**discussion:** Chapter 6

**y_max**

**argument:** real value, greater than zero

**default:** 1 cm

**units of:** length

**default units:** cm

**set:** globally

**description:** Use this option to set the maximum \( y \)-thickness allowed along the cross section. Use `y_max` to make a partial wedge (i.e., a wedge over part of the cross section).

**discussion:** Chapter 6
**y_min**

- **argument:** real value, greater than zero
- **default:** 1 cm
- **units of:** length
- **default units:** cm
- **set:** globally
- **description:** Use this option to set the minimum $y$-thickness allowed along the cross section.
- **discussion:** Chapter 6

**y_RHS**

- **argument:** real value, greater than zero
- **default:** 1 cm
- **units of:** length
- **default units:** cm
- **set:** globally
- **description:** Use this option to set the $y$-thickness of the cross section at its right-hand side. Use $y_{LHS}$ and $y_{RHS}$ to make a wedge-shaped cross section.
- **discussion:** Chapter 6

**Z_average**

- **a.k.a.:** kzmodel, kzmod1
- **argument:** arithmetic, geometric, harmonic, or special
- **default:** harmonic
- **units:** none
- **set:** globally or by strat unit and/or well
- **description:** This keyword specifies the averaging technique to be applied along the $z$-direction in strat units composed of more than one rock type. These averaging techniques are used by Basin2 to determine the permeability, thermal conductivity, and dispersion coefficient of nodal blocks. The outdated special option for $Z_{average}$ is the same as for $X_{average}$.
- **discussion:** Chapter 4
## Appendix 2 Units Recognized

### About Basin2 units

Basin2 recognizes the following units in assignment and column statements. Unit names may appear in upper or lower case, and embedded underscores are ignored. To set a reciprocal unit, precede the unit name by a slash (e.g., /km or /hour).

### Basin2 units

<table>
<thead>
<tr>
<th>Unit</th>
<th>Keyword(s)</th>
<th>Conversion</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Length</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>meters</td>
<td>m</td>
<td>–</td>
</tr>
<tr>
<td>centimeters</td>
<td>cm</td>
<td>$ \times 10^{-2}$</td>
</tr>
<tr>
<td>kilometers</td>
<td>km</td>
<td>$ \times 10^3$</td>
</tr>
<tr>
<td>inches</td>
<td>in</td>
<td>$ \times 0.0254$</td>
</tr>
<tr>
<td>feet</td>
<td>ft</td>
<td>$ \times 0.3048$</td>
</tr>
<tr>
<td>miles</td>
<td>mi</td>
<td>$ \times 1609.344$</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Centigrade, °C</td>
<td>C</td>
<td>–</td>
</tr>
<tr>
<td>Fahrenheit, °F</td>
<td>F</td>
<td>$ -32 \times \frac{5}{9}$</td>
</tr>
<tr>
<td><strong>Temperature change</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta$°C</td>
<td>delta_C</td>
<td>–</td>
</tr>
<tr>
<td>$\Delta$°F</td>
<td>delta_F</td>
<td>$ \times \frac{5}{9}$</td>
</tr>
<tr>
<td><strong>Time</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>seconds</td>
<td>sec, secs, second, seconds</td>
<td>–</td>
</tr>
<tr>
<td>minutes</td>
<td>min, mins, minute, minutes</td>
<td>$ \times 60$</td>
</tr>
<tr>
<td>hours</td>
<td>hr, hrs, hour, hours</td>
<td>$ \times 3600$</td>
</tr>
<tr>
<td>days</td>
<td>day, days</td>
<td>$ \times 86400$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>years</td>
<td>yr, yrs, year,</td>
<td>$\times 31.5576\times 10^6$ years</td>
</tr>
<tr>
<td>millions of years</td>
<td>my, m.y.</td>
<td>$\times 31.5576\times 10^{12}$</td>
</tr>
<tr>
<td>billions of years</td>
<td>by, b.y.</td>
<td>$\times 31.5576\times 10^{15}$</td>
</tr>
</tbody>
</table>

**Pressure**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>atmospheres</td>
<td>atm</td>
<td></td>
</tr>
<tr>
<td>bars</td>
<td>bar</td>
<td>$\times .9869233$</td>
</tr>
<tr>
<td>psi</td>
<td>psi</td>
<td>$\times .0680460$</td>
</tr>
<tr>
<td>megapascals</td>
<td>MPa</td>
<td>$\times 9.869233$</td>
</tr>
</tbody>
</table>

**Heat flow**

<table>
<thead>
<tr>
<th></th>
<th>HFU</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat flow units</td>
<td>cal/cm² sec</td>
<td>$\times 10^6$</td>
</tr>
<tr>
<td>milliwatts/m²</td>
<td>mW/m²</td>
<td>$\times 0.0239006$</td>
</tr>
</tbody>
</table>

**Energy/mole**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Joule/mole</td>
<td>J/mol</td>
<td></td>
</tr>
<tr>
<td>kiloJoule/mole</td>
<td>kJ/mol</td>
<td>$\times 10^3$</td>
</tr>
<tr>
<td>calories/mol</td>
<td>cal/mol</td>
<td>$\times 4.184$</td>
</tr>
</tbody>
</table>

**Density**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>g/cm³</td>
<td>g/cm³</td>
<td></td>
</tr>
<tr>
<td>kg/cm³</td>
<td>kg/m³</td>
<td>$\times 10^{-3}$</td>
</tr>
<tr>
<td>pound/in³</td>
<td>lb/in³</td>
<td>$\times 27.67$</td>
</tr>
<tr>
<td>pound/ft³</td>
<td>lb/ft³</td>
<td>$\times .01601$</td>
</tr>
</tbody>
</table>

**Permeability**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>darcy</td>
<td>darcy</td>
<td></td>
</tr>
<tr>
<td>μm²</td>
<td>μm²</td>
<td>$\times 1.01316$</td>
</tr>
<tr>
<td>cm²</td>
<td>cm²</td>
<td>$\times 1.01316\times 10^8$</td>
</tr>
<tr>
<td>m²</td>
<td>m²</td>
<td>$\times 1.01316\times 10^{12}$</td>
</tr>
<tr>
<td>square inches</td>
<td>in²</td>
<td>$\times 6.53660\times 10^8$</td>
</tr>
<tr>
<td>square feet</td>
<td>ft²</td>
<td>$\times 9.41260\times 10^{10}$</td>
</tr>
</tbody>
</table>

**Log permeability**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>log darcy</td>
<td>log_darcy</td>
<td></td>
</tr>
<tr>
<td>log μm²</td>
<td>log_um²</td>
<td>+.00568</td>
</tr>
<tr>
<td>log cm²</td>
<td>log_cm²</td>
<td>+ 8.00568</td>
</tr>
<tr>
<td>log m²</td>
<td>log_m²</td>
<td>+ 12.00568</td>
</tr>
<tr>
<td>log square inches</td>
<td>log_in²</td>
<td>+ 8.81535</td>
</tr>
<tr>
<td>log square feet</td>
<td>log_ft²</td>
<td>+ 10.97371</td>
</tr>
</tbody>
</table>

**Thermal conductivity**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>cal/cm·sec °C</td>
<td>cal/cm·secC</td>
<td></td>
</tr>
<tr>
<td>Joules/cm·sec °C</td>
<td>J/cm·secC</td>
<td>$\times .239006$</td>
</tr>
</tbody>
</table>

**Heat capacity**
calories/gram °C \( \text{cal/g°C} \) –  
Joules/gram °C \( \text{J/g°C} \) \( \times 0.239006 \)

**NaCl salinity**

molality \( \text{molal} \) –  
parts per million \( \text{ppm} \) \( \times 10^3/(M_W (10^6 – \text{ppm})) \)
mg/kg solution \( \text{mg/kg} \) \( \times 10^3/(M_W (10^6 – \text{mg/kg})) \)

\( M_W \) is NaCl molar weight, 58.4428 g/mol

**Isotope concentration**

molality \( \text{molal} \) –  
parts per million \( \text{ppm} \) \( \times 10^{-3} / M_W \)
mg/kg solution \( \text{mg/kg} \) \( \times 10^{-3} / M_W \)
dissolved gas volume \( \text{cm}^3 \text{STP/cm}^3 \) \( \times 10^3 / 22414 \)

\( M_W \) is 3.016 g/mol for \(^3\)He, 4.0026 for \(^4\)He, 35.968 for \(^{36}\)Cl, 35.968 for \(^{36}\)Ar, 39.962 for \(^{40}\)Ar

\(^1\)Important: unit conversions to molal are valid only for dilute fluids. When salinity is not small, use molal units to prescribe isotope concentrations accurately. The conversion to \(\text{cm}^3 \text{ STP/cm}^3\) further assumes that the fluid density is 1 g/cm\(^3\).

**Viscosity**

centipoise \( \text{cp} \) –  
poise \( \text{poise} \) \( \times 10^2 \)
grams/cm sec \( \text{g/cm sec} \) \( \times 10^2 \)

**Solute flux**

moles/cm\(^2\) sec \( \text{mol/cm}^2\text{sec} \) –  
moles/cm\(^2\) yr \( \text{mol/cm}^2\text{yr} \) \( \times 3.1688 \times 10^{-8} \)
Appendix 3 Mathematical Notation

About mathematical notation

The table below summarizes the mathematical notation used within this Guide.

Symbols used

\( \alpha_f \) Fluid isobaric coefficient of thermal expansion
\( \alpha_L, \alpha_T \) Longitudinal and transverse dispersivity
\( \beta \) Compressibility of a rock’s reducible pore volume
\( \beta_f \) Fluid isothermal coefficient of compressibility
\( \beta_{ul} \) Compressibility of reducible pore volume during unloading
\( \theta \) Time weighting variable
\( \Lambda_i \) Release factor for isotope \( i \)
\( \lambda_i \) Decay constant for isotope \( i \)
\( \mu \) Fluid viscosity
\( \rho \) Groundwater density
\( \rho_o \) Oil density
\( \rho_{sm} \) Bulk density of the saturated medium (sediment)
\( \sigma_E \) Effective stress
\( \sigma_i \) Neutron absorption cross-section for element \( i \)
\( \sigma_T \) Total stress
\( \sigma_{\text{max}} \) Greatest effective stress experienced at a point
\( \tau \) Hydrologic residence time
\( \tau_{i,j} \) A transmissivity between nodes \( i,j \) and \( i+1,j \)
\( \tau_{z_{i,j}} \) A transmissivity between node \( i,j \) and underlying node
\( \phi \) Sediment porosity
\( \phi_o \) Reducible porosity
\( \phi_i \) Irreducible porosity
\( \phi_{\text{min}} \) Minimum porosity experienced by a sediment
\( \Phi \) Hydraulic potential
\( \Phi_n \) Neutron flux within the medium
\( \chi \) Intermediate term in calculating fluid density
\( \chi_{UR} \) Under-relaxation variable
ψ  An arbitrary field variable
χ  Fraction of an element made up of isotope i
A, B, C, D, E, a1, a2, a3, c1, c2, c3  Regression coefficients
Ao  Pre-exponential factor in maturation models
A\textsubscript{1,4He}  Moles of \(^4\)He produced per \(\mu\)g of U, per year
A\textsubscript{1,40Ar}  Moles of \(^{40}\)Ar produced per \(\mu\)g of K, per year
A\textsubscript{1,\text{flux}}  Number of neutrons produced per \(\mu\)g of U, per year
A\textsubscript{2,4He}  Moles of \(^4\)He produced per \(\mu\)g of Th, per year
A\textsubscript{2,\text{flux}}  Number of neutrons produced per \(\mu\)g of Th, per year
b  Compaction coefficient
b\textsubscript{ul}  Compaction coefficient under conditions of unloading
C  Fluid salinity
CI  Concentration of an isotope
C\textsubscript{m}  Concentration of unreacted component m in vitrinite model
C\textsubscript{m}^0  Initial concentration of component m in vitrinite model
C\textsubscript{P}  Heat capacity
D\textsuperscript{*}  Diffusion coefficient
D\textsubscript{x}, D\textsubscript{z}  Coefficient of hydrodynamic dispersion along x and z
E\textsubscript{A}  Activation energy in maturation models
E\textsubscript{B\textsubscript{x}}, E\textsubscript{B\textsubscript{z}}  Buoyant forces for oil migration along x and z
E\textsubscript{H\textsubscript{x}}, E\textsubscript{H\textsubscript{z}}  Hydrodynamic forces for oil migration along x and z
f\textsubscript{m}  Stoichiometric coefficients for vitrinite model
F  Extent of reaction for vitrinite model
F\textsubscript{i}  Mass fraction of element i in the rock grains
g  Acceleration of gravity
i  Node index along x
i  Index for an element or isotope
j  Node index along z
J\textsubscript{i}  Production rate of isotope i, per gram of rock per year
J\textsubscript{i}^r  Production rate of isotope i from rock grains alone, expressed per gram of rock per year
J\textsubscript{k}  Anisotropy \(k_x/k_z\) in permeability
J\textsubscript{K}  Anisotropy \(K_x/K_z\) in thermal conductivity
k  Reaction rate constant in maturation models
k  As a subscript, mineral index
k\textsubscript{x}, k\textsubscript{z}  Permeability along and across stratigraphy
k\textsubscript{ave}  Averaged permeability
(k), (k+1)  Indices of iteration levels
K\textsubscript{H}  Hydraulic conductivity
K\textsubscript{ex}, K\textsubscript{z}  Thermal conductivity along and across stratigraphy
m\textsubscript{k}  Molal solubility of mineral k
M\textsubscript{F}  Molar volume of mineral
M\textsubscript{W}  Molar weight of a mineral, or atomic weight of an
<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n, n+1$</td>
<td>Indices of time levels</td>
</tr>
<tr>
<td>$N_i$</td>
<td>Number of atoms of element $i$ per gram of rock</td>
</tr>
<tr>
<td>$P$</td>
<td>Fluid pressure</td>
</tr>
<tr>
<td>$P_{atm}$</td>
<td>Atmospheric pressure</td>
</tr>
<tr>
<td>$P_H$</td>
<td>Hydrostatic pressure</td>
</tr>
<tr>
<td>$P_n$</td>
<td>Neutron production rate per gram of rock per year</td>
</tr>
<tr>
<td>$q_x, q_z$</td>
<td>Specific discharge along $x, z$</td>
</tr>
<tr>
<td>$q_A$</td>
<td>Adveective heat or solute flux</td>
</tr>
<tr>
<td>$q_D$</td>
<td>Solute flux due to diffusion and dispersion</td>
</tr>
<tr>
<td>$q_{iu}$</td>
<td>Conductive heat flux</td>
</tr>
<tr>
<td>$Q_x, Q_z$</td>
<td>Net flux of fluid, energy, or solute between nodal blocks</td>
</tr>
<tr>
<td>$R$</td>
<td>Gas constant</td>
</tr>
<tr>
<td>$R_i$</td>
<td>Production rate of isotope $i$, per volume of saturated sediment per year</td>
</tr>
<tr>
<td>$R_i^v, R_i^w$</td>
<td>Production rate of isotope $i$ from within the rock grains alone, or fluid phase alone, per unit volume of saturated medium per year</td>
</tr>
<tr>
<td>$R_o$</td>
<td>Vitrinite reflectance</td>
</tr>
<tr>
<td>$S_i$</td>
<td>Mass stopping power of element $i$</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$T_{1/2}$</td>
<td>The half-life of an isotope</td>
</tr>
<tr>
<td>$T_K$</td>
<td>Absolute temperature</td>
</tr>
<tr>
<td>$TDS$</td>
<td>Total dissolved solids</td>
</tr>
<tr>
<td>$TTI$</td>
<td>Time-temperature index of organic maturity</td>
</tr>
<tr>
<td>$v_x, v_z$</td>
<td>Fluid velocity along Cartesian $x, z$</td>
</tr>
<tr>
<td>$v_x', v_z'$</td>
<td>Fluid velocity along curvilinear $x, z$</td>
</tr>
<tr>
<td>$v_{on}$</td>
<td>Subsidence velocity</td>
</tr>
<tr>
<td>$V_k$</td>
<td>Dissolved volume of mineral $k$ per unit volume of groundwater</td>
</tr>
<tr>
<td>$X_{rk}$</td>
<td>Volume fraction of rock type in strata</td>
</tr>
<tr>
<td>$X_o$</td>
<td>Oil generated by bed as fraction of capacity</td>
</tr>
<tr>
<td>$Y_k$</td>
<td>Cementation by mineral $k$, as fraction of bed’s volume</td>
</tr>
<tr>
<td>$Y_{ih}, Y_{iU}$</td>
<td>Neutron yields of element $i$ per ppm of Th and U in the rock grains, per year</td>
</tr>
<tr>
<td>$z$</td>
<td>Depth below sea level</td>
</tr>
<tr>
<td>$Z$</td>
<td>Burial depth</td>
</tr>
<tr>
<td>$Z_E$</td>
<td>Effective burial depth</td>
</tr>
<tr>
<td>$Z_{max}$</td>
<td>Maximum $Z$ or $Z_E$ experienced by a sediment</td>
</tr>
</tbody>
</table>
Appendix 4 Transmissivities and Fluxes

About transmissivities and fluxes

Basin2 uses variables $\tau_x$ and $\tau_z$, known as transmissivities, to calculate net mass and energy fluxes among neighboring nodal blocks. The program carries three types of transmissivities: hydraulic transmissivities that give the volume flux of groundwater by Darcy flow, thermal transmissivities that give the heat flux due to conduction, and solute transmissivities that give the solute flux due to diffusion and hydrodynamic dispersion.

By convention, an $x$-direction transmissivity $\tau_x$ with indices $i,j$ applies to a lateral flux between nodes $i,j$ and $i+1,j$. A transmissivity $\tau_z$ along $z$ with indices $i,j$ applies to a vertical flux between node $i,j$ and its underlying node. The underlying node is indexed $i,j+1$ unless a hiatus (i.e., a stratigraphic unit of zero thickness) falls below $i,j$.

The net groundwater flux between nodes in cm$^3$/sec can be calculated from hydraulic transmissivity, pressure, and fluid density according to

$$Q_x = -\tau_x \left[ (P_{i+1,j} - P_{i,j}) - \frac{\rho_{i+1/2,j} g}{1.013 \times 10^6} (z_{i+1,j} - z_{i,j}) \right]$$

and

$$Q_z = -\tau_z \left[ (P_{i,j+1} - P_{i,j}) - \frac{\rho_{i,j+1/2} g}{1.013 \times 10^6} (z_{i,j+1} - z_{i,j}) \right]$$

(A4.1)

Here, pressure $P$ is in atm, $\rho_{i+1/2,j}$ and $\rho_{i,j+1/2}$ are averaged fluid densities in g/cm$^3$, $g$ is the acceleration of gravity (980.1 cm/sec$^2$), and $z$ is depth in cm.

In runs that take fluid density to be constant, the equations above can be rewritten in terms of hydraulic potential as

$$Q_x = -\tau_x \left( \Phi_{i+1,j} - \Phi_{i,j} \right)$$

and
\[ Q_i = -\tau_{z,ij} (\Phi_{z,jd} - \Phi_{z,i}) \]  

(A4.2)

where \( \Phi \) is in atm.

The conductive heat flux in cal/sec is given from temperature differences according to

\[ Q_i = -\tau_{x,ij} (T_{x1,i} - T_{x,i}) \]

and

\[ Q_j = -\tau_{x,ij} (T_{x,jd} - T_{x,j}) \]  

(A4.3)

where temperature \( T \) is in °C. Similarly, the solute flux due to diffusion and hydrodynamic dispersion is given in mol/sec from concentration differences as

\[ Q_i = -\tau_{z,ij} (C_{z1,i} - C_{z,i}) \]

and

\[ Q_j = -\tau_{z,ij} (C_{z,jd} - C_{z,j}) \]  

(A4.4)

where concentration \( C \) is given in mol/cm³.
Appendix 5 Bibliography and Further Reading

About literature references

The following literature references, selected from the many hundreds that have been published, provide a starting point for further reading on various aspects of basin modeling and its applications.

Basin2 and its application


---

**Basin hydrology**


Groundwater flow


Gridding and numerical solutions


Thermal maturation


### Hydrologic properties


**React geochemical software; mineral solubilities**


**Groundwater age**


**Isotope transport**


Torgersen, T., 1980, Controls on the pore-fluid concentration of $^4$He and
$^{222}$Rn and the calculation of $^{4}$He/$^{222}$Rn ages. Journal Geochemical.
Exploration. 13, 57–75.

Torgersen, T., M. A. Habermehl, F. M. Phillips, D. Elmore, P. Kubik, B.
G. Jones, T. Hemmick, and H. E. Gove, 1991, Chlorine 36 dating of very
old groundwater 3. Further studies in the Great Artesian Basin. Australia,
Water Resources Research 27, 3201–3213.

Zailowski, A., Kosanke, B.J., and Hubbard, N., 1987, Noble gas
composition of deep brines from the Palo Duro Basin, Texas.
Geochimica et Cosmochimica Acta 51, 73–81.

Zhao, X., T.L.B. Fritzel, H.A.M. Quinodoz, C.M. Bethke and T.
Torgersen, 1998, Controls on the distribution and isotopic composition of
helium in deep ground-water flows. Geology 26, 291–294.

Niger Delta

Burke, C. K., T. F. J. Dessauvagie and A. J. Whiteman, 1971, The
opening of the Gulf of Guinea and the geological history of the Benue

Bustin, R. M., 1988, Sedimentology and characteristics of dispersed
organic matter in Tertiary Niger delta: origin of source rocks in a deltaic
environment. American Association of Petroleum Geologists Bulletin 72,
227–298.

Evamy, B. D., J. Haremboure, P. Kamerling, W. A. Knaap, F. A. Molloy

Weber, K. J., 1971, Sedimentological aspects of oil fields in the Niger

Whiteman, A., 1982, Nigeria: its petroleum geology, resources, and
potential. Vols. 1 and 2, London, Graham, and Trotman, Ltd, 176 p. and
238 p.