**User guide of database conversion program for MIN3P**

|  |  |  |
| --- | --- | --- |
| File state：  [ x ] Manuscript  [ ] Revision  [ ] Released | File tag： |  |
| Version： | 1.0.26 |
| Authors： | Danyang Su |
| Date： | 2013/04/10 |
| Email: | [dsu@eos.ubc.ca](mailto:dsu@eos.ubc.ca); [danyang.su@gmail.com](mailto:danyang.su@gmail.com) |

Contents

[1. Introduction 3](#_Toc353397792)

[2. Input files 3](#_Toc353397793)

[1) Input parameter file 3](#_Toc353397794)

[3. Output files 6](#_Toc353397795)

[4. Installing and Running 7](#_Toc353397796)

[1) How to run the program: 7](#_Toc353397797)

[5. Important note 7](#_Toc353397798)

[1) Reaction of minerals 7](#_Toc353397799)

[2) Important notes for Phreeqc database 7](#_Toc353397800)

[a) Section label 7](#_Toc353397801)

[b) Data storage format 8](#_Toc353397802)

[c) Charge value 8](#_Toc353397803)

[d) Molecular weight 8](#_Toc353397804)

[e) Density of minerals 8](#_Toc353397805)

[f) Sample database for Phreeqc 8](#_Toc353397806)

# Introduction

Database conversion program for MIN3P is an efficient tool to convert geochemistry databases. Current version (V1.0.26) can convert Toughreact database, Crunchflow database and Phreeqc database to MIN3P database. It can aslo used to change the master variable for reactions, switch specified components and output specified data with pre-defined order.

# Input files

Input files include input parameter file (\*.inp), database files and alias file. The input parameter file and database files are indispensable while the alias file is optional.

|  |  |  |  |
| --- | --- | --- | --- |
| Type | File name | Description | Requirement |
| Input parameter file | Prefix.inp | General input parameters for database conversion. | Required |
| Database files | \*.\* | Database file of Toughreact, Crunchflow and Phreeqc. Path of these database should be specified in the input parameter file. | Required |
| Alias.dbs | Alias.dbs contains all the alias of the long name that cannot accepted by min3p. Original name and alias is seperated by semicolon ";". If the species name does not include blank space, you can also use blank space as a separator. | Optional |

## Input parameter file

!

!This input file contains parameters used in database conversion.

!This file is not case-sensitive.

!--------------------------------

**!Block 1: Database settings**

!--------------------------------

!set source database type, ***required.***

**source database type**

**phreeqc**

!crunchflow

!toughreact

!set source database path, ***required.***

**source database path**

**Phreeqc-1.dat**

!--------------------------------

**!Block 2: Conversion settings**

!--------------------------------

!Set target database temperature, ***required for Toughreact and Crunchflow*** database .

**target database temperature**

**25**

!Set target master variable, ***optional***. Can be h2(aq), o2(aq) or 'same as source database'.

!If not provided, use the same master variable in the source database.

!**Note 1**: if the target master variable is the same as the the master varialbe in the source database,

!you can comment out this command or provide ‘same as source database’.

!**Note 2**: this only works for toughreact and crunchflow database.

!For Phreeqc, please use "switch component" (bellow) instead.

**target database master variable**

**h2(aq)**

!o2(aq)

!Switch reaction component

!This is an extended function of change master variable. This switched component can be master specie,

!secondary sepcies, phases and any expression you wanted.

!The first line after the command line is the number of components that need to be switched and

!number of log\_k values. The data line start with switched component, followed by reaction equation

!and log\_k values.

!**Note 1**: The switched component should be in the first position in the left or right side of "=".

!The coefficient of the switched component should be 1..

!For the reaction, keep at least one blank space before the connector "+", "-", and "=".

!The first blank space and coefficient of 1.0 can be omitted.

!The reaction equation can be association or disassociation.

!Keep in mind that the sign of log\_k should be in correspondence with reaction direction.

!**Note 2**: The switched component should be in the right order. First come, first service.

!Example

! switch reaction component

! 1 4 ;number of components that need to be switched, number of logK (temperature points)

! H2(aq); H2(aq) = H2O - 0.5O2(aq); log\_k 50.4436 46.0719 40.94 36.1423 (A: correct)

! H2(aq); H2O - 0.5O2(aq) = H2(aq); log\_k -50.4436 -46.0719 -40.94 -36.1423 (B: correct)

! The above data (A and B) means reaction expressed by H2(aq) will be switched to O2(aq).

! The following is incorrect because H2(aq) is not in the first location and the coefficient is -2.0, not 1.

! H2(aq); O2(aq) = 2 H2O - 2H2(aq); log\_k 100.8872 92.1438 81.8800 72.2846 (C: incorrect)

**switch reaction component**

**4 1 ;number of components that need to be switched, number of logK (temperature points)**

**SiO2(OH)2-2; +1.000Si(OH)4 -2.000H+ = SiO2(OH)2-2; log\_k -23.1397**

**SiO(OH)3-; +1.000Si(OH)4 -1.000H+ = SiO(OH)3-; log\_k -9.80974**

**Al(OH)4-; +1.000Al+3 +4.000H2O -4.000H+ = Al(OH)4-; log\_k -22.8786**

**OH-; +1.000H2O -1.000H+ = OH-; log\_k -13.9998**

!--------------------------------

**!Block 3: Output settings**

!--------------------------------

!set target database type, ***required.***Currently the database type can only be min3p.

**target database type**

**min3p**

!Set targer database path, ***optional.***

!if not provided, use the current path as the output location.

**target database path**

**Phreeqc2min3p\_h2aq\_1**

!Sort the output data by ascending lexical order, ***optional***.

!This is useful when you need to compare the databases converted from different databases.

!**sort data by lexical order**

!Export the specied species only, ***optional***.

!This is useful when you need to compare the databases converted from different database.

!**export following species only**

!**3**

!**'species1**'

!**'species2**'

!**'species3'**

# Output files

Output files include the log file, the converted database file and name truncation data file.

|  |  |  |  |
| --- | --- | --- | --- |
| Type | File name | Description | Requirement |
| Log file | Prefix.log | Log file for database conversion. All the conversion information, warning and error messages can be found in this file | Required |
| Database files | \*.dbs | MIN3P database files. | Required |
| Name\_truncation.txt | This file contains all the truncated long name that cannot accepted by min3p. This file can be used to set alias file. | Optional |

# Installing and Running

The program is developed by Intel Visual Fortran for Windows. The program is a single executable file dbs\_conversion.exe that can run on Windows box. Double click the executable file or run through command line to start the program. Type in the input parameter file (\*.inp) to start database conversion.

## How to run the program:

1. Run the main program dbs\_conversion.exe, type in the input parameter file, e.g., “phreeqc2min3p.inp”.
2. The program will read in the input parameters and alias database (if exists) and then convert the database, write the output files. You may find warnings /errors during the first run.
3. Check the name truncation data. When the program find the name needs truncation, it will use the first 12 (can be specified in source codes) characters as the truncate name and output the original name and the truncate name into name\_truncation.txt file. You can see from the log files if there is duplicate truncate name or name conflict with the original name. Modify the truncate name to make the name readable and then copy all the name pairs into alias.dbs.
4. Rerun the main program, repeat the steps 1 to 3 until all the errors are resolved. When no error occurs, there will be no name–truncation pair in the file name\_truncation.txt.

**IMPORTANT: Be sure there is no error in the log file unless the error can be ignored. If there is error, try to fix it. The error information in the log file will help you.**

# Important note

## Reaction of minerals

By default, the program export all the reactions of mineral to “reversible “, you need to manually change it if the reaction is “irreversible” or others.

## Important notes for Phreeqc database

Toughreact database and Crunchflow database are well formatted that you do not need to change anything in the database. But Phreeqc database is so flexible that you need to add some label to the Phreeqc database before converting

### Section label

The format of Phreeqc database is so flexible that some keywords need to be **MANUALLY ADDED** to the database. These keywords are **NOT** case-sensitive and start with “#section:” (quotation mark “ is not included).

The following keywords are recognized: “#section: solution master species” , “#section: pmatch master species”, “#section: pmatch secondary master species”, “#section: gases”, “#section: minerals”, “#section: end”. Each section should end with “#section: end”.

### Data storage format

There are two formats of data storage in Phreeqc database. Data for the secondary species, gases, and minerals can be in the same line or in different lines, just keep the original format.

### Charge value

Not all the charge value of species/components is provided. In the conversion program, the charge value is estimated from the specie name in the database (e.g., nh4+, so3-2, ch4).

### Molecular weight

Not all the molecular weight of species/components is provided. The conversion program calculates the molecular weight following two steps.

(a) For the user-defined species/components, the molecular weight cannot be calculated by the specie name (e.g., Uranyl+2, AmmH+, where Urany and Amm are user-defined specie names). The program will search the section “#section: solution master species ” to extract molecular weight for the these specified species/components.

**Note**: To be strict, the name of user-defined species must contain at least two characters and cannot be the same as the name of elements in periodic table.

(b) For the “standard-expressed” species/components, the molecular weight is calculated from molecular formula (e.g., Ca+2, CaSO4(H2O)5, Uranyl(OH)2(H2O)2). The species should be in standard format, only alphabet (e.g, a to z and A to Z), number(e.g., 0-9, 1.5), user-defined names and bracket pair() are allowed. Molecular formula is **CASE-SENSITIVE** in calculating molecular weight, otherwise, the formula may not be recognized or the result may be incorrect. E.g., CaSO4:5H2O or CaSO4(h2o)5 is not allowed, use CaSO4(H2O)5 instead.

(c) For the mixed-format specie/component name such as AmmH+, the molecular weight is calculated by “Amm” plus “H”, both (a) and (b) are needed in calculation.

**Note**: When export to min3p database, all the names are converted to lower case.

### Density of minerals

Density of mineral is not available in Phreeqc database and this value is set to 1 g/cm3. You should **MANUALLY** modify this value if necessary.

### Sample database for Phreeqc

**#Section: SOLUTION\_MASTER\_SPECIES**

# elemen species alk gfw\_formula element\_gfw atomic

# number

H H+ -1.0 H 1.008 # 1

H(0) H2 0.0 H #

H(1) H+ -1.0 H #

E e- 0.0 0.0 0.0 #

O H2O 0.0 O 15.999 # 8

O(0) O2 0.0 O #

O(-2) H2O 0.0 O #

C HCO3- 1.0 C 12.011 # 6

C(+4) HCO3- 1.0 HCO3- #

Uraninite Uraninite 0.0 Uraninite 270.029

U U+4 -4.0 U 238.029

U(4) U+4 -4.0 U

#...

**#Section: End**

**#Section: PMATCH MASTER SPECIES**

H+ = H+

log\_k 0.0

-gamma 9.00 0.064

e- = e-

log\_k 0.0

H2O = H2O

log\_k 0.0

-gamma 0.00 0.0#64

HCO3- = HCO3-

log\_k 0.0

-gamma 5.40 0.064

Uraninite = Uraninite

log\_k 0.0

U+4 = U+4

log\_k 0

#...

**#Section: End**

#Section: PMATCH SECONDARY MASTER SPECIES

#format 1: all data in the same line

+1.000Al+3 +1.000SO4-2 = AlSO4+ ; -gamma 4.00 0.064 ; log\_K 3.900111 ; -analytical\_expression -59.74759294081 0 2048.61497066133 22.9451885920 0

+2.000H+ +2.000e- = H2 ; -gamma 0.00 0.0 ; log\_K -3.10597 ; -analytical\_expression -55.35493262717 0 2808.32060172984 20.0675686240 0

+2.000H2O -4.000H+ -4.000e- = O2 ; -gamma 0.00 0.0 ; log\_K -85.9855 ; -analytical\_expression -30.79426700990 0 -27925.53838584180 10.0321005086 0

#format 2: data in different lines

CO3-2 + 10 H+ + 8 e- = CH4 + 3 H2O

log\_k 41.071

delta\_h -61.039 kcal

-dw 1.85e-9

SO4-2 + H+ = HSO4-

log\_k 1.988

delta\_h 3.85 kcal

-analytic -56.889 0.006473 2307.9 19.8858 0.0

-dw 1.33e-9

**#Section: End**

**#Section: Gases**

#format 1: all data in the same line

CH4(g) ; CH4 = +1.000CH4 ; log\_K -2.8565 ; -analytical\_expression -89.63393582234 0 4440.29675525994 29.0478933816 0

H2S(g) ; H2S = +1.000HS- +1.000H+ ; log\_K -8.00993 ; -analytical\_expression 37.63799849734 0 -2225.98872774971 -15.4105293036 0

#format 2: data in different lines

CH4(g)

CH4 = CH4

log\_k -2.860

delta\_h -3.373 kcal

NH3(g)

NH3 = NH3

log\_k 1.770

delta\_h -8.170 kcal

**#Section: End**

**#Section: Minerals**

#format 1: all data in the same line

SiO2am ; SiO2 + 1OH- + 1H2O = SiO(OH)3- ; log\_K 1.475988 ; -analytical\_expression -2.14181238156 0 664.05554528339 0.5620295123 0

CSHtob1 ; (CaO)2(SiO2)2.4(H2O)3.2 + 1.2 H2O = 2 Ca++ + 2.4 SiO(OH)3- + 1.6OH- ; log\_K -19.1991 ; -analytical\_expression 240.84653128714 0 -13954.21726608490 -86.1775378224 0

#format 2: data in different lines

Melanterite

FeSO4:7H2O = 7 H2O + Fe+2 + SO4-2

log\_k -2.209

delta\_h 4.910 kcal

-analytic 1.447 -0.004153 0.0 0.0 -214949.0

Alunite

KAl3(SO4)2(OH)6 + 6 H+ = K+ + 3 Al+3 + 2 SO4-2 + 6H2O

log\_k -1.400

delta\_h -50.250 kcal

Uraninite

UO2 + 4H+ = U+4 + 2H2O

log\_k -4.88

log\_k 1.42 #biogenic uraninite

**#Section: End**