MIN3P Database Version Control

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MIN3P currently use ASCII format database. Any user can edit the database and run the simulation. This is a potential risk if the parameters in the database are changed and then passed to other users without notification since most users will not check whether the database is correct.

In the current approach, MD5 hashcode is used to verify the database version. This MD5 value is calculated based on the function implemented in MIN3P-TD code. It is not the same as the MD5 value of a file. Instead, only the valid value in the file (e.g., without empty lines) are used to calculate MD5.

When MIN3P simulation is launched, MD5 hashcode will be calculated for each database file and then compared against MIN3P database repository hosted on github. If a matched version is found, the version number and MD5 hashcode will be written to the log file and screen output. If no matched version if found, a warning information “***Caution: you are using a database not available in the repository.***” will be written before the MD5 hashcode.

# System requirements:

1. The operation system should have ‘wget’ executable file installed. ‘wget’ will be used to fetch version information from MIN3P database repository .

*https://raw.githubusercontent.com/Terradot/min3p-database/refs/heads/main/version.xml*

1. The operation system should have internet access.

If the above system requirements are not met, MIN3P code will continue to run. However, the database version information cannot be verified.

# Format of database version information

Database version information is saved in xml format, as shown below. The required fields are version id, description, path and md5 for each database. The version id and path should be unique.

<?xml version="1.0"?>

<database>

<version id="0.0">

<description>MIN3P default database</description>

<path>./default</path>

<md5>

<comp.dbs>F09EB4D1BC1B76196689C6B644C8C790</comp.dbs>

<complex.dbs>ED6C302EB390465F6EDC127D6C151ACF</complex.dbs>

<gases.dbs>5EF06A2FC632811FCF8F3746665AEB5D</gases.dbs>

<mineral.dbs>1C7E20164105949C9ADCC7174E346444</mineral.dbs>

<redox.dbs>85794CF5246ABE8BEBB2E2AE66B52282</redox.dbs>

<sorption.dbs>83A508EE DF72C52FD4B41E324577F8</sorption.dbs>

</md5>

</version>

<version id="0.1">

<description>MIN3P organic database</description>

<path>./organic</path>

<md5>

<comp.dbs>65F2C8F0723489564BF312A6F06419CA</comp.dbs>

<complex.dbs>CE7F55848E3575756E218F8BEA4C8B42</complex.dbs>

<gases.dbs>CEEE6191B632B617F779DC382867348A</gases.dbs>

<mineral.dbs> FBA21CE 8148383F214246364163F1</mineral.dbs>

<redox.dbs>B5CF94014599A2BF5BB5AE6DA2C91E6A</redox.dbs>

<sorption.dbs>EE2E771B1C8D93B467670868EB9BE3FE</sorption.dbs>

</md5>

</version>

</database>

# How to add database and version information

The database version information is saved as version.xml in the root folder of MIN3P database repository <https://github.com/Terradot/min3p-database>. Please note this is a public database so that database version information can be verified by any MIN3P users.

Step 1:

To add database version information, user needs to run the latest MIN3P code to calculate MD5 hashcode for each database file, which is available in the screen output and log file. An example is shown below:

Database version information

Caution: you are using a database not available in the repository.

comp.dbs, MD5: 6B9A213C6E9F41196F7CDA124AE2E207

complex.dbs, MD5: 916A3A2E2A15ACEDDFE9A10B8247A8AC

mineral.dbs, MD5: 82EF90BF62077B378912A11CCB8368DE

gases.dbs, MD5: 5EF06A2FC632811FCF8F3746665AEB5D

redox.dbs, MD5: 6D2EB4A9ACFA8104F481425B58264D83

sorption.dbs, MD5: 60C95F23A45B6FAF3C0CAFADDFEC1E1B

End of database version information

Because this is a new database, there is a warning information ‘Caution: you are using a database not available in the repository.’

Step 2:

Check MIN3P database from repository <https://github.com/Terradot/min3p-database>. Add the new database to the folder ./database and specify a new folder name, e.g., ./database/cdr\_database\_v1.

Edit version.xml file and add the MD5 hashcode value obtained in Step 1. User also needs to specify the version, description and path of the database. An example based on the above MD5 value is shown below.

<?xml version="1.0"?>

<database>

<version id="0.0">

<description>MIN3P default database</description>

<path>./database/default</path>

<md5>

<comp.dbs>F09EB4D1BC1B76196689C6B644C8C790</comp.dbs>

<complex.dbs>ED6C302EB390465F6EDC127D6C151ACF</complex.dbs>

<gases.dbs>5EF06A2FC632811FCF8F3746665AEB5D</gases.dbs>

<mineral.dbs>1C7E20164105949C9ADCC7174E346444</mineral.dbs>

<redox.dbs>85794CF5246ABE8BEBB2E2AE66B52282</redox.dbs>

<sorption.dbs>83A508EE DF72C52FD4B41E324577F8</sorption.dbs>

</md5>

</version>

<version id="0.1">

<description>MIN3P organic database</description>

<path>./database/organic</path>

<md5>

<comp.dbs>65F2C8F0723489564BF312A6F06419CA</comp.dbs>

<complex.dbs>CE7F55848E3575756E218F8BEA4C8B42</complex.dbs>

<gases.dbs>CEEE6191B632B617F779DC382867348A</gases.dbs>

<mineral.dbs> FBA21CE 8148383F214246364163F1</mineral.dbs>

<redox.dbs>B5CF94014599A2BF5BB5AE6DA2C91E6A</redox.dbs>

<sorption.dbs>EE2E771B1C8D93B467670868EB9BE3FE</sorption.dbs>

</md5>

</version>

<version id="0.2">

<description>MIN3P-TD cdr database v1</description>

<path>./database/ cdr\_database\_v1</path>

<md5>

<comp.dbs>6B9A213C6E9F41196F7CDA124AE2E207</comp.dbs>

<complex.dbs>916A3A2E2A15ACEDDFE9A10B8247A8AC </complex.dbs>

<gases.dbs>C5EF06A2FC632811FCF8F3746665AEB5D</gases.dbs>

<mineral.dbs>82EF90BF62077B378912A11CCB8368DE</mineral.dbs>

<redox.dbs>6D2EB4A9ACFA8104F481425B58264D83</redox.dbs>

<sorption.dbs>60C95F23A45B6FAF3C0CAFADDFEC1E1B</sorption.dbs>

</md5>

</version>

</database>

After new database folder and version information are added, user can merge the changes to the repository.

# Demonstration of database version information

If the database used in current simulation is same as one of the database version in the repository, the version information together with MD5 hashcode will be found in the log file and screen output. An example is shown below.

Database version information

Version: 0.0

comp.dbs, MD5: F09EB4D1BC1B76196689C6B644C8C790

complex.dbs, MD5: ED6C302EB390465F6EDC127D6C151ACF

mineral.dbs, MD5: 1C7E20164105949C9ADCC7174E346444

gases.dbs, MD5: 5EF06A2FC632811FCF8F3746665AEB5D

redox.dbs, MD5: 85794CF5246ABE8BEBB2E2AE66B52282

sorption.dbs, MD5: 83A508EE DF72C52FD4B41E324577F8

End of database version information

If no matched database version is found, or if there is no internet access to the database repository, user will get a warning information in the log file and screen output, together with MD5 hashcode for each database file. An example is shown below.

Database version information

Caution: you are using a database not available in the repository.

comp.dbs, MD5: 6B9A213C6E9F41196F7CDA124AE2E207

complex.dbs, MD5: 916A3A2E2A15ACEDDFE9A10B8247A8AC

mineral.dbs, MD5: 82EF90BF62077B378912A11CCB8368DE

gases.dbs, MD5: 5EF06A2FC632811FCF8F3746665AEB5D

redox.dbs, MD5: 6D2EB4A9ACFA8104F481425B58264D83

sorption.dbs, MD5: 60C95F23A45B6FAF3C0CAFADDFEC1E1B

End of database version information