If not specified, all the files are in the same location with the program.

**Update log:**

2012-12-20

1. Add additional format check in database conversion, output detail information if error is detected.
2. Blank line is ignored, whatever the location is.
3. Modify bug in reading AKCOP optional dataset.
4. Add support to the name includes blank space.
5. Update alias database format. Use semicolon “;” as separator. Blank space can be used as a separator only if the species name does not include blank space.
6. Update output format of truncation name list, separated by semicolon “;” instead of blank space.

**Files input:**

1. Touthreact database, e.g., “thermoddem.txt”
2. Alias database , e.g., “alias.dbs”. This file contains all the alias of the long name that cannot accepted by min3p. File is optional. 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.

**Files output:**

1. Log file, e.g., “thermoddem.log”. File name is the generated by program, the same with toughreact database.
2. Component database of min3p, “ comp.dbs”.
3. Complex database of min3p, “complex.dbs”.
4. Gases database of min3p, “gases.dbs”.
5. Mineral database of min3p, “mineral.dbs”.
6. Redox database of min3p, “redox.dbs”. At present, all the aqueous species in toughreact database go into complex database in min3p.
7. Name truncation data, “name\_truncation.txt”.

**Output information:**

1. Warning. The program can give out the following warning information:
2. (a) name conflicts in alias.dbs, if the name and alias conflict with each other, the conflict name or alias will be ignored;
3. (b) name conflicts in name truncation data, this information indicates that the automatic truncation (e.g., the first 12 characters) generate the same alias name or the alias name is the same with the origional full name;
4. (c) number of components exceeds 5. In toughreact, the number of reactant or product may exceeds 5, but in min3P, the maximum number of reactant or product is five (see from database write format in min3p user manual). In this case, only 5 reactant or product are exported to min3p database. This warning can be treated as error.
5. Errors. The program can give out the following error information:
6. File open/write error;
7. Name error in reading toughreact database. This error occurs when the program find the name has already been used as an alias in alias.dbs.

Please see the log file for the detail information

Sample of Errors:

For example, minerals "hsaponite(feca)" and "hsaponite(fek)" will have the same truncated short name "hsaponite(fe" if not using alias. In the log file, the following information can be found:

---

Name truncation: hsaponite(feca) to hsaponite(fe

New name and truncation added: hsaponite(feca) hsaponite(fe

...

Error(ignored): Truncate name duplicated, the same truncate name already exist: hsaponite(fe

New name and truncation added: hsaponite(fek) hsaponite(fe

---

And in the mineral.dbs, you will find the two minerals with the same name but different parameters

---

!

! hsaponite(fe

! equilibrium constant, gram formula weight from TOUGHREACT database and enthalpy change is set to 0

'hsaponite(fe'

'surface'

497.4140 2.2570

7 'h+1' -1.340 'ca+2' 0.170 'mg+2' 2.000 'h2o' 3.790 'alo2-' 0.340 'hsio3-' 3.660 'feoh+' 1.000

'reversible' 29.5008 0.0000

!

! hsaponite(fe

! equilibrium constant, gram formula weight from TOUGHREACT database and enthalpy change is set to 0

'hsaponite(fe'

'surface'

459.0360 2.5656

7 'h+1' -1.340 'h2o' 1.300 'k+' 0.340 'mg+2' 2.000 'alo2-' 0.340 'hsio3-' 3.660 'feoh+' 1.000

'reversible' 28.7034 0.0000

---

You should manually change the truncated name and add "long name-truncated name" to alias.dbs.

**IMPORTANT: Be sure there is no error in the log file.**

**How to run the program:**

1. Run the main program dbs\_conversion.exe, type in the toughreact database name, e.g., “thermoddem.txt”.
2. The program will read in the toughreact database 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.