Setting Up THAMES v5.0 Input

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This document provides guidance on how to prepare input files for THAMES v5.0. Special attention is given to common pitfalls to avoid and some troubleshooting recommendations for fixing improper input files.

1 Software Requirements

The following software must be installed and running properly on your computer:

- GEMS3K standalone library 3.4.1: http://gems.web.psi.ch/GEMS3K/downloads/index.html
- THAMES v5.0: https://github.tamu.edu/jwbullard/THAMES.git
- (Optional) GEM-Selektor 3.6.0 or 3.7.0: http://gems.web.psi.ch/GEMS3/downloads/index.html

2 Categories of THAMES Input

Throughout this document, it will be assumed that your THAMES simulation will happen in a working directory called `$WORKDIR`.

THAMES requires three categories of input files:

1. The initial 3D microstructure of the material system
2. Thermodynamic data input files produced by GEM-Selektor
3. Microstructure input file and file linking microstructure phases to GEM phases

4. Files to specify calculation times and microstructure output times
5. (Optional) File containing standard input to redirect to the program

Each of these will be detailed in the following sections.

2.0.1 Microstructure initial 3D arrangement

The microstructure representation is a digitized 3D image with `X_Size` voxels in the x direction, `Y_Size` in the y direction, and `Z_Size` in the z direction. Each voxel is a physical dimension of `Image_Resolution` in micrometer units. This is a normal ASCII text file. The first few lines of an example microstructure are given below.

```
#THAMES:Version: 5.0
#THAMES:X_Size: 100
#THAMES:Y_Size: 100
#THAMES:Z_Size: 100
#THAMES:Image_Resolution: 1.0
1
1
1
2
1
2
1
.
.
.
```

The meaning of the five lines of header information follows:

- `#THAMES:Version` is the THAMES version with which these data should be compatible. It is not currently used in the code but is only for informational purposes;
- `#THAMES:X_Size`, `#THAMES:Y_Size`, and `#THAMES:Z_Size` are the system dimensions, in voxel units, in all three Cartesian directions;
- `#THAMES:Image_Resolution` is the linear dimension of each cubic voxel, in μm units.

After the five-line header to this file, each line contains a single integer corresponding to the ID of one of the microstructure phases (not the GEM phases). The rows have a `z-y-x` nesting convention, by the first voxel is $(0, 0, 0)$, the x coordinates vary most quickly and the z coordinates vary most slowly.

One way to generate such a file is to create a virtual 3D microstructure using VCCTL, which produces a `.img` file in much the same format as just shown. However, the VCCTL phase ID numbers (Table 1) are different than the ones required by THAMES. Therefore, one must replace the VCCTL ID numbers with the corresponding THAMES microstructure id numbers. A C program called `vcctl2thames` has been provided to assist with this, but the program may need to be edited as needed to be consistent with the THAMES microstructure definition file described later in this document.

Table 1: VCCTL 9.5 phase identification numbers

Phase	ID	Phase	ID	Phase	ID
Water	0	Gypsum	7	$Ca(OH)_2$	19
Void	55	Bassanite (Hemihydrate)	8	C−S−H	20
Alite	1	Anhydrite ($CaSO_4$)	9	C_3AH_6	21
Belite	2	Silica Fume	10	Ettringite	22
C_3A	3	Inert	11	$Fe(OH)_3$	25
C_4AF	4	Silica glass	16	Pozzolanic C−S−H	26
K_2SO_4	5	Monosulfate	24	Friedel salt	29
Na_2SO_4	6	Monocarboaluminate	34	$CaCl_2$	28
$CaCO_3$	33	Strätlingite	30	Brucite	35

2.1 Thermodynamic data input

THAMES 5.0 comes with the thermodynamic data files you will need to run most of the simulations you want. This includes systems with temperatures ranging from 283 K to 333 K and including most of the important components of portland cement, portland limestone cement, and oil well cement. It also includes most of the iron sulfides needed for simulations involving pyrrhotite oxidation, as well as some common supplementary cementitious materials (SCMs) including silica fume and proxies for the main glassy and crystalline phases found in fly ashes. A full list of all the phases included can be found in the appendix.

The thermodynamic data files can be found in any of the various test cases provided with THAMES 5.0, located in subfolders of the `tests` folder:

- `alite-298K-sealed-wc35`
- `highvolume-silicafume`
- `PC-Carbonate-200`
- `PC-FlyAsh-200`
- `portcem-298K-sat-wc45`
- `portcem-298K-sealed-alk-wc45`
- `portcem-298K-sealed-wc45`
- `pyrragg-298K-sat`
- `pyrrcem-296K-sat`

The first seven test cases in this list all have the exact same thermodynamic data files, a collection of five files that all start with `thames-` The last two test cases have data files that contain chlorinated phases such as Friedel's salt and Kuzel's salt, but they do not contain the glassy and crystalline fly ash components.

If you need a system that cannot be modeled with these thermodynamic data files, you will need to use the GEM-Selektor software specified in Section 1 and follow its documentation for creating recipes and exporting data files.

2.1.1 Meaning of GEMS3K the File Contents

For normal usage of THAMES, one does not need to be concerned with most of the contents of the GEMS3K files. However, a few noteworthy items are as follows:

- The `-dat.lst` file contains that string that the GEMS3K library reads when performing a calculation so that it knows which other files contain the thermodynamic data it needs to run.
- The `-dch.dat` file contains the names of the independent components in the `<ICNL>` field, the names of the dependent components in the `<DCNL>` field, and the names of the phases in the `<PHNL>` field. You will need these names when correlating microstructure phases with GEM phases. This file also contains the parameters needed to calculate the molar volumes and densities of the dependent components as a function of temperature and pressure.
- The `-dbr.dat` file contains information about the calculated state of the system calculated using GEM Selektor, such as the activity coefficients, and phase abundances. But these will change with subsequent calculations in THAMES and so they are not of concern in the great majority of cases.
- The `-ipm.dat` file contains information about the numerical parameters used in the calculations, and are not of immediate concern for using THAMES.

2.2 Simulation Parameters

2.2.1 Microstructure phase definition section

THAMES defines a collection of phases that can potentially be present in its 3D microstructure. These are called "(THAMES) microstructure phases," and they can be defined as one or more of the phases recognized in the thermodynamic data files from GEMS. For example, one microstructure phase could be defined for each of the multiple phases in AFm family that GEMS recognizes, or one microstructure phase could be defined as the collection of all of those AFm phases. The user has the liberty to define these microstructure phases, and it is not necessary to include every phase recognized by GEMS within the collection of microstructure phases. If you know that silica fume will never be present within your simulation, it does not need to be defined in any microstructure phase that you create. However, two non-negotiable microstructure phases **must** always be defined: *void space* and *electrolyte* (the aqueous pore solution).

The other information that must be given is the final age of the system to be simulated and the specific times that you want to output microstructure images. These are both given in units of days.

The file for specifying these simulation parameters in a JSON file, which you can name anything you want but which has a default name of `simparams.json`. The documentation for JSON syntax can be found at https://www.json.org. We will examine the typical contents of this file for a portland cement paste with some pyrrhotite included.

2.2.2 Environment section.

The first section is called `environment` and contains information about the curing conditions and any boundary conditions on the electrolyte composition. An example is shown below, with extra annotations that are not included in the actual JSON file

```
{
  "environment": {
    "temperature": 296.15,        # Curing temperature (K), required
    "reftemperature": 298.15,     # Reference temperature (K) for kinetics, required
    "saturated": 1,               # 1 = saturated pores, 0 = sealed pores,
    "electrolyte_conditions": [   # (optional)
      { "DCname": "Ca(CO3)@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "AlO2H@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "CaSiO3@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "Fe(CO3)@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "MgSiO3@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "KOH@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "Ca(SO4)@", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "K+", "condition": "initial", "concentration": 2.0e-6 },
      { "DCname": "SO4-2", "condition": "initial", "concentration": 1.0e-6 },
      { "DCname": "Na+", "condition": "initial", "concentration": 0.672 },
      { "DCname": "ClO-", "condition": "initial", "concentration": 0.672 }
    ],
  },
  .
  .
  .
}
```

The `temperature`, `reftemperature`, and `saturated` lines are required for every simulation. The `electrolyte_conditions` section is techincally optional, but it is a good idea to have it. The GEMS library used by THAMES is more likely to properly converge if there is at least a little bit of each independent component in the electrolyte at the beginning. As shown, this can be done by including small amounts of different dependent components (DCs) that contain the ICs.

The list of all available DCs can be found in the `DCNL` section of the thermodynamic DCH file (usually called `thames-dch.dat`). The required options for any electrolyte component are:

- `DCname`, must exacdtly match a name in the `DCNL` section of the `-dch.dat` file.
- `condition` can be "initial" if the component's concentration is to be set initially but can vary as the simulation proceeds, or "fixed" if the component's concentration is to remain at the same value throughout.
- `concentration` is the molal concentration for the component in units of moles per kilogram of water.

Please be aware that the net electrical charge of the electrolyte must be zero, and it is the user's reponsibility to ensure that the concentrations are set in a way to balance the charge. If the charge is **not** balanced, the simulation will throw an exception and exit.

2.2.3 Microstructure phase definitions

The next section is called `microstructure` and defines each of the phases (or collection of phases) that can potentially exist within the 3D microstructure. The characteristics of a microstructure phase definition are

- its name,
- a unique numerical identification number (id) (**Note** that each id appearing in the initial 3D microstructure image file must be equal to the numerical id for one of the microstructure phases defined here),
- whether or not it is considered to be part of the cementitious material or is some other component in the mixture,
- its relation to phases defined in the thermodynamic data,
- its internal, or "subvoxel" porosity (assumed to be zero if not given),
- its internal pore size distribution (optional),
- information about its kinetic behavior (more details to follow below), and
- the color it should have in visualizations produced by THAMES

The section opens with its name (microstructure) and the number of microstructure phases that are defined

```
"microstructure": {
  "numentries": 23,
  .
  .
  .
},
```

In this example there are going to be 23 microstructure phases defined. Remember that every phase in the microstructure must be defined here, but that not every phase defined here must appear in the microstructure. Immediately after the `numentries`, each phase is defined sequentially in a collection named `phases`.

The void phase. The first defined phase *must* be "Void" which is just empty porosity within the microstructure. This phase is unique because it is the only one that does not have any associated thermodynamic phase. The meaning of each entry is

```
  "phases": [
    {
      "thamesname": "Void",
      "id": 0,
      "cement_component": 0,
      "display_data": { "red": 0.0, "green": 0.0, "blue": 0.0, "gray": 0.0 }
    },
    .
    .
    .
  ],
},
```

The meaning of each entry is

- `thamesname` is any string in quotes to designate the phase. The void phase **must** be named `Void` and the pore solution phase **must** be named `Electrolyte`, but you are free to choose the names of all other microstructure phases.
- `id` is the unique numerical identification number, which must be a non-negative integer. The void phase **must** have `id` of 0 and the pore solution **must** have `id` of 1, but you are free to choose the `id` of all other microstructure phases. Just remember that the phase identificatino numbers in the 3D microstructure image file must correspond to the correct microstructure phase `id` here.
- `cement_component` is 1 for any phase that is solid and that belongs to the cementitious material, such as cement clinker phases, gypsum, alkali sulfates, free lime, *etc*, and is 0 for other phases such as void, electrolyte, silica fume, fly ash phases, and any solid hydration products such as C−S−H gel. This distinction is needed for internal calculations of water/cement ratio and water/solids ratio.
- `display_data` is a set of red/green/blue/gray values that specify the color of the phase in THAMES visualizations. Many microstructure phases, though not all, have default colors assigned already according to predefined `thamesname` names, so this entry is only needed if you are defining a new microstructure phase, changing the name of an existing phase, or if you wish to override the default color.

The electrolyte phase. The next phase after the void phase **must** be the pore solution, which has the name `Electrolyte`:

```
{
  "thamesname": "Electrolyte",
  "id": 1,
  "cement_component": 0,
  "gemphase_data": [
    {
      "gemphasename": "aq_gen",
      "gemdc": [
        { "gemdcname": "Al(SO4)+", "gemdcporosity": 1.0 },
        { "gemdcname": "Al(SO4)2-", "gemdcporosity": 1.0 },
        { "gemdcname": "Al+3", "gemdcporosity": 1.0 },
        { "gemdcname": "AlO+", "gemdcporosity": 1.0 },
        { "gemdcname": "AlO2-", "gemdcporosity": 1.0 },
        { "gemdcname": "AlO2H@", "gemdcporosity": 1.0 },
        .
        .
        .
      ],
    }
  ]
}
```

This phase definition starts just like the void phase, with a `thamesname`, a unique `id`, and the designation that it is **not** to be considered a cement component. After these three, there is a section called `gemphase_data` that tells THAMES how to relate this microstructure phase to one or more phases in the thermodynamic system definition (`-dch.dat` file).

- `gemphasename` is the name of the corresponding GEMS system phase found in the `PHNL` section of the `-dch.dat` file. It must match exactly.

- gemdc is a list of all the GEMS dependenct components (DCs) that are assigned to this GEM phase. Each entry has two characteristics:
  - gemdcname is the name of the DC, which must actually belong to the GEM phase and which must also exactly match the name in the DCNL section of the -dch.dat file. Note that these correspondences of GEM phases and GEM DCs are already set up in the -dch.dat file, but they are listed here primarily for solid solutions where the internal pore space of a phase may depend on its composition (see below).
  - gemdcporosity is the volume fraction of non-solid space associated with this DC. It must be a real number on the interval $[0, 1]$.

Note that the electrolyte phase has many DCs, one for each possible dissolved component; only a small fraction of them are shown here for brevity.

The names of all the DC components for a GEM phase must be placed within gemdc field, and there must be one of these fields for each GEM phase that you wish to link to the microstructure phase. In addition, the gemphasename must exactly match one of the <PHNL> entries in the -dch.dat file, and *all* of the DCs associated with that phase must immediately follow that phase as shown in this example. Determine which GEM DCs are associated with a given phase by consulting the <nDCinPH> field of the -dch.dat file.

To illustrate, Figure 1 shows a portion of a real -dch.dat file. In the figure, there are *nine* phases listed in the <PHNL> field and 26 DCs listed in the <DCNL> field. The numbers in the <nDCinPH> field relate the two. Notice that there are *nine* numbers in <nDCinPH>, one for each phase. The ordering of the numbers is the same as the ordering of phase names in the <PHNL> field. So there are 13 DCs in the first phase, which is aq_gen. In addition, those 13 DCs are the *first* 13 DCs in the <DCNL> list. Moving on, we see that there are three DCs in the next phase, which is gas_gen, and those three DCs are the next three after the first 13 in the <DCNL> list, namely 'H2', 'O2', and 'H2O' (the last being the water vapor molecule, not liquid water which is H2O@[1]

Solid microstructure phases. Solid microstructure phases may be "simple" (one phase, one DC, and possibly some impurities), "solid solution" (one phase, multiple DCs that may be present in any mole fraction to give a phase with nonstoichiometric composition, such as C−S−H gel), or "composite" (multiple thermodynamic phases combined for simplicity or computational efficiency).

An example of a "simple" microstructure phase is alite, which is usually a monoclinic form of tricalcium silicate (Ca_3SiO_5) with some impurities to stabilize the monoclinic polymorph.

```
{
  "thamesname": "Alite",
  "id": 2,
```

[1] In GEMS, the '@' symbol is reserved to designate a zero-charge liquid solvent or a zero-charge dissolved component. Gas molecules do not have this symbol even though they also have zero charge.

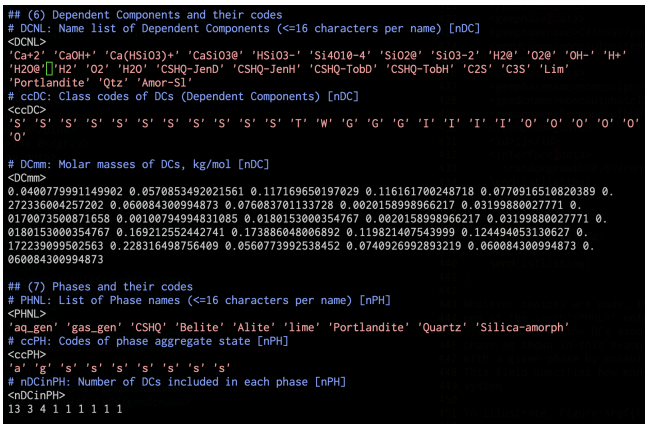

Figure 1: Portion of a DCH input file showing the definitions of GEM phases and DCs.

```
  "cement_component": 1,
  "interface_data": { }
  "gemphase_data": [
    {
      "gemphasename": "Alite",
      "gemdc": [{ "gemdcname": "C3S" }]
    }
  ],
  "impurity_data": {
    "k2ocoeff": 0.00087,
    "na2ocoeff": 0.0,
    "mgocoeff": 0.00861,
    "so3coeff": 0.007942
  },
  "kinetic_data": {
    .
    .
    .
  }
},
```

This entry indicates three more features of a solid phase, namely data about its interface with other phases, its impurity content, and its kinetic behavior:

- `interface_data` in the above entry for alite is empty, but can have information about the affinity the phase has for growing on one or more other substrate phases, using the name of the substrate phase and the thermodynamic contact angle between the two:
  - `affinityphase` must be the `thamesname` of another *microstructure* phase defined in this file
  - `contactangle` is the equivalent thermodynamic contact angle for the two phases in units of degrees, and must be a real number on the interval $[0, 180]$, where $0°$ is perfect wetting and $180°$ is complete nonwetting.

- `impurity_data` contains data on the amounts of four different possible impurities, namely potassium, sodium, magnesium, and sulfur, in terms of the *mole fractions* of their equivalent oxides, namely K_2O, Na_2O, MgO, and SO_3. Currently these are the only four impurities that are recognized by THAMES.
- `kinetic_data` is optional and will be described in detail in a later section. For now, the presence of this section indicates that the rates of reaction of this phase will be controlled by a kinetic rate equation. If this section is not provided, the amounts of this phase at any time will be determined solely by thermodynamic equilibrium as calculated by GEMS.

An example of a more complicated composite microstructure phase could be a collection of carbonated AFm phases, which would include all the monocarbonates, hemicarbonates, and tricarboaluminate phases:

```
{
  "thamesname": "AFmc",
  "id": 14,
  "cement_component": 0,
  "interface_data": {
    "affinity": [
      { "affinityphase": "Alite", "contactanglevalue": 180 },
    ]
  },
  "gemphase_data": [
    {
      "gemphasename": "C4Ac0.5H105",
      "gemdc": [{ "gemdcname": "hemicarb10.5" }]
    },
    {
      "gemphasename": "C4Ac0.5H12",
      "gemdc": [{ "gemdcname": "hemicarb" }]
    },
    {
      "gemphasename": "C4Ac0.5H9",
      "gemdc": [{ "gemdcname": "hemicarb9" }]
    },
    {
      "gemphasename": "C4AcH11",
      "gemdc": [{ "gemdcname": "monocarb" }]
    },
    {
      "gemphasename": "C4AcH9",
      "gemdc": [{ "gemdcname": "monocarb9" }]
    }
  ]
},
```

The absence of impurities or kinetic data in this example indicate that the phase is to be considered pure and that its amount in the microstructure at any time will be determined solely by thermodynamic equilibrium with the electrolyte. Also note that each of the DCs associated with this phase default to having zero porosity, so there will be no subvoxel or interhydrate porosity associated with this microstructure phase.

Finally, a solid solution with internal porosity can be defined, such as C−S−H gel:

```
{
  "thamesname": "CSHQ",
  "id": 11,
  "cement_component": 0,
  "interface_data": {
```

```
    "affinity": [
      { "affinityphase": "Alite", "contactanglevalue": 30 },
      { "affinityphase": "AFmc", "contactanglevalue": 90 },
    ]
  },
  "gemphase_data": [
    {
      "gemphasename": "CSHQ",
      "gemdc": [
        { "gemdcname": "CSHQ-JenD", "gemdcporosity": 0.4935 },
        { "gemdcname": "CSHQ-JenH", "gemdcporosity": 0.4935 },
        { "gemdcname": "CSHQ-TobD", "gemdcporosity": 0.2004 },
        { "gemdcname": "CSHQ-TobH", "gemdcporosity": 0.2004 },
        { "gemdcname": "KSiOH", "gemdcporosity": 0.1825 },
        { "gemdcname": "NaSiOH", "gemdcporosity": 0.1825 }
      ]
    }
  ],
  "poresize_distribution": [
    { "diameter": 0.23228, "volumefraction": 0.01684781722375019 },
    { "diameter": 0.49089, "volumefraction": 0.02276126023357459 },
    .
    .
    .
  ],
  "Rd": [
    { "Rdelement": "K", "Rdvalue": 0.42 },
    { "Rdelement": "Na", "Rdvalue": 0.42 }
  ]
},
```

Two more sections can be found in this example. First, the pore size distribution can be defined as a normalized probability density function, with the differential volume fraction (`volumefraction`, dimensionless) given for each effective pore size dimension (`diameter`) given in nanometer units. The second new section is the impurity partition section, with the name `Rd`, that describes the proportion of impurities that will be drawn from the surrounding electrolyte if available:

- `Rdelement` is the name of an independent component (IC) found in the `ICNL` section of the `-dch.dat` file.
- `Rdvalue` is the partition coefficient defined for alkalis by Hong and Glasser (*Cem Concr Res*, 29 (1999), 1893–1903; *Cem Concr Res*, 32 (2002), 1101-1111.) which is defined

$$R_{\mathrm{d}} = \frac{c_s w}{c_d s} \qquad (\text{units of } \mathrm{L\,kg^{-1}}) \tag{1}$$

  where c_s is the concentration of the impurity in the solid phase (units $\mathrm{mol\,L^{-1}}$), c_d is the concentration of the impurity in the electrolyte (units $\mathrm{mol\,L^{-1}}$), and w/s is the water-solids ratio in units of $\mathrm{L\,kg^{-1}}$

2.2.4 Calculation and output times

The final section of this file is called `time_parameters` and defines both the final age of the material to simulate and the simulation times at which THAMES should write data for visualization and for assessing the pore size distribution and saturation state. This section is fairly simple:

```
"time_parameters": {
  "finaltime": 56.0,
  "outtimes": [0.01, 0.1,0.5,1.0,3.0,7.0,14.0,28.0]
}
```

The meaning of the parameters are as follows:

- `finaltime` is the final time, in days, to attempt simulating the microstructure evolution. For various reasons the simulation may not complete the full requested age—for example, the microstructure could be completely depleted of electrolyte and so not be able to perform any other reactions—but the simulation will definitely stop after this time is reached.
- `outtimes` is a list of times, in days, at which THAMES should output the microstructure state, which includes
  - the full 3D microstructure image (an `.img` file),
  - a 2D image of a slice of the microstructure (both `.ppm` and `.png` files), and
  - the current pore size distribution and saturation state.