

Getting Started with F0AM

Note: It is recommended that new users read the F0AM_readme.pdf file as well.

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Using MATLAB

Users will need some knowledge of the MATLAB language and environment. At a minimum, new users should be familiar with:

- MATLAB desktop panes: Command Window, Editor, Workspace, Current Folder, Help Window
- The MATLAB search path
- Difference between a “script” and a “function”
- Variable classes: numerical arrays, character arrays (strings), logical arrays, cell arrays, structures
- Basic syntax: how to call a function, how to index an array, etc.

There are many resources available online and elsewhere for learning the basics. If nothing else, try typing “getting started” into the MATLAB help window search bar. Surprisingly enough, MATLAB Help is an excellent first stop for many questions.

Downloading F0AM

Presumably you have already figured this out if you are reading this file, but just in case...

1. Go to <https://sites.google.com/site/wolfegm/code-archive> and download the F0AM zip file.
2. Unzip the file and put the folder somewhere that you can remember.

Adding the Model to Your Search Path

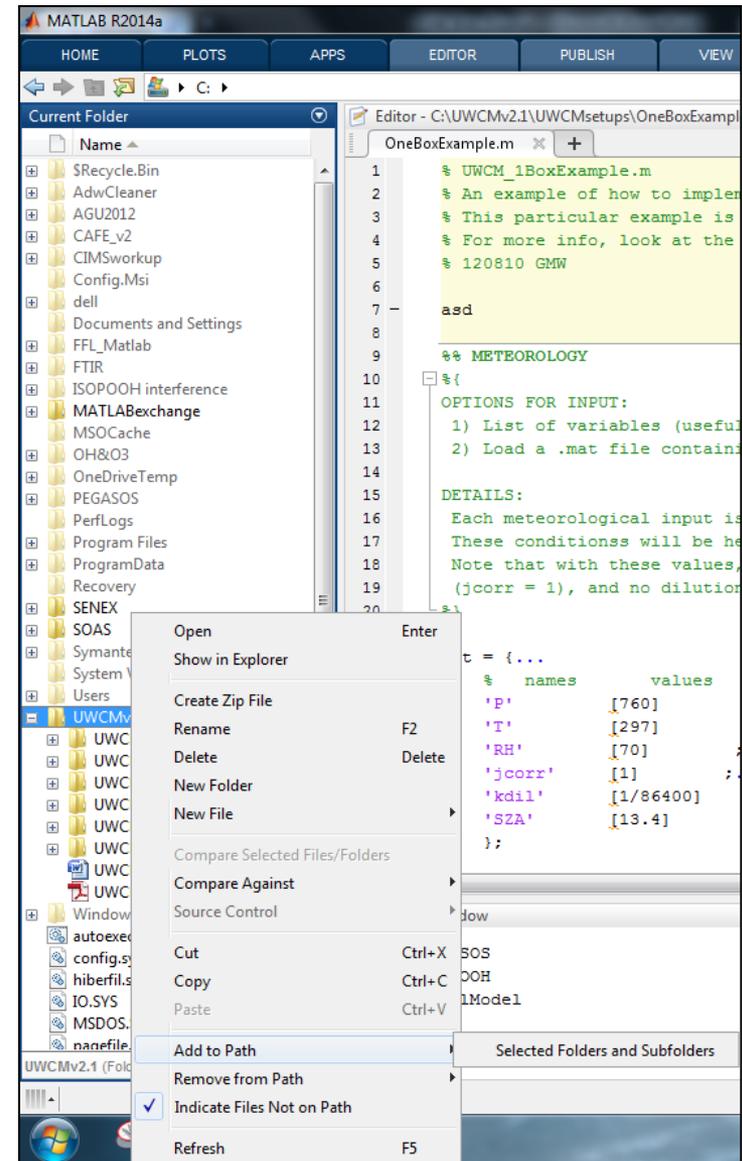
MATLAB can only “see” files that are on its search path. To add the model to your search path:

1. Navigate to the FOAM folder in the Current Folder window
2. Right click the folder → Add to Path → Selected Folders and Subfolders

Alternatively, you can add the model folders by entering the following in the command window:

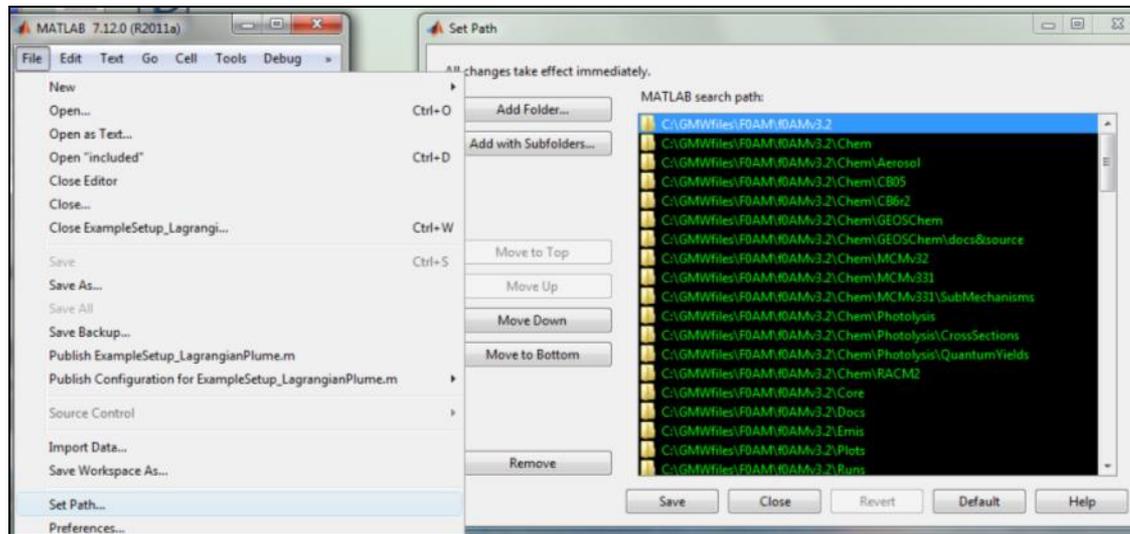
```
addpath(genpath(FOAMdir));
```

Here, *FOAMdir* is the full directory name, e.g. C:\Science\F0AMv3.1.



Notes on Search Paths

- You can see which folders are in your search path (and add/remove/rearrange them) by going into the file menu (top of screen) and choosing “Set Path...” to get to the Set Path Dialog.



- MATLAB resets the search path every time you restart it. If you want to keep the FOAM directories on your search path, type “savepath” (without quotes) into the command window or use the Set Path Dialog.
- MATLAB searches the folders in the set path sequentially. If you have multiple functions or scripts with the same name, only the first one (in the search path) will be called. If you think you have an error stemming from redundant file names, use the “which” command to see which file is being called.

Running the Examples

There are five example setup scripts in the Setups/Examples/ folder:

- ExampleSetup_Chamber.m
- ExampleSetup_DielCycle.m
- ExampleSetup_FlightSS.m
- ExampleSetup_LagrangianPlume.m
- ExampleSetup_MechCompare.m

The last example shows how to loop through multiple mechanisms before calling the FlightSS example, so ignore it for now.

Try to run one of the examples: type a script name into the Command Window and hit ENTER. Some of the examples can take several minutes to execute, depending on your hardware. The example should run without errors and generate a bunch of figure windows. Next, read through the example script that you ran and try to get an understanding of the inputs and outputs. The scripts are heavily commented to walk you through the setup. The FOAM_ReadMe is also helpful here.

Repeat for all examples.

Making your Own Setup Script

The example setups encompass a range of standard applications. Generally, it is easiest to start with the one that most closely matches your research problem and modify the inputs as needed.

Don't forget to save the new script under a different name!

Troubleshooting Setups

```
>> ExampleSetup_LagrangianPlume
INITIALIZING MODEL...
??? Error using ==> FOAM_ModelCore at 143
FOAM_ModelCore: ChemFiles input "FURFURAL_FURN" not found on search path.

Error in ==> ExampleSetup_LagrangianPlume at 150
S = FOAM_ModelCore(Met, InitConc, ChemFiles, BkgdConc, ModelOptions);

>>
```

Errors are not improbable when trying to run one of the examples, and they are even more likely when running your own setups. Learning to debug is part of becoming a proficient modeler. Keep calm and debug like so:

1. **Check for obvious errors first.** The error shown above is just a typo.
2. **Read the error message** and try to decipher the problem. MATLAB usually provides clues, and FOAM includes input checking to screen out common mistakes.
3. **Click the link** to go to the error location. Insert a breakpoint and run the code to this point, then look at the variables in the local workspace to find issues (wrong size, wrong type, NaNs, etc.).
4. **Ask someone for help**, but only after you've tried to debug yourself.

MCM Extraction

The MCM is big, and it is rare that users will need all of the species contained therein. You can extract a portion of the mechanism for use in FOAM as follows.

MCM Extraction

1. Go to the MCM website, <http://mcm.leeds.ac.uk/MCM/>
2. Near the top, click “Browse.”
3. Check all species that you want to include and click the “Add Selection to Mark List” button.
4. Species should then be added to the Mark List (note: may not work properly on all browsers).

The screenshot displays the MCM website interface. At the top, a navigation bar includes links for Home, Browse, Search, Extract, Download, Constraints, method, AlChem, Tools, Feedback, Links, Citation, Contributors, Funding, MCM v3.2, and CRI. The 'Browse' link is circled in red. Below the navigation bar, a 'Mark List' box is highlighted with a red oval, containing checkboxes for CH3OH and C2H5OH, along with 'Delete' and 'Clear' buttons. The main content area is divided into sections: 'Generic rate parameters' (with links for Complex rate coefficients, Simple rate coefficients, and Photolysis rates), 'Select a primary VOC' (with a grid of category links including Inorganic Section, Alcohols and Glycols, Aldehydes, Alkanes, Alkenes, Alkynes, Aromatics, Chloro and Hydrochlorocarbons, Diaalkenes, Esters, Ethers and Glycol Ethers, Hydrobromocarbons, Ketones, Monoterpenes, Sesquiterpenes, Organic Acids, and Unclassified), 'Inorganic Chemistry' (with links for Thermal gas-phase reactions, Gas-particle reactions, and Photolysis reactions), and 'Alcohols and Glycols' (with a list of species including METHANOL, ETHANOL, and 1-PROPANOL, each with a checkbox and its InChI string). The 'Check All' and 'Uncheck All' buttons are visible. The 'Add Selection to Mark List' button at the bottom right is also circled in red.

You can also add species using the search tools on the MCM website.

MCM Extraction

5. Near the top, click “Extract.”
6. Select “FACSIMILE input format.”
Also, check the “Include inorganic reactions?” box.
7. Click the “Extract” button to download the mechanism subset to a text file (mcm_subset .fac).
8. Give this file a more descriptive name and move it to somewhere on your MATLAB search path, e.g. FOAMv31\Chem\MCMv331\Alcohols.fac).

The screenshot shows the 'Extract Sub-Mechanisms' page of a web application. The navigation bar at the top includes 'Home', 'Browse', 'Search', 'Extract', 'Download', 'Construction method', 'AtChem', 'Tools', 'Feedback', and 'Links'. The 'Extract' link is circled in red. Below the navigation bar is a 'Mark List' section with checkboxes for 'CH3OH' and 'C2H5OH', and 'Delete' and 'Clear' buttons. The main heading is 'Extract Sub-Mechanisms', followed by a descriptive paragraph. A section titled 'Select the format in which you would like to generate the sub-mechanism:' contains several radio button options. The 'FACSIMILE input format, suitable for inserting into a FACSIMILE model.' option is circled in red. Below this is a link to a 'FORTRAN converter zip file'. Further down, a section titled 'Select which options you require:' contains a checked checkbox for 'Include inorganic reactions?' and an unchecked checkbox for 'Include generic rate coefficients? FACSIMILE, FORTRAN and KPP formats only'. Both checkboxes are circled in red. At the bottom, the instruction 'Click below to generate the sub-mechanism.' is followed by an 'Extract' button, which is also circled in red.

Home Browse Search **Extract** Download Construction method AtChem Tools Feedback Links

Mark List
 CH3OH C2H5OH Delete Clear

Extract Sub-Mechanisms

You can extract a subset of the MCM using your mark list as the set of primary species. All subsequent reaction mechanisms.

Select the format in which you would like to generate the sub-mechanism:

- HTML, displaying MCM species names.
- HTML, displaying SMILES strings.
- FACSIMILE input format, suitable for inserting into a FACSIMILE model.
- FORTRAN format, suitable for use with a FORTRAN numerical integrator.

Download the files needed to convert existing FACSIMILE files to FORTRAN compatible format or experimental [FORTRAN converter zip file](#).

- XML, experimental XML format.

View the Schema [mcm.xsd](#) against which the XML file can be validated.

- KPP, experimental KPP format.
- FACSIMILE with RDF metadata, experimental (CM).
- Molecular Weights for all species in a subset.

Select which options you require:

- Include inorganic reactions?
- Include generic rate coefficients? FACSIMILE, FORTRAN and KPP formats only

Click below to generate the sub-mechanism.

Extract

MCM Extraction

9. In the MATLAB command window, call the **FAC2FOAM** function, e.g.:

```
FAC2FOAM('Alcohols.fac')
```

This will create a script that contains properly formatted reactions, with the same name and in the same directory(e.g. Alcohols.m).

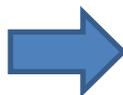
10. Add the mechanism to your ChemFiles input.

Note: DO NOT USE MULTIPLE MCM-EXTRACTED MECHANISMS SIMULTANEOUSLY!

This will lead to duplicate reactions.

TROUBLESHOOTING: the FAC2FOAM script will sometimes fail if the .fac file is not formatted properly, which can happen. In this case, you will need to scroll through the .fac file in a text editor and fix aberrant lines.

```
% 9.20D-12*0.39 : INDOOH + OH = INDO2 ;  
% J<41> : INDOOH = INDO + OH ;  
% 1.80D+13*(TEMP/298)@1.7*EXP(-4733/TEMP) : INDO = ACETOL + HOCH2CHO  
+ NO2 ;% 1.80D+13*(TEMP/298)@1.7*EXP(-4079/TEMP) : INDO = HCHO + HO2 +  
MVKNO3 ;% 5.60D-12 : INDOH + OH = INDHCHO + HO2 ;  
% J<41> : C590OH = C590 + OH ;  
% J<22> : C590OH = HOCH2CO3 + ACETOL + OH ;  
% 3.60D-12 : OH + C590OH = C5902 ;
```



```
% 9.20D-12*0.39 : INDOOH + OH = INDO2 ;  
% J<41> : INDOOH = INDO + OH ;  
% 1.80D+13*(TEMP/298)@1.7*EXP(-4733/TEMP) : INDO = ACETOL + HOCH2CHO + NO2 ;  
% 1.80D+13*(TEMP/298)@1.7*EXP(-4079/TEMP) : INDO = HCHO + HO2 + MVKNO3 ;  
% 5.60D-12 : INDOH + OH = INDHCHO + HO2 ;  
% J<41> : C590OH = C590 + OH ;  
% J<22> : C590OH = HOCH2CO3 + ACETOL + OH ;  
% 3.60D-12 : OH + C590OH = C5902 ;
```