AQcast: SCICHEM User’s Guide

Revision 3.1

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1. Introduction

AQcast: SCICHEM’s user interface (UI) allows novice and experienced users to more easily set parameters for a SCICHEM model run. The UI presents a set of simplified and default settings that a user can select which AQcast maps to the NAMELISTS input option for SCICHEM (i.e. *.inp, *.msc, *.scn files). This method allows the user more options for model input choices, and provides examples of standard selections, all of which can be set from the AQcast: SCICHEM UI. Once the user hits “Submit” all programs shown in Figure 1 are sent to an Amazon Web Services (AWS) queue for processing. The Results tab of the UI shows what parameters were submitted to the model run as well as the status of the run (i.e. SUCCESSFUL, FAILED, or RUNNING). An email is sent to the user once the run is completed, and a short summary and some vital plots are shown on the Results Tab. There is also a link to download a compressed file of all essential modeling input, intermediate, and output files (excluding the larger .puf, .ados, .dos, and .dep files, which can be downloaded upon request).

![Figure 1](image_url)

**Figure 1. AQcast: SCICHEM – Process Container Flow. (Orange boxes and arrows denote optional processes. Columns represent processes that are parallelized within AWS).**

2. Maps

Contained in the UI are two maps. The first map (example shown in Figure 2) in the UI is where the user can draw or upload files of their fence line and another for all building locations as well as see an overview of the facility location and sources input to be modeled. (Note: any area source will plot the center point provided and not show the full size of the source.) A fence line (or property line) can be added to be used by SCICHEM. The system will create receptor points along the fence line at 25-meter intervals and then include those receptor points in running SCIDOSPOST. (See “Section 6: Receptors” for more information.) Buildings can also be drawn or uploaded. All buildings are given a default height of...
3 meters which can be edited by clicking on each building. When “Submit” has been clicked, these shapefiles will be saved for use in a future run via a drop-down-menu on the UI shown in Figure 2. These respective files are saved with the project description in their name.

Open the map below to upload building/fenceline shapefiles in WGS84 projection or to draw buildings/fencelines on the map. Clicking a building will allow you to change its height (the default value is 3 meters). NOTE: To remove uploaded files, change the Previously Created dropdown below to ‘None’. Buildings/fencelines drawn on the map will take precedence over uploaded shape files.

Figure 2. AQcast: SCICHEM UI screenshot of fence line and building location interface.

The next map (example shown in Figure 3) in the UI is used for selecting the surface and upper air stations for processing METSCI. Clicking the “Find Closest Meteorological Sites” button will search the NOAA station list for the five closest surface sites with recent data including ASOS one-minute data and the five closest upper air sounding stations. The resulting sites will be shown on the map and are selectable by the user. When a previous project has been selected to load, click the “Find Closest Meteorological Sites” button and the NWS stations used in the previous project will be selected if MMIF or onsite options were not chosen. (Note: this option is not required, as stored WRF data, processed using MMIF, can be used instead. See “Section 6: Meteorology Options” for more information.)
3. Background Data

Background data on chemical concentrations is processed automatically using EPRI’s program CTM2SCICHEM. This program utilizes AQcast’s archived 3D EPA CMAQ data for CONUS at 12 km resolution. If NO₂ is being modeled, CTM2SCICHEM is run for a few select species including NO, NO₂, NO₃, and O₃. For other species, CTM2SCICHEM is run for all species that correctly map to the CMAQ data used and are found in SCICHEM files, for example HONO, PAN, ANO₃I, NH₃, or SO₂. The model outputs all species’ background information into a single ambient file (*.amb), which is then used in SCICHEM. (see Section 5. Pollutants for more information)
4. WRF and MMIF

Checking this option in the meteorology section of the UI will process and use WRF output as the meteorology option. AQcast includes archived 12 km WRF data for North America from 2014 through 2018. Using this, MMIF will be run for the modeling time selected assuming it’s within the years of available archived data. (An mmif run set outside of the stated years will fail.) The modeling domain must be greater than 20 km in each direction. If either modeling domain dimension is greater than 46 km, this option will be used by default. TERSCI will be processed for a subregion of the modeling domain to provide much finer resolution elevation data to the model. Elevation data is included in the *.mcw file created by MMIF, but is at a resolution of 12 km.

5. Pollutants

AQcast: SCICHEM has the option to model four separate pollutant species, including NO$_2$, SO$_2$, PM$_{2.5}$, and Ozone (O$_3$). Figure 4 shows and example of the chemistry input portion of the UI. Once selected, each pollutant triggers other parameters to match. If NO$_2$ is selected, the file containing the chemical mechanisms (*.imc) contains only basic information for a select few species, whereas if any of the other pollutants were selected the model would include a full chemical mechanism file with nearly 150 species. For each pollutant the SCIDOSPOST output parameters are specific. For example, the National Ambient Air Quality Standards (NAAQS) for NO$_2$ is the highest 8th high concentration of 1 hour daily maximum concentrations, while SO$_2$ is the highest 4th high concentration of 1 hour daily maximum concentrations. Depending on the pollutant selected, the appropriate values are extracted and plotted.

![Figure 4. AQcast: SCICHEM UI screen shot of the chemistry options and source inputs](image)

6. UI options

**Load Previous Project** – This option will provide a list of all previously run SCICHEM projects. A user can load a previous project selecting one from the list and all input options from that project will be loaded into the rest of the UI. After loading, the various parameters can be modified. Note that to load
properly, the previous project must have completed. When rerunning a project, it is suggested that a user edit the “Project Description” as it will create a set of new project files instead of overwriting the previous ones.

**Project Description** – This string is used for reference only and is how the user will select the results from this specific run. This name will also be used when referencing this run to use previous meteorology, stack parameters, fence line, or building files. (We suggest including the location or facility name, date of run, and MMIF/NOAA to make clear the source of the meteorological data.)

**Run Option** – “Default” simply runs the model with the parameters chosen and creates figures and summaries comparable to the Significant Impact Level (SIL) and the NAAQS. “Setup Only” will run all aspects of the model setup and stop before running SCICHEM itself. Files will be compressed and available in the *Results Tab* upon completion. “Meteorology Only” will process the meteorology option chosen in the UI then provide any processed files in the *Results Tab* upon completion. (Note: source parameters are not needed for the “Meteorology Only” option.)

**Time Input Option** – Choose the format to input the model run time. The dates must be in the format YYYYMMDDHH. It is recommended to run at least 1 week of data.

**Time Zone** – Select the appropriate time zone for the location of the facility.

**Project Coordinates (CONUS)** – Input the coordinates for the facility to be modeled. This is used to find the nearest meteorological station as well as where to plot final results. Note: the coordinates must be in the contiguous United States.

**Modeling Domain/Grid** – Input the modeling domain dimensions in kilometers (km). A square domain is common, but not necessary. This domain will be centered over your project coordinates. If either of the domain dimensions is greater than 46 km, the WRF-MMIF option will automatically be used for the meteorological data. AQcast includes archived WRF data at 12 km resolution for North America for the years 2014-2018. The model spacing parameter will not be used in that case.

**Chemistry Option** – At least one pollutant must be selected. This determines the level and type of chemistry to be used in the model run. There must be a corresponding source with emissions for the selected pollutant or precursors (see “Source Parameters and Emissions” below). Multiple components will be included for only those species with emissions greater than zero. See Section 5 for more information.

**Source Parameters and Emissions** – For each source to be modeled, the user needs to fill out the section under “Create New Source”. The “Source Type” denotes the option to choose if it is a point source (continuous stack, “CS”) or an area source (continuous area, “CA”). Not all parameters are needed for each source type. Parameters are noted with “(a)” area or “(p)” point if they are required only one source type. Proceed to fill out the corresponding parameters and emissions in the stated units provided on the UI. More than one source is possible, and to add another simply click the button “Add Another Source”. An hourly emissions file is optional. See the SCICHEMv3.2 User Guide for more information. Note: the file must be formatted correctly, for a successful run. An example of the format is here:
Previously Created Source Parameter File – A previously created source file (named by the project description) can be used by selecting from a dropdown menu below the source inputs. The selected file will be loaded into the UI and plotted on the map.

Building Locations – The user can upload a zipped file of all files pertaining to a GIS shapefile. This includes *.shp, *.dbf, *.sbn, *.shx among others. (NOTE: the projection of this shapefile must be WGS84. To check, open the *.prj file in a text editor and “WGS_1984” should be present a few times. The shapefile must be type POLYGON and not POLYGON ZM.) The user can also draw the buildings individually on the map in the UI. After buildings are either drawn or uploaded the user must click on each building to verify the height in meters. The default is 3 meters, which is an average one-story building. After the map, there is an option where the user can specify a previously drawn or uploaded building file named by project description and whether it was drawn or uploaded. Any previously selected file will be loaded into the map and at this time the user can add a building to it to be used in the current run. To clear uploaded files, choose the “Previously Created Building File” to be “None”, and to clear drawn files click the “Clear Drawings” button near the map (Note: this will clear previously drawn fence lines). If a building was uploaded and drawn the resulting filename will contain “UploadAll” and contain all buildings for the run.

Fence line Location – Similar to building locations, the user can either draw the fence line or upload a zipped file of the GIS shapefiles. (See “Building Locations” above for information on shapefiles.) After the fence line is either drawn or uploaded to the map the user can specify a previously drawn or uploaded fence line file named by project description and whether it was drawn or uploaded. AQcast: SCICHEM creates receptor points at 25-meter intervals along the fence line (See Receptors below). Any previously selected file will be loaded into the map and at this time the user can add a fence line to it to be used in the current run. To clear uploaded files, choose the “Previously Created Fence Line File” to be “None”, and to clear drawn files click the “Clear Drawings” button near the map (Note: this will clear previously drawn buildings).

Previously Created Fenceline File – A previously created fenceline file (named by the project description) can be used by selecting from a dropdown menu below the map. The selected file will be loaded into the UI and plotted on the map. A drawn fenceline can be added to any loaded shapes.

Previously Created Building File – A previously created building file (named by the project description) can be used by selecting from a dropdown menu below the map. The selected file will be loaded into the UI and plotted on the map. Drawn buildings can be added to any loaded shapes.

Meteorology Options – One of the below must be selected. These are listed by priority. (For example, if ‘Previous Met.’ was selected, any selected stations in the map would be ignored.) When loading a previous project, click the “Find Closest Meteorological Sites” button and the NWS stations used will be selected when the list loads.

1. WRF and MMIF – If selected, AQcast: SCICHEM will run MMIF on AQcast’s archived WRF data for the selected run period, which must be in the range of available archived data (currently 2014-2018). The modeling domain must be greater than 20 km in each direction.
2. **Meteorology from previous job** – The user has the option to use previously processed meteorology, such as MMIF or METSCI data from a previously submitted project, by selecting the project description in the dropdown menu.

3. **Onsite Meteorology** – An onsite meteorology file is optional to include via the UI and should contain the latitude, longitude, base elevation option in meters, and precipitation. This data will be supplemented by NOAA FSL upper air data. The format **MUST** be correct for a successful run. For more information on the format refer to SCICHEM v3.2 User Guide. The format is as follows:

```
OSYR OSMO OSDY OSHR PRES SLVP PAMT TT01 WS01 WD01 SA01 RH01
```

4. **Default meteorology stations** – AQcast: SCICHEM will select the nearest NOAA surface (with ASOS one-minute data) and upper air stations to the user provided coordinates for processing in METSCI.

5. **Selected Meteorology stations** – The user can choose to search for the 5 closest surface and upper air stations to their provided coordinates. From that list the user can select which station to use. See Section 2.

**Receptors** - AQcast: SCICHEM utilizes the EPA's AERMAP program to extract the elevation at specific locations for use in calculating concentrations. These will include any fence line receptors and sensitive receptors if the user has selected these options. Sensitive Receptors include churches, schools, parks, and hospitals in the modeling domain and are used as receptor locations for final outputs.

**Advanced Options** – This portion of the UI includes nearly all variables used in running the SCICHEM model. Their names and descriptions are identical to those listed in the SCICHEM v3.2 User’s Guide. The default values seen on the UI are the values used in a general run, and **DO NOT** need to be filled in unless the user specifically desires to change a setting.

6. **Output**

After successful completion of AQcast: SCICHEM an email will be sent to the user notifying them the project is complete. The **Results Tab** will provide a final summary of the maximum concentrations and design value for the selected pollutant along with some plots. A link to download a tar ball of the outputs and model setup files will also be provided on the **Results Tab** as well. A list of example files is provided in Appendix A. The user will get concentration plots (e.g., Figure 5), an elevation plot for the modeling domain, fence line and stack location plots, and some time-series plots for where the maximum concentration occurred (e.g., Figure 6).
Figure 5 Maximum Concentration for 1-hr NO₂.
Figure 6. Time Series plot for where the maximum plume design concentration of PM$_{2.5}$ occurred. $y$-axis is in $\mu$g/m$^3$.

7. References

SCICHEM Model and Documentation: [https://github.com/epri-dev/SCICHEM](https://github.com/epri-dev/SCICHEM)

EPA’s MMIF Model: [https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#mmif](https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#mmif)

EPA’s AERMAP Processor: [https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#aermap](https://www.epa.gov/scram/air-quality-dispersion-modeling-related-model-support-programs#aermap)
Appendix A
Sample File List for User Download

**Bpip**
- Bpip.inp/bpip.out – files used to run the building downwash program

**OTHER**
- Output/domainBox – a GIS shapefile that covers your modeling domain.
- Output/Fenceline – a GIS shapefile that represents the border between private and public land for your modeling case
- Output/bldg – a GIS shapefile that represents the buildings in your project area
- NED/data/Elevation data – USGS elevation data downloaded for use in tersci
- StackParams.csv – All stack data for this project.

**Tersci**
- Ter.inp – input parameter file used by tersci
- Terrain.ter – output file from tersci with elevation data for use in SCICHEM

**Metsci**
- METSCI*.SFC and METCI*.PRF - final metsci output files used in SCICHEM
- Metsci*.inp – input parameter file used to run metsci
- *ISH and *FSL files – raw NOAA surface and upper air station data respectively, used as input to metsci
- ONSITE.OBS/OSITE.DAT – files used for onsite meteorology data

**Scichem**
- *.inp, *.msc, *.scn – input parameter files used in SCICHEM
- *.sam – sampler file used in calculating receptor concentrations used in SCIDOSPOST
- Met.lis – file use in scichem listing input meteorological files
- sciDOSpost_plume and sciDOSpost_cumu .inp – input parameter files for SCIDOSPOST for the plume and cumulative concentrations respectively
- *.amb – any ambient concentration files created by CTM2SCICHEM
- AER.* - project files created by scichem.

*Note:* direct output of SCICHEM files *.ados, *.dep, *.dos, and *.puf will **NOT** be included in the tar.gz file as they can be very large. They are available for download upon request. (To request, e-mail AQcast@aer.com and include the project Job ID found on the UI Results Tab).

**Figures**
- Elevation.png – image with the modeling domain and elevation with the facility location in the middle.
• metSites.png – (non MMIF only) image with the surface and upper air stations relative to the facility location.
• Facility.kml – A Google Earth file plotting the facility, sources, buildings, and fence lines if provided.
• Windrose*.png - (non MMIF only) image of the surface winds for the surface station and modeling period selected.
• *DesignConcPlots*.png – images of the design concentrations for the plume and cumulative impacts respectively as well as zoomed in images of the impact area.
• *MaxDailyConcPlot.png – images of the maximum concentrations for the pollutant over the modeling period
• *tseries*.png – time series plots for the cumulative and plume maximum impact locations
• SensitiveReceptor.png – (if selected) image of the sensitive receptor locations

Summary Files
• Output/Summary.txt – summary of the maximum and design values and locations from your facility.
• Metsci/MetSummary.txt – summary of the surface and upper air stations used in metsci
• CMAQ_Summary.txt – summary of the CMAQ run and domain used for creating the background data file used in SCICHEM. (TBD)
• AERMAP/SensitiveReceptor_Descriptions.txt – list of sensitive receptor locations and names
• Scichem.info.txt – MMIF output