SCICHEM Version 3.3

As of December 2021, the SCICHEM model has been updated to Version 3.3. Significant improvements have been made to the building downwash calculation as well as methods implemented to speed-up non-chemistry calculations. Following are the code changes associated with the release.

- A bug using building downwash with multicomponent sources was fixed. The cavity fraction was not applied properly, which may have resulted in large over predictions. Note that this bug would have affected all calculations using an IMC file.

- Plume rise calculations with building downwash were modified. Previously, if the plume was determined to not be influenced by downwash, a separate plume rise calculation was utilized. However, it was determined that this often resulted in over predictions as well as giving inconsistent results as varying wind directions changed building influence. Now, the PRIME plume rise calculation is always used, with very small “buildings” defined for wind directions giving no building downwash.

- A “no chemistry” mode has been implemented to speed-up calculations. This is controlled by the “step_chemistry” flag in the IMC file. The default is ‘.true.’; setting this to ‘.false’ lets SCICHEM skip chemistry calculations that are irrelevant for inert reactions.

- Non-chemistry calculations have been parallelized (multi-threaded) using OpenMP. This can be used for calculations in “no chemistry” mode or those not using an IMC file. The number of threads is set by the parameter NumThreads in SCIPUFF.ini. This capability has the greatest impact for calculations involving many thousands of puffs and large meteorological grids. It has been found generally that up to 8 threads results in significant speed-up in such cases; there is little benefit beyond that due to the overhead associated with each thread.

- A bug in the chemistry calculation has been fixed. The impact is expected to be small, but a full assessment has not been made.