Dataset Name: Fallout Super-droplet Method Output

Citation Requests

Please cite the final paper in JGR: Atmospheres:

McGuffin, D. L., Lucas, D. D., Morris, J. P., Spriggs, G. D., and Knight, K. B.(2022) "Super-droplet Method to Simulate Lagrangian Microphysics of Nuclear Fallout in a Homogeneous Cloud", *JGR: Atmospheres 128*(18) DOI: 10.1029/2022JD036599.

Abstract: Predict the particle size distribution of nuclear fallout in a post-detonation cloud using the super-droplet method (SDM) to simulation fallout microphysics.

Source: This data was created under work funded by the Laboratory Directed Research and Development Strategic Initiative "Influence of the Environment on Post-Detonation Chemistry and Debris Formation" with tracking code 20-SI-006. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and is released under number LLNL-MI-839946. Refer to our published paper or contact dana.lynn.mcguffin at gmail.com for dataset questions.

Dataset Information

The dataset contains output from the model described in the published paper to create Figures 7 – 11. The compressed tar file contains three directories: *Section3.1, Section3.2, Section3.3*. Figures 7 and 8 can be reproduced from the data set in Section3.1. Figure 9 can be reproduced from the data sets in Section3.2. Figures 10 and 11 can be reproduced from the data sets in Section3.3. All data sets are zipped NumPy files (npz) including key/value pairs for the various model output arrays. To extract the data set in python, use the NumPy package's load function.

Attribute Information

Section3.2: There are four subdirectories here that correspond to the four different studies listed in Table 1 of the publication. Each study represents a set of simulations across a different range of model inputs: system explosive energy and mass. The naming convention is Data_NoX_YYsims/Data_NoX_scenarioZZZ.npz where X represents the study number from 1 to 4, YY represents the total number of simulations performed for that study, and ZZZ is the scenario number. Data from the z^{th} simulation in a study is accessed from loading the npz data. In the following arrays, T is the number of time steps and NF is the number of super-droplets at the final time step.

Keys representing the data include:

- **Mass_kg:** model input system mass in kilograms (scalar)
- **Yield_kt:** model input explosive energy in kilotons (scalar)
- **time_sec:** time steps for all time series in seconds (Tx1 array)
- **Temperature_K**: boundary condition for cloud temperature in Kelvin timeseries (Tx1 array)
- **Volume_cm3:** boundary condition for cloud volume in cm3 timeseries (Tx1 array)
- **Ntot_cm3:** predicted number concentration of fallout in #/cm3 timeseries (Tx1 array)
- **Dpm_nm:** Predicted mean particle diameter of fallout in nanometers timeseries (Tx1 array)
- **Dpg_nm:** Predicted median particle diameter of fallout in nanometers timeseries (Tx1 array)
- **vapor_g:** Predicted mass of vapor in grams timeseries (Tx1 array)
- **vaporCondensed_frac:** Predicted cumulative vapor condensed normalized by initial vapor mass (Tx1 array)
- **SDradius_nm:** Predicted radius of super-droplets at final time in nanometers (NFx1 array)
- **SDmult_cm3:** Predicted number concentration represented by each super-droplet at final time in #/cm3 (NFx1 array)

Section3.3: This directory contains several datasets, each corresponding to a different sensitivity simulation. We simulated four different high yield tests listed in Table 2 of the publication (cases 1 – 4). For each case, we varied the species (FeO or SrO) and two scaling factors: applied to the coagulation rate (coag) and another applied to both condensation and nucleation rate (CondNuc). The naming convention for each simulation's dataset is: CaseX_Out_SPEC_CondNucSPEC_xY_coagZ_Nsd20_NF.npz where X is the case number, SPEC is either FeO or SrO, Y is the CondNuc scaling factor, Z is the coag scaling factor, and NF is the final number of super-droplets in the simulation. Each dataset file includes the same key/value pairs listed in the previous section for *Section3.2.*

Section3.1: This directory contains one dataset for a single simulation with model inputs of 10 kt and 1500 kg system. The data is structured the same as described above in *Section3.2*, but we include additional diagnostics to produce the more detailed figures. The additional key/values are:

- **MMD_nm:** Predicted mass mean diameter of fallout in nanometers timeseries (Tx1 array)
- **Saturation_ratio:** Predicted saturation ratio of the condensing species timeseries (Tx1 array)
- **vaporNucleated_frac:** Predicted cumulative vapor lost in nucleation normalized by initial vapor mass (Tx1 array)
- **timeseries_SDradius_nm:** Predicted radius of super-droplets in nm at each timestep (TxNF array)
- **timeseries_SDmult_cm3:** Predicted number concentration represented by each super-droplet in #/cm3 at each timesetp (TxNF array)
- **timeseries_time_sec:** Array listing timestep in seconds for super-droplet timeseries arrays (TxNF array)