

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](https://doi.org/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@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 timestep (TxNF array)
- **timeseries_time_sec:** Array listing timestep in seconds for super-droplet timeseries arrays (TxNF array)