Project 013 Microphysical Modeling and Analysis of Access 2 Aviation Exhaust Observations

Stanford University

Project Lead Investigator
Name: Mark Z. Jacobson
Title: Professor
Department: Civil and Environmental Engineering
University: Stanford University
Mailing Address: Yang & Yamazaki Environment and Energy Building, 397 Stanford, CA 94305
Phone: 650-723-6836
email: jacobson@stanford.edu

University Participants

Stanford University
- P.I.(s): Mark Z. Jacobson, professor; co-I Sanjiva K. Lele, professor
- Air Transportation Center of Excellence Agreement 13-C-AJFE-SU Amendments No. 001, 002]
- Period of Performance: October 1, 2013 – September 30, 2014.
- Task(s):
    1. Update GATOR-GCMOM and LES models to simulate ACCESS 2 data
    2. Obtain ACCESS 2 data / determine best data for model comparison
    3. Simulate data with models and compare with Aerodyne
    4. Write up results for conferences and peer-reviewed publications

Project Funding Level
$200,000 from FAA plus $200,000 in cost-sharing by Stanford University.

Investigation Team
The team performing the research during this period included Prof. Mark Z. Jacobson (PI), Prof. Sanjiva K. Lele (co-I), Mary A. Cameron (a Ph.D student), and Aniket R. Inamdar (a Ph.D student). We are also collaborating with other groups for goals 1-3. The PIs are overseeing the project (Tasks 1-4). The graduate students are performing the research described under Tasks 1-4.

Project Overview
NASA's Alternative Fuel Effects on Contrails and Cruise Emissions (ACCESS-2) field experiment, held in the summer of 2014 in California, *measured* a number of aviation exhaust parameters *during flight* that are useful to study the chemical and physical evolution of exhaust gases. A detailed knowledge of the composition and evolution of exhaust gases and particles in free flight is necessary to study their interaction with solar and thermal radiation to estimate aviation climatic effects. The main goal of this project was to simulate the measured short-term, near- and far-field evolution of aircraft exhaust aerosol and contrail particles and gases with two computer models – GATOR-GCMOM and an LES model. Thus these two models together would simulate phenomena spanning a very large range in spatial scales from the smallest turbulent scales (a few millimeters) to the largest planetary scales (a few thousand kilometers). During the exercise, we would validate and improve detailed microphysical processes in the models so that the models could provide more credible estimates of impacts on climate and atmospheric composition (useful for air quality impact studies) when used at the regional and global scale. The studies were also designed to tease out characteristics of near-field aerosol and contrail evolution not available from data alone. Model simulations with GATOR-GCMOM were proposed to simulate the evolution of aerosol and contrail particle size distributions for comparison with data and with Aerodyne model results (obtained in a

parallel study). The LES model CDP-IF2 were supposed to be run to provide parameters for plume spreading and shearing to GATOR-GCMOM and the Aerodyne model. Results were to be obtained following the analysis of data from six aircraft flights.

Task 1. Update GATOR-GCMOM and LES models to simulate ACCESS 2 data

Stanford University

Objective(s)

The main goal of this task is to update the GATOR-GCMOM and LES models to simulate ACCESS 2 data.

Research Approach

Simulations with two different models are being run. One model is an LES model and the second, a Reynolds-Averaged Navier-Stokes (RANS) model that treats subgrid plumes. Near-field simulations are being run with both models from 1 second to 20 minutes.

The LES model is CDP-IF2, an incompressible turbulent flow solver, with Boussinesq approximation for buoyancy effects and Euler-Lagrangian treatment for ice-microphysics. Potential temperature and water vapor concentration are treated as Eulerian fields. The model treats emissions of aerosol, which are tracked for the primary purpose of simulating contrail development. Water vapor deposition on aerosol particle nuclei is based on local supersaturation. The model treats multiple ice crystal-habits (Inamdar et al., 2013). It has been used for process studies of persistent aircraft contrails and has supported the development of subgrid-plume model for use with global circulation models.

The RANS model is GATOR-GCMOM, a one-way nested, online gas-aerosol transport, radiation, general-circulation, mesoscale, and ocean model. It treats gas photochemistry, spectral radiative transfer, size- and composition-resolved aerosol and cloud microphysics and chemistry, dynamical meteorology, and ocean and soil processes. With respect to aircraft, GATOR-GCMOM treats the subgrid evolution of aircraft exhaust from individual flights with an analytical plume expansion model coupled with a size-and-composition-resolved aerosol and contrail module. The model also treats subgrid gas chemistry. Emissions from individual flights worldwide are obtained from the 2006 chorded Volpe emission inventory.

For the present study, the models were updated to simulate the ACCESS 2 data. For GATOR-GCMOM, this involved shrinking the model to a box-model version in each of many layers of a 1-D model and adjusting input such that a single flight with a specified initial plume cross section and emissions profile was specified. The initial plume axes were determined from the LES model output for ACCESS 2 ambient conditions and aircraft characteristics. The LES model updates included setting up the model under the ambient conditions of the field campaign, adjusting emission indices for different engines, and including a multimodal initial particle PDF to replace the initial uniform distribution. During the LES simulations, the impact of fuel sulfur content is modeled by varying the initialized PDF of activated particles.

Task 2. Obtain ACCESS 2 data / determine best data for model comparison

Stanford University

Objective(s)

The goal of this task is to obtain as much ACCESS 2 data as possible then to aggregate the data in the best way possible so as to compare model results.

Research Approach

Data were obtained from NASA's Alternative Fuel Effects on Contrails & Cruise Emissions (ACCESS 2) field experiment. ACCESS 2 involved six, 3-hour long flights and was designed to measure the aircraft exhaust composition and contrail characteristics as it burned (1) JP-8 with low sulfur, (2) a 50/50 blend of low S JP-8 and HEFA fuel, and (3) high sulfur JP-8. The flights were in the 31,000-38,000 ft. altitude range.

GATOR-GCMOM and LES simulations are being initialized using measurements of ambient conditions taken by the NASA DC-8 4-engine aircraft. Within each flight, some ambient conditions needed for model simulations (temperature, pressure, and humidity) varied during the flight, creating a large number of test cases spanning the observed parameter values. To decrease the parameter space needed for simulations, four test cases that were most likely to result in contrail formation were chosen.

Exhaust measurements from the NASA DC-8 source aircraft were made by the NASA HU-25 Falcon sampling aircraft. For two flight days, May 27 and May 29, 2014, short-lived contrails were sampled and the corresponding aerosol and contrail size distributions were provided. Mach number and separation distance, also provided, were used to calculate the age of the exhaust plume for each test case, providing a time-resolved size distribution for up to ~2 minutes. These size distributions are used for comparison with GATOR-GCMOM and LES model results from the four test cases.

Task 3. Simulate data with models and compare with Aerodyne

Stanford University

Objective(s)

The goal of this task is to perform simulations of the evolution of aircraft exhaust under conditions that the data were valid for in order to compare model results with the data and with the Aerodyne model results.

Research Approach

Several iterations of comparisons are needed. Following the first comparison, the models must be updated further. The four GATOR-GCMOM and LES 20-minute simulations described under Task 2 have been run but require further refinement to compare directly the number of activated particles, ice mass, and optical properties resulting from each model simulation.

To match GATOR-GCMOM results with measured data, it may be necessary to start the model simulation within 1 second after exhaust leaves the aircraft rather than one minute or to assume a smaller initial plume size. Another change may be to assume a different initial size distribution of particles to ensure the modeled size distribution is not so far off the observed one initially. Once Stanford has compared sufficiently with data, we will compare with results from the Aerodyne model ensemble-averaged quantities including dilution ratio from LES, ice mass, ice area, and particle size distribution.

Task 4. Write up results for conferences and peer-reviewed publications

Stanford University

Objective(s)

This task involves determining the most important information to present publicly through conferences proceedings and talks as well as in peer-reviewed publications.

Research Approach

Some results will already by presented at the October 14, 2015 Ascent meeting and at the American Geophysical Union 2015 annual fall meeting in San Francisco, CA.

Milestone(s)

The milestones reached to date include the setting up of the GATOR-GCMOM and LES models to simulate individual aircraft plumes, the gathering and analysis of size-resolved aerosol data, and the preliminary simulation of the data with the models. Some results have been graphed for presentation for the October 14, 2015 Ascent Meeting. The four GATOR-GCMOM and LES model inter-comparison cases will be presented at the American Geophysical Union 2015 fall meeting, December 2015.

In addition to LES comparisons with GATOR-GCMOM, a separate reduced order ODE box model for contrail ice habit formation was developed to predict bulk contrail properties, including total ice mass and number density, total ice area, median particle size, and inferred optical depth. The ODE model is computationally inexpensive, so simulations lasting up to 20 minutes can be run and compared with GATOR-GCMOM. Results from common 20-minute test cases performed by the LES, GATOR-GCMOM, and reduced-order ODE model will be compared and presented at the 2015 AGU fall meeting.

Major Accomplishments

The major accomplishments to date are the setting up of the GATOR-GCMOM and LES models to simulate individual aircraft plumes, the gathering and analysis of size-resolved aerosol data, and the preliminary simulation of the data with the models. Some results have been graphed for presentation at the October 14, 2015 Ascent Meeting. A comparison of GATOR-GCMOM, LES, and reduced-order ODE model results will be presented at the 2015 AGU fall meeting.

Publications

Peer-reviewed publications

Gettleman, A., C.C. Chen, M.Z. Jacobson, M.Z. Cameron, D.J. Wuebbles, A. Khodayari, and D. Phoenix, Climate effects from 2050 projected aviation emissions, Atmospheric Environment, in review, 2015.

Cameron, M.A., M.Z. Jacobson, S. R. H. Barrett, H. Bian, C.-C. Chen, S. D. Eastham, A. Gettelman, A. Khodayari, Q. Liang, D. Phoenix, H. B. Selkirk, N. Unger, D. J. Wuebbles, Model intercomparison study of effects of aircraft on surface air quality, in preparation, 2015.

Conference proceedings

Inamdar, A.R., S.K. Lele, and M.Z. Jacobson, LES of Contrails with Ice Habit Treatment Using the Fickian-Distribution Model, 4th Joint US-European Fluids Engineering Division Summer Meeting, American Society of Mechanical Engineers 2014 Conference, August, 2014.

Technical reports

Gettelman, A., C.-C. Chen, M.Z. Jacobson, M.A. Cameron, D.W. Wuebbles, and A. Khodayari, Climate forcing effects from 2050 projected aviation, Federal Aviation Administration Office of Environment and Energy, Washington, D.C., March 31, 2015.

Jacobson, M.Z., M.A. Cameron, S.R.H. Barrett, S.D. Eastham, A. Gettelman, C.-C. Chen, H.B. Selkirk, H. Bian, Q. Liang, N. Unger, D.W. Wuebbles, A. Khodayari, and D. Phoenix, Surface air quality effects of cruise emissions, Federal Aviation Administration Office of Environment and Energy, Washington, D.C., March 31, 2015.

Outreach Efforts

Cameron, M.A., M.Z. Jacobson, and S.K. Lele, Evaluating the photochemical effects of aircraft emissions in the upper-troposphere/lower stratosphere, Atmospheric Chemical Mechanisms conference, University of California, Davis, December 10-12, 2014.

Cameron, M.A., M.Z. Jacobson, and S.K. Lele, Quantifying the spatial and temporal distribution of aircraft emissions in the upper troposphere/lower stratosphere, American Geophysical Union Fall Meeting, San Francisco, California, December 15-19, 2014.

Cameron, M.A., M.Z. Jacobson, and S.K. Lele, Quantifying the spatial and temporal distribution of aircraft emissions in the upper troposphere/lower stratosphere, 2015 CRC mobile-source air toxics workshop, Sacramento, California, Feb. 17-19, 2015.

Cameron, M.A., M.Z. Jacobson, S. R. H. Barrett, H. Bian, C.-C. Chen, S. D. Eastham, A. Gettelman, A. Khodayari, Q. Liang, D. Phoenix, H. B. Selkirk, N. Unger, D. J. Wuebbles, X. Yue, An intercomparative study of the effects of aircraft on surface air quality, American Geophysical Union Fall Meeting, San Francisco, California, December 14-18, 2015.

Inamdar, A.R., M.A. Cameron, S.K. Lele, and M.Z. Jacobson, Reduced order ODE model for linear contrails, American Geophysical Union Fall Meeting, San Francisco, California, December 14-18, 2015.

Jacobson, M.Z., J.T. Wilkerson, S. Balasubramanian, W.W. Cooper, Jr., and N. Mohleji, The effects of rerouting aircraft around the Arctic Circle on Arctic and global climate, Climatic Change, 115, 709-724, doi:10.1007/s10584-012-0462-0, 2012.

Inamdar A.R., Lele S.K., Jacobson M.Z., A Probabilistic Ice Habit Model for LES of Contrails, 5th Atmos. & Space Env. Conference, AIAA control number 1586391, 2013.

Cameron, M.A., M.Z. Jacobson, A.D. Naiman, and S.K. Lele, Effects of plume-scale versus grid-scale treatment of aircraft exhaust photochemistry, Geophys. Res. Lett., 40, 5815-5820, 2013. Projects

Studying the effects of aircraft exhaust on global and regional climate, ASCENT Aviation Sustainability Center Advisory Meeting, Alexandria, Virginia, March 10, 2015 (presented remotely).

Studying the effects of aircraft exhaust on global and regional climate, ASCENT Aviation Sustainability Center Advisory Meeting, Seattle, Washington, October 14, 2015.

Awards

Outstanding student poster award, Atmospheric Sciences, Mary Cameron, American Geophysical Meeting Fall 2014 Meeting, http://ospa.agu.org/ospa/2014-fall-meeting-ospa-winners/. Cameron, M.A., M.Z. Jacobson, and S.K. Lele, Quantifying the spatial and temporal distribution of aircraft emissions in the upper troposphere/lower stratosphere, American Geophysical Union Fall Meeting, San Francisco, California, December 15-19, 2014.

Outstanding presentation award for the poster, "Quantifying the Spatial and Temporal Distribution of Aircraft Emissions in the Upper Troposphere/Lower Stratosphere," Cameron, M.A., M.Z. Jacobson, and S.K. Lele, at the Opportunity Job Fair Reception at Stanford University, January 23, 2015.

First place in student poster competition at the MSAT workshop, "Quantifying the Spatial and Temporal Distribution of Aircraft Emissions in the Upper Troposphere/Lower Stratosphere," Cameron, M.A., M.Z. Jacobson, and S.K. Lele, February 19, 2015.

Student Involvement

Mary Cameron (PhD student) has been working to compare GATOR-GCMOM box-model simulation results of the evolution of the aerosol size distribution with ACCESS 2 data. She has updated the model, obtained, analyzed, and aggregated some data, and performed some initial comparisons. She will now compare with additional data and update the model to simulate the data more accurately. She will also write up results for publication.

Aniket Inamdar (PhD student) has been working to compare LES 3-D model simulation results with ACCESS 2 data, and has developed the reduced-order ODE contrail model. He has updated the LES model, helped to analyze and plot data, and compared model predictions with some data. He will now compare with additional data and GATOR-GCMOM results and update the model to simulate the data more accurately. He will also write up results for publication.

Plans for Next Period

We requested and received a no-cost extension until September 30, 2016 to complete the uncompleted work for the project at no additional cost. The main remaining tasks are to finish model comparisons with data and Aerodyne results and to write up papers for publication.