Project 020 Development of NAS wide and Global Rapid Aviation Air Quality Tools

Massachusetts Institute of Technology (MIT)

Project Lead Investigator

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- FAA Award Number: 13-C-AJFE-MIT, Amendment Nos. 007, 018, 025, and 032.
- Period of Performance: Aug. 19, 2014 to Aug. 31, 2018 (reporting with the exception of funding levels and cost share only for period from October 1, 2016 to September 30, 2017)
- Tasks:
    1) Extend second-order sensitivities to future years
    2) Evaluate sources of uncertainty within the tool
    3) Extend North American nested grid focused to represent Canadian impacts
    4) Develop nested grids for Europe and southeast Asia

Project Funding Level

Project Funding Level: $800,000 FAA funding + $50,000 Transport Canada funding = 850,000 total sponsored funds, with just $800,000 matching funds required. Sources of match are that same $50,000 Transport Canada funding (it constitutes both matching funds itself, as well as being sponsored funds that do not need to be matched), plus approximately $215,000 from MIT, and 3rd party in-kind contributions of $114,000 from Byogy Renewables, Inc. and $421,000 from Oliver Wyman Group.

Investigation Team (all MIT)

Principal Investigator: Prof. Steven Barrett
Co-Principal Investigator: Dr. Raymond L. Speth
Co-Investigator: Dr. Florian Allroggen
Research Scientist: Dr. Sebastian Eastham
Graduate students: Irene Dedoussi, Guillaume Chossière, Kingshuk Dasadhikari

Project Overview

The aim of this project is to develop tools that enable the rapid assessment of the health impacts of aviation emissions. The focus of the project is on aviation-attributable $PM_{2.5}$ and ozone at the NAS-wide and global scales. These tools should allow for rapid policy analysis and scenario comparison. The adjoint method, which the tools are based on, provides a computationally efficient way of calculating the sensitivities of an objective function with respect to multiple model inputs. The project enhances the existing tools in terms of the domains and impacts covered, and in terms of uncertainty quantification. The enhanced tools support the FAA in its strategic vision to reduce the significant health impacts of aviation emissions, and allow for detailed and quantified policy analyses.

Tasks for Current and Next Period

Current Period (AY2016-2017)

- **Task 1:** Extend second-order sensitivities to future years
- **Task 2:** Evaluate sources of uncertainty within the tool
- **Task 3:** Extend North American nested grid focused to represent Canadian impacts
- **Task 4:** Develop nested grids for Europe and southeast Asia

Next Period (AY2017-2018)

- **Task 1:** Continue work on the development of nested domains and provide tool validation
- **Task 2:** Incorporate the nested domains into a single user friendly framework
- **Task 3:** Support and assist the nvPM standard team on consistency-checking input data and interpreting results
- **Task 4:** Finalize and project uncertainty in ammonia emissions onto aviation impact sensitivities
- **Take 5:** Perform scoping of work for developing a multi-scale adjoint tool

Objectives

The aim of the project is to enhance the capabilities of the existing rapid assessment tool. The main objectives of this cycle are aligned with the aforementioned tasks. Specifically:

1. To provide a quantitative estimate of the relationship between aircraft emissions, background emissions and health impacts. By working on second order sensitivities, the impacts of aviation can be understood in the context of the background in which they act, and the relative benefits that can be achieved through policy action on aviation or non-aviation emissions.
2. To quantify the sensitivity of the tool's impact calculations to uncertainties in model inputs. This will ensure that the calculated impacts can be communicated in the context of the known sources of uncertainty, providing a more policy-relevant impact estimate.
3. To provide additional context for North American aviation emissions by incorporating the impacts on additional stakeholders. The ability to simultaneously calculate impacts for Canadian and US residents will allow multiple perspectives on impacts from the same emissions, adding a multinational dimension.
4. To bring high-resolution impact calculations for multiple regions into the net impact calculation. This provides additional validation for the global model results while also allowing high-fidelity estimation of local-scale impacts attributable to aviation for regions beyond the North American domain.

Research Approach

As documented in previous reports, the central tool for this project is the GEOS-Chem adjoint. A major, and unanticipated, focus of this period has been the diagnosis and correction of issues which resulted from an upgrade of the adjoint tool to the most recent version, GEOS-Chem adjoint version 35. Therefore, many of the results presented here are focused on structural improvements, which can be conducted in parallel with the adjoint diagnosis process, or are results which have been produced on a temporary basis using the previous version of the adjoint. Although the majority of the issues with v35 of the adjoint have now been resolved, this has occurred too late in the cycle to permit the production of updated sensitivity maps for this report.

Extension of calculations outside of original time range

The first task for this period of performance was concerned with extending our second-order sensitivity calculations beyond the original domain of interest. Prior sensitivity calculations had been performed almost exclusively using year 2006 meteorology. This resulted in the potential for unacknowledged bias in the results, and excluded the possibility of correctly accounting for the effects of interannual variability on either the model sensitivity or the associated uncertainty. In addition to meteorological variability, there have also been changes in the background emissions which will affect the sensitivity of surface conditions to aviation (the second-order sensitivity).

In response to this, the analysis has been extended to additional years and used to estimate the second order sensitivity of surface air quality to aviation emissions and to changes in background conditions. Formally, this can be expressed as

$$\text{Second order sensitivity} = \frac{\partial^2 J}{\partial E_{av} \partial C_{BG}}$$

where the cost function J is some metric of air quality impact, E_{av} is the rate of aviation emissions at a given point, and C_{BG} is some metric of the background conditions. This is a continuation of results presented previously, which focused on 2011 compared to 2006. With the upgrade to version 35 of the adjoint, sensitivities can be calculated using meteorology generated by the current-generation GEOS-FP output from the GEOS-5 model. This allows the re-calculation of sensitivities on an ongoing basis, up to and including the current day. An early result has been that ~7% of the sensitivity changes between the years of 2006 and 2011are estimated to be the result of changes in meteorology, compared to ~10% changes attributable to changes in population.

Evaluate additional sources of uncertainty within the tool

Following a literature review and feasibility analysis, a key (and, as yet, unquantified) source of uncertainty that has been identified within the current method is the potential impact of uncertainty in ammonia emissions on the sensitivity of air quality to aviation emissions. The rate of near-surface $PM_{2.5}$ formation is known to be highly sensitive to local concentrations of ammonia, which acts to neutralize acidic aerosol and thereby increase the total aerosol mass. However, no study has yet incorporated the known high uncertainty in ammonia emissions into their estimates of health impacts from aviation.

A new strategy has been developed to estimate the impact of uncertainty in ammonia emissions on the sensitivity of average surface-level air quality to aviation emissions. This constitutes an application of the second order sensitivity of aviation's impacts with respect to both aviation emissions and ammonia emissions, making use of the combined power of adjoint sensitivity calculation and forward differencing.

The impact of this uncertainty will be estimated by taking second order sensitivities of population exposure with respect to ammonia emissions, with and without aviation emissions. A typical example is shown in Figure 1, in this case for the sensitivity of surface-level mean $PM_{2.5}$ with respect to ammonia emissions in the baseline environment. These second order sensitivities can then be multiplied with the estimated uncertainty in ammonia emissions to give the impact that uncertainty in ammonia emissions have on aviation's contribution to ground-level $PM_{2.5}$

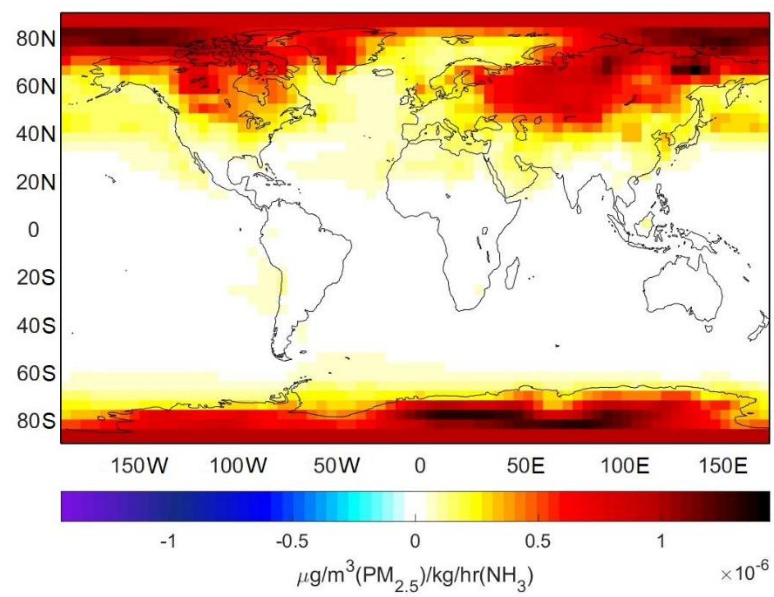

Figure 1: Sensitivities of mean surface-level $PM_{2.5}$ concentration to surface-level emissions of ammonia

In order to obtain the uncertainty in ammonia emissions, a literature review has been conducted to identify previously-derived estimates for the uncertainty, on both a global and regional scales. Thus, values of uncertainty have been obtained across several literature studies. Although some estimates suggest a low level of uncertainty in the overall global ammonia budget, with ~5% uncertainty in global emissions, regional studies have found that the local budgets are much more uncertain, with estimates of ~80% uncertainty for the U.S. (Zhu et al. 2013) and ~50% for China (Zheng et al. 2012, Xu et al. 2016). Multiplying these uncertainty percentages with input ammonia emissions for GEOS-Chem for each domain then gives the emissions uncertainties for post-multiplication with the second order sensitivities.

Incorporation of alternative stakeholders in estimation of North American impacts

All previous estimates of impacts within the North American nested domain had used as their receptor maps either the total population of the contiguous United States, or the total population within the domain. However, this resulted in a loss of nuance with regards to the specific distribution of impacts. While this is to some extent an inevitable result of using adjoint, rather than forward difference, methods, the dimensionality of the analysis can be increased by providing alternative cost functions which take into account the needs of different stakeholders.

To this end, a new receptor region has been implemented for the Canadian portion of GEOS-Chem Adjoint's North American nested grid, including incorporation of the population map for Canada (Figure 2). This enables computation of the sensitivity of average population exposure to $PM_{2.5}$ in Canada to aviation emissions, which can be used to calculate health impacts and costs in Canada attributable to aviation emissions. At present, all structural work necessary for this capability extension has been completed, in addition to the production of preliminary sensitivities for the Canadian nested region. However, full validation of sensitivities to certain emissions species is yet to be completed, pending output from the updated v35 adjoint model.

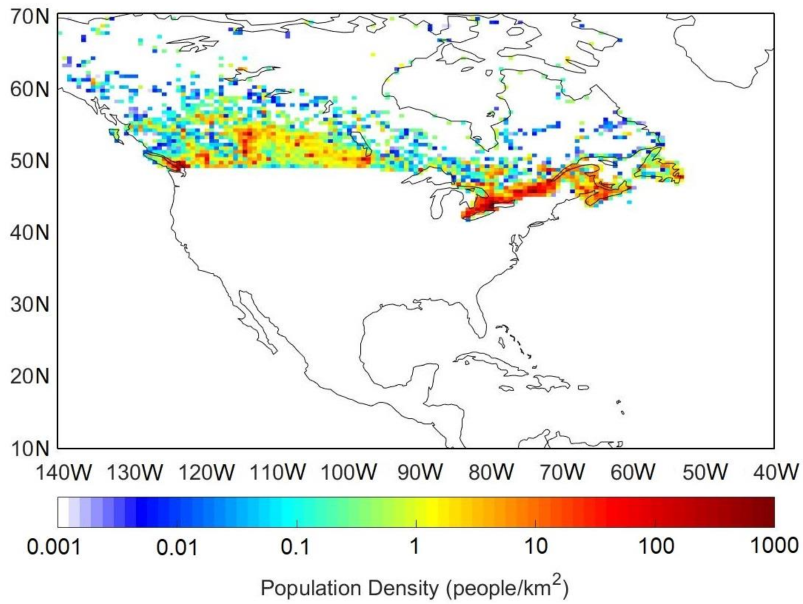

Figure 2: Population distribution used for calculation of sensitivity of Canadian air quality with respect to aviation emissions

Development of additional nested region domains

Given the global nature of aviation, much of the MIT research to date has focused on global impacts using global models with global population maps used to define the receptor regions and weighting. However, investigations using the North American nested domain have revealed that there are significant advantages to higher-resolution simulation over smaller domains. Capture of near-airport impacts is impossible with the coarse (~400 km) resolution at which the global model is run, while the finer (~50 km) resolution of the nested model is sufficient to isolate chemical and dynamical non-linearity associated with urban and coastal regions. This is complemented by further studies, such as Barrett et al (2010) and Eastham et al (2016), which show that the greatest impacts of aviation on surface air quality are incurred not in North America but rather in Western Europe and South Asia.

Accordingly, two additional nested domains have been developed for use with the GEOS-Chem adjoint. The first is the South-East Asia nested domain. This domain, modeled at a resolution of 0.5x0.667 degrees, allows impacts of aviation to be finely resolved throughout India, China, Indonesia, and the rest of the South-East Asian domain. A similar grid has been developed and implemented for Europe.

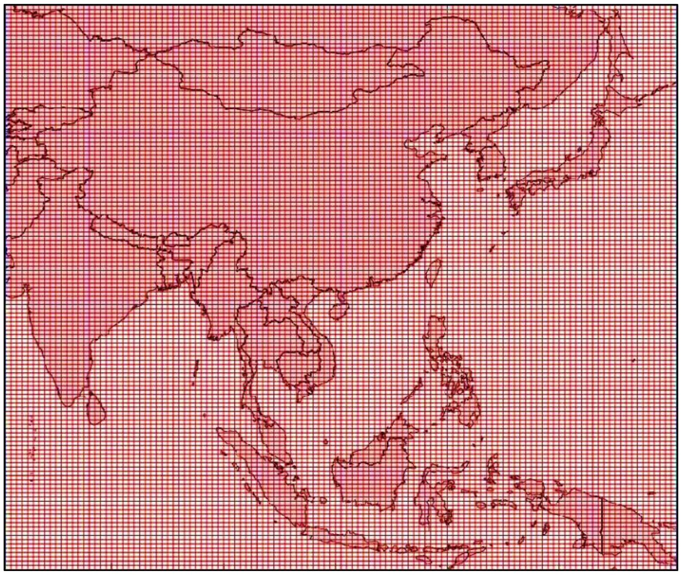

Figure 3: Population distribution used for calculation of sensitivity of Canadian air quality with respect to aviation emissions

These developments are complemented by a focused effort to improve the background emissions in these regions. As mentioned previously, the relative impact of aviation on surface air quality is dictated by the chemical environment encountered by both the LTO and cruise-level emissions, both in the region of production and along the path to their impacts. Although the standard inventories for Europe present in GEOS-Chem are relatively recent (e.g. the European EMEP project), those for China are over a decade old, based on the 2006 estimate by Zhang et al (2009). Use of these emissions would provide a poor representation of the local chemical environment. Accordingly, the most recent version of the EDGAR global anthropogenic emissions inventory (v4.3) has been acquired and implemented, relevant to the base year 2010. Since this is still too old to take into account recent policy, technology, and behavioral changes in the South-East Asian region, an ongoing follow-up project is the production of an updated emissions inventory for this domain using an activity-based updating method.

The calculation of the ozone impacts of aviation emissions required a careful definition of the metric used to measure exposure. On that front, MIT have collaborated with the ASCENT 18 project contributors. Jon Levy and his team suggested an appropriate metric for ozone exposure, and assisted with the choice of the concentration-response function to be used. The one that was chosen ensures consistency with previous FAA work.

The results for ground-level $PM_{2.5}$ from the forward model of this domain using the pre-existing emissions inventories have been validated against observational data from several urban centers in this region, as well as against satellite data for ground-level $PM_{2.5}$, and we are currently awaiting full validation of adjoint sensitivities.

Milestones

- *Extend second-order sensitivities to future years:* Work has continued on evaluating second order sensitivities for years beyond 2006.
- *Evaluate sources of uncertainty within the tool*: an assessment of uncertainty in ammonia emissions, considered to be key to all $PM_{2.5}$ formation, has been performed and will be propagated into impact sensitivities as part of the next project period. Other sources of uncertainty, such as those from variations in emissions and meteorology, have been evaluated and propagated.
- *Extend North American nested grid focused to represent Canadian impacts*: the relevant receptor region has been developed and tested, with final results pending simulation with the frozen, stable adjoint version.
- *Develop nested grids for Europe and southeast Asia:* These grids have been developed, with final validation pending simulation with the frozen, stable adjoint version.

Major Accomplishments

During this period of performance, the adjoint model was upgraded to the recently-released adjoint version 35. This also resulted in an extensive diagnostic effort, identifying, isolating, and resolving multiple unexpected software and data integrity issues present in version 35. An assessment of ammonia emissions uncertainty has been completed, revealing a potentially significant source of uncertainty in all existing estimates of aviation impacts on air quality. Additional nested domains and receptor regions have also been implemented in the adjoint model. Wherever possible, these improvements have been passed back to the adjoint community.

References

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Zhang, Q., Streets, D. G., Carmichael, G. R., He, K. B., Huo, H., Kannari, A., … Yao, Z. L. (2009). Asian emissions in 2006 for the NASA INTEX-B mission. Atmospheric Chemistry and Physics, 9(14), 5131–5153.

Outreach Efforts

Presented results at the ASCENT spring and fall meetings.
Presented air quality impacts mechanism at an ECMWF seminar.

Student Involvement

Graduate students involved in this project are: Irene Dedoussi, a PhD candidate in the Department of Aeronautics and Astronautics at MIT and Kingshuk Dasidhakari and Guillaume Chossière, Master's students in the Department of Aeronautics and Astronautics at MIT.

Plans for Next Period

Over the next period of this project (2017-2018), a frozen, stable version of the GEOS-Chem Adjoint rapid policy assessment tool will be generated which can be applied to both the problem of aviation impacts and the broader problems faced by the atmospheric modeling community. This version of the tool will incorporate multiple features not currently available to the community, such as the multiple consistent nested domains discussed above. The tool will also have been fully validated for multiple simulation years. The experience of the past project year has demonstrated the importance of independent validation of the community adjoint model which can be held stable and used for consistent policy analysis.

A key outcome of this testing and validation effort will be the development of a user-friendly framework for rapid policy assessment and analysis using the results from these new grids. A specific development priority will be a MATLAB-based tool which can accept a slate of policy options and return an estimate of impacts. Although previous work has focused on the global and North-American domain, these tools will incorporate results from all three of the now-available nested domains in parallel with the global results, while also incorporating the additional dimensionality of the division between US and Canadian impacts within the same nested domain.

These tools will also incorporate the results of another key task for the next period: the finalization of uncertainty in aviation sensitivities which has been propagated from underlying uncertainty in ammonia emissions. With an initial literature review now complete, significant existing uncertainty in the quantity of ammonia emitted within the target regions has been demonstrated. This will be combined with the existing work on assessing the impacts of background changes in emissions and in meteorology, providing a multidimensional assessment of the sensitivity of aviation impacts to variability and uncertainty.

The next period will see the launch of an ambitious multi-scale adjoint modeling assessment. The primary objective will be to scope out the benefits, requirements, and achievability of different approaches to investigating aviation impacts using adjoint models at multiple scales. Potential avenues of investigation include the use of multiple uncoupled global scales, internally coupled nested and global models, propagation of sensitivities through nested domain boundary conditions, or even the application of high performance computing techniques which have recently been mooted by the GEOS-Chem adjoint development team. Once this assessment is complete, a viability estimate will be produced for a specific approach to multi-scale adjoint modeling of aviation impact sensitivities.

In addition to these core research efforts, support will be provided for the non-volatile PM (nvPM) standards team, with a specific focus on ensuring consistency of upstream inputs. This will include the validation of gridded emissions data, a priority which intersects well with efforts to update and improve the emissions data within the adjoint model. Assistance will also be provided to the nvPM standard team in results interpretation and policy assessment using the tools described.

Collaboration will continue with the research teams that will be continuing ASCENT projects 18 and 19 to maintain consistency between assumptions and inventories in the rapid assessment tools, health impacts assessments and airport-specific analyses, as has been successfully done in the past with the groups of Prof. Levy at Boston University and Prof. Arunachalam at University of North Carolina. MIT will also continue to assist the teams (e.g. currently ASCENT 48 for the non-volatile PM standard work and ASCENT 39 for the assessment of naphthalene removal from jet fuel) who are either applying or require contributions from the adjoint tool for air quality analyses.

Finally, within the next period a deep refresh of the MIT computing infrastructure will be performed. The GEOS-Chem model is highly computationally intensive, and has become more so over time. Recent versions require significantly more computational power and disk space for the same simulated period. This affects the time taken for a production run but it also slows debugging efforts. The current generation of servers used for this work were purchased in 2010, and are reaching their effective end of life. As such, they will be replaced with a new generation of servers, in addition to higher-capacity network interconnects designed to better cope with the overwhelming data communication burden imposed by the adjoint.