U.S. Department of Transportation
Federal Aviation Administration

FINAL PROJECT REPORT

Form Approved:
O.M.B. No. 2120-0559
9/30/2013

PART I - PROJECT IDENTIFICATION INFORMATION

1. Institution and Address
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, MA 02139

2. FAA Program
ASCENT

3. FAA Award Number
13-C-AJFE-MIT, #7, 18, 25, 32, 41

4. Award Period
From 2014 To 2020

5. Cumulative Award Amount
850,000

6. Project Title
Development of NAS Wide and Global Rapid Aviation Air Quality – 20

PART II - SUMMARY OF COMPLETED PROJECT (For Public Use)

The project developed tools that enable rapid assessment of NAS wide and global impacts of aviation emissions on aviation-attributable PM, ozone, and resultant health outcomes for different policy scenarios. 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 enhanced the existing tools in terms of the domains and impacts covered, and in terms of uncertainty quantification. The project also packaged the tools in user-friendly code to be used internally by the FAA. In addition, this project provided data and technical support to ASCENT projects 14 and 48. The enhanced tools help support the FAA in its strategic vision to reduce the significant health impacts of aviation emissions, by providing a rapid way of assessing the significant health impacts of any present or future aviation emissions scenario.

PART III - TECHNICAL INFORMATION (For Program Management Uses)

1. **ITEM** (Check appropriate blocks)	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (X)	Approx. Date
a. Abstracts of Theses		☒			
b. Publication Citations		☒			
c. Data on Scientific Collaborators		☒			
d. Information on Inventions	☒				
e. Technical Description of Project and Results	■	☒			
f. Other (specify)	■				

2. Principal Investigator/Project Director Name (Typed)
Steven BARRETT

3. Principal Investigator / Project Director Signature

4. Date
10-30-2020

FAA Form 9550-5 (03-03) Supersedes Previous Edition

Part III – Technical Information

Thesis Abstracts

Kingshuk Dasadhikari (S.M., 2020)
Asia-Pacific anthropogenic emissions have changed rapidly in recent years due to industrialization, increasing mobility, and emissions controls. Although these changes have altered the region's burden of premature mortalities due to ambient fine particulate matter ($PM_{2.5}$), the contribution of each sector and effectiveness of different policy measures has not yet been quantified. Such data would inform future decision-making on both policy effectiveness and the relative importance of controlling emissions from different sectors. This study estimates changes in regional anthropogenic emissions by industrial sector between 2010 and 2015, based on sector-level activity indicators and enacted emission controls. These factors are applied to an existing high-resolution emissions inventory for 2010 to estimate emissions up to 2015. Using a chemical transport model, the effects of changes in each sector's contribution to total $PM_{2.5}$-driven premature mortalities are calculated for 2010 - 2015, in addition to the total contribution of each sector to premature mortality in 2015. 2,000,000 (95% CI: 1,740,000- 2,260,000) annual global $PM_{2.5}$-driven premature mortalities are attributed to Asia-Pacific anthropogenic sectoral emissions in 2015. The agricultural, industrial, and residential sectors constitute the top three sources of these total impacts. Between 2010 and 2015, sustained economic and activity growth, particularly in South and Southeast Asia, have led to 129,000 (95% CI: 106,000-166,000) additional annual premature mortalities, primarily across India, Indonesia, and Bangladesh. The energy and industrial sectors, in particular, cause 38,000 and 45,000 additional annual premature mortalities across these three countries respectively. Simultaneously, falling activity rates in other countries due to structural changes such as electrification of railroads, as well as newly introduced abatement measures over this period, including China's Action Plan on the Prevention and Control of Air Pollution as well as region-wide adoption of Euro IV/V/VI-compliant road vehicle emission and fuel quality standards have led to a total reduction of 95,000 (95% CI: 76,000-129,000) annual premature mortalities, primarily across East Asia, including China and Japan. These opposing drivers result in a net change of an additional 34,000 (95% CI: 23,000-47,000) $PM_{2.5}$-driven annual premature mortalities between 2010 and 2015 due to Asia-Pacific anthropogenic emissions.

Irene Dedoussi (Ph.D.), 2018
Combustion emissions impact the environment through chemical and transport processes that span varying temporal and spatial scales. Numerical simulation of the effects of combustion emissions and potential corresponding mitigation approaches is computationally expensive. Atmospheric adjoint modeling enables the calculation of receptor-oriented sensitivities of environmental metrics of interest to emissions, overcoming the numerical cost of conventional modeling. This thesis applies and further develops an existing adjoint of a chemistry-transport model to perform three evaluations, where the high number of inputs (due to the nature of the problem or the associated uncertainty) prevented comprehensive assessment in the past. First, this thesis quantifies the pollution exchange between the US states for seven major anthropogenic combustion emissions sectors: electric power generation, industry, commercial/residential, aviation, as well as road, marine, and rail transportation. This thesis presents the state-level fine particulate matter ($PM_{2.5}$) early death impacts of combustion emissions in the US for 2005, 2011 and 2018 (forecast), and how these are driven by sector, chemical species, and location of emission. Results indicate major shifts in the chemical species and sectors that cause most early deaths, and opportunities for further improving air quality in the US. Second, this thesis quantifies how changes in emissions impact the marginal atmospheric $PM_{2.5}$ response to emissions perturbations. State-level annual adjoint sensitivities of $PM_{2.5}$ population exposure to precursor emissions are compared for the years of 2006 and 2011, and correlated with the magnitude of emissions reduction and the background ammonia mixing ratio. Third, this thesis presents the development and evaluation of the discrete adjoint of the GEOS-Chem unified tropospheric-stratospheric chemistry extension (UCX), which enables the calculation of stratospheric sensitivities and the examination of the entire design space of high altitude emissions impacts. To illustrate its potential, sensitivities of stratospheric ozone to precursor species are calculated. This development expands the span of atmospheric chemistry- transport questions (including inversions) that this open-source model can be used to answer. The assessments performed in this thesis span spatial scales from the regional to the global and demonstrate the ability of this approach to provide information on both bottom-up and top-down mitigation approaches.

Publication Citations

Papers

Grobler, Carla, Philip J. Wolfe, Kingshuk Dasadhikari, Irene C. Dedoussi, Florian Allroggen, Raymond L. Speth, Sebastian D. Eastham, et al. 2019. “Marginal Climate and Air Quality Costs of Aviation Emissions.” Environmental Research Letters 14 (11): 114031. https://doi.org/10.1088/1748-9326/ab4942.

Dasadhikari, Kingshuk, Sebastian D. Eastham, Florian Allroggen, Raymond L. Speth, and Steven R. H. Barrett. 2019. “Evolution of Sectoral Emissions and Contributions to Mortality from Particulate Matter Exposure in the Asia-Pacific Region between 2010 and 2015.” Atmospheric Environment 216 (November): 116916. https://doi.org/10.1016/j.atmosenv.2019.116916.

Datasets

Grobler, Carla, Philip J. Wolfe, Kingshuk Dasadhikari, Irene C. Dedoussi, Florian Allroggen, Raymond L. Speth, Sebastian D. Eastham, et al. 2019. Marginal Climate and Air Quality Costs of Aviation Emissions - Supplementary Dataset. https://doi.org/10.6084/m9.figshare.9944954

Dasadhikari, Kingshuk, Sebastian D. Eastham, Florian Allroggen, Raymond L. Speth, and Steven R. H. Barrett. 2019. Estimated changes in anthropogenic emissions from the Asia-Pacific region from 2010 to 2015. https://doi.pangaea.de/10.1594/PANGAEA.899705

Theses

Dasadhikari, Kingshuk, 2019. Attribution of $PM_{2.5}$ Health Impacts in Asia-Pacific. Sm. Thesis. Massachusetts Institute of Technology. http://hdl.handle.net/1721.1/120383

Dedoussi, Irene, 2019. Adjoint sensitivity analysis of the atmospheric impacts of combustion emissions. PhD Thesis, Massachusetts Institute of Technology. http://hdl.handle.net/1721.1/120414

Data on Scientific Collaborators

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

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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University Participants

Massachusetts Institute of Technology

- P.I.: Steven R. H. Barrett
- FAA Award Number: 13-C-AJFE-MIT, Amendment Nos. 007, 018, 025, 032, and 041
- Period of Performance: Aug. 19, 2014 to Aug. 31, 2020 (via No-Cost Extension)
- Tasks:
    - Task 1. Develop a rapid air quality assessment tool to calculate the sensitivity of surface $PM_{2.5}$ and ozone globally and in the US to aviation emissions
    - Task 2. Expand the air quality assessment tool to include nested geographic domains
    - Task 3. Validate the rapid air quality assessment tool
    - Task 4. Operationalize the air quality assessment tool for internal use by FAA
    - Task 5. Calculate and analyze second-order sensitivities
    - Task 6. Investigate the effect of changing ammonia emissions on aviation impacts
    - Task 7. Support and assist the nvPM standard team (ASCENT 48) and ICAO CAEP CO2 standard (ASCENT 14)
    - Task 8. Perform scoping of work for developing a multi-scale adjoint tool

Project Funding Level

$800,000 FAA funding + $50,000 Transport Canada funding = 850,000 total sponsored funds, of which only the FAA funded $800,000 portion requires matching funds. 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

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

Project Overview

The project developed tools that enable rapid assessment of NAS wide and global impacts of aviation emissions on aviation-attributable PM, ozone, and resultant health outcomes for different policy scenarios. 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 enhanced the existing tools in terms of the domains and impacts covered, and in terms of uncertainty quantification. The enhanced tools help support the FAA in its strategic vision to reduce the significant health impacts of aviation emissions, by providing a rapid way of assessing the significant health impacts of any present or future aviation emissions scenario.

Task 1. Develop a rapid air quality assessment tool to calculate the sensitivity of surface $PM_{2.5}$ and ozone globally and in the US to aviation emissions

Objective(s)

Develop a computationally efficient way of evaluating the sensitivity, or first-order derivative, of a given metric (e.g., population exposure to fine particulates) with respect to inputs such as emissions of different aviation-relevant chemical species at all relevant altitudes. This approach allows to overcome the computational burden of classical atmospheric modeling and provides policymakers with information on where and when emissions reductions matter most.

Research approach

The first task involved extending the GEOS-Chem adjoint model to include the calculation of the sensitivity of global and US-level $PM_{2.5}$ and ozone to aviation emissions. This capability complements the $PM_{2.5}$ capability and allows for more extensive analysis. As a result, the global rapid air quality assessment tool allows us to distinguish LTO from non-LTO impacts and capture differential scenarios. This also allows the study of transport of cruise emissions between regions in the global domain (Koo et al. 2013). The grid decomposition used globally and in the nested US domain is shown in in Figure 1 and Figure 2.

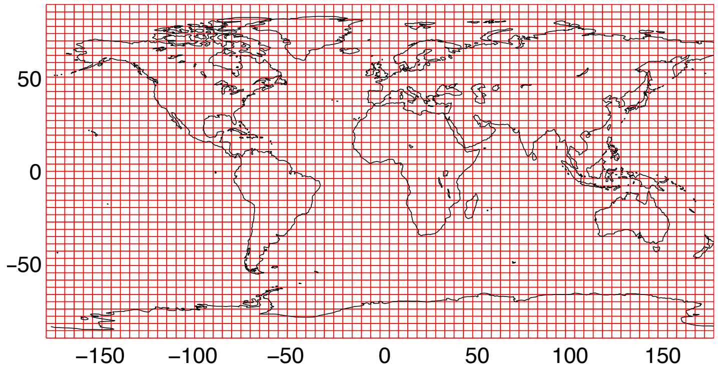


Figure 1: GEOS-Chem global 4°×5° grid

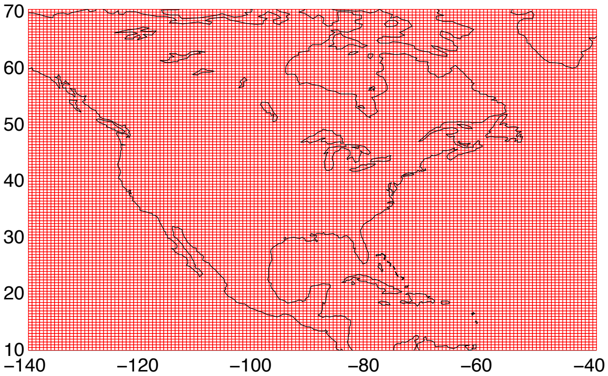


Figure 2: GEOS-Chem NA nested 0.5°×0.667° grid

In order to complete this task, we updated the version of the GEOS-Chem model that we are using and produced up-to-date results. The aviation emissions inventory used in our calculations also needed to be updated, and we worked with the Volpe Center to obtain and validate the new inventory data.

In order to capture impacts of aviation on ozone which are relevant to health, we needed to modify the adjoint to capture health-relevant metrics of ozone concentrations. Whereas $PM_{2.5}$ impacts are usually given as a function of 24-hour average surface concentration, ozone impacts are typically quantified based on the 8 or 1-hour maximum daily average concentration. The time of day of the ozone maximum requires *a-priori* evaluation, and the adjoint model needed to be modified to be able to capture this. The forward GEOS-Chem was used to identify the portion of each day when O_3 contributes to health impacts in each location, and a modified adjoint objective function was developed which could utilize this information.

We collaborated with the ASCENT 18 project contributors to identify the optimal metric for ozone health impacts. Jon Levy and his team suggested an appropriate metric for ozone exposure, and helped us with the choice of the concentration-response function to be used. The one that was chosen, based on the 1-hour daily maximum concentration, ensures consistency with the current health impact assessment standards.

Once these data were obtained and the model properly updated and validated, we needed to implement the calculation of the ozone impacts in the code, test our implementation, and finally run the model to obtain sensitivities. The computational process is shown in Figure 3.

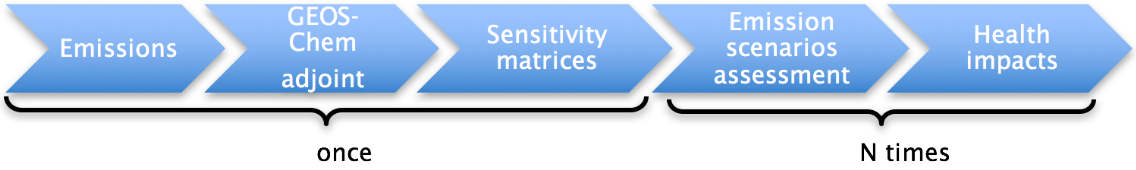


Figure 3: Computational workflow

The sensitivities calculated allow us to quantify the speciated, temporal, and spatial origins of the population exposure to $PM_{2.5}$ and ozone. Specifically, they allow us to decouple the LTO and non-LTO impacts, as well as to calculate what percentage of the total aviation impacts originates from each aviation emissions species. In terms of the temporal aspect, they allow us to see if there is any seasonality in the importance of emissions in driving the $PM_{2.5}$ exposure and hence premature morality impacts. Specifically, we find that the SO_2 sensitivity over the full flight altitude layers exhibits significant seasonality. Emissions over the summer months (April to September) are approximately twice as impactful in terms of $PM_{2.5}$ exposure than those over the winter months (October to March). This implies that the benefit of sulfur emissions control (e.g. using alternative fuels, or low sulfur jet fuel) over the summer is twice as high as that of the winter.

$$\frac{\partial \mathrm{J}}{\partial(\mathrm{SO_2})}(i,j,k,t)$$

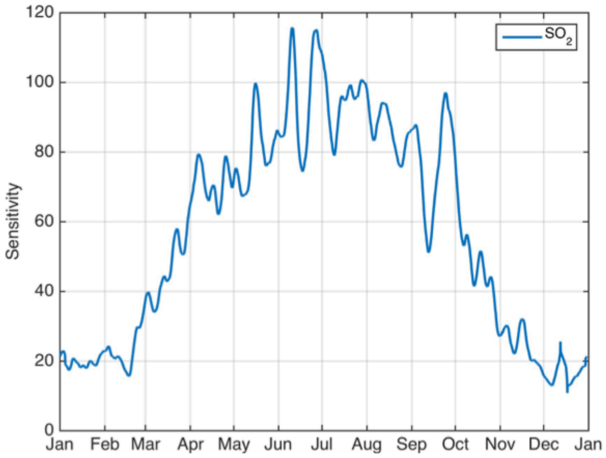


Figure 4: Seasonality in the SO2 sensitivity

The 3D sensitivity matrices can be used to assess the impacts of different emissions scenarios. The health impacts associated with a specific emissions scenario are given by the inner matrix multiplication of the sensitivity matrix with the emissions matrix as shown in Figure 5. This computation is of negligible computational cost, compared to the 3D Chemical Transport Model (CTM) tools that have been conventionally used until now in assessing air quality impacts of different emissions. This is the main benefit of the adjoint approach.

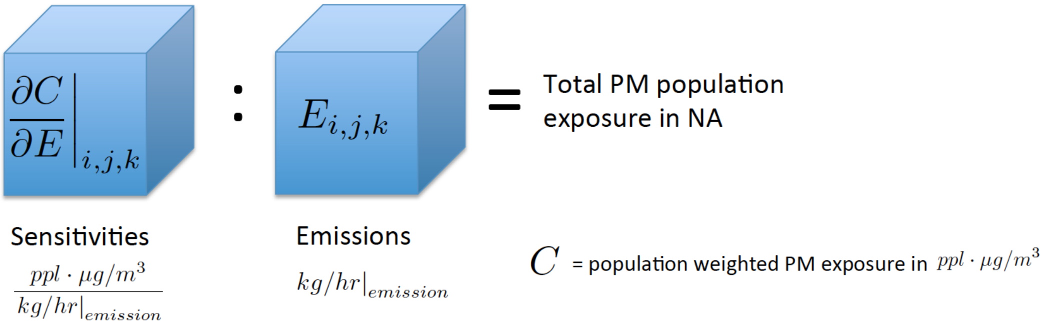
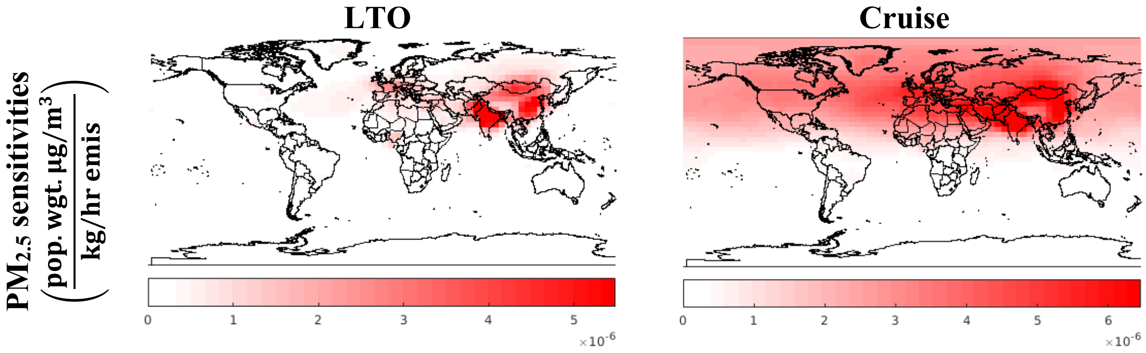


Figure 5: Application of sensitivities

As a result of the work completed under this task, we produced and made available to the FAA the following maps of sensitivity to NO_x emissions. Similar maps for SO_2 and black carbon have been produced and made available to the FAA.



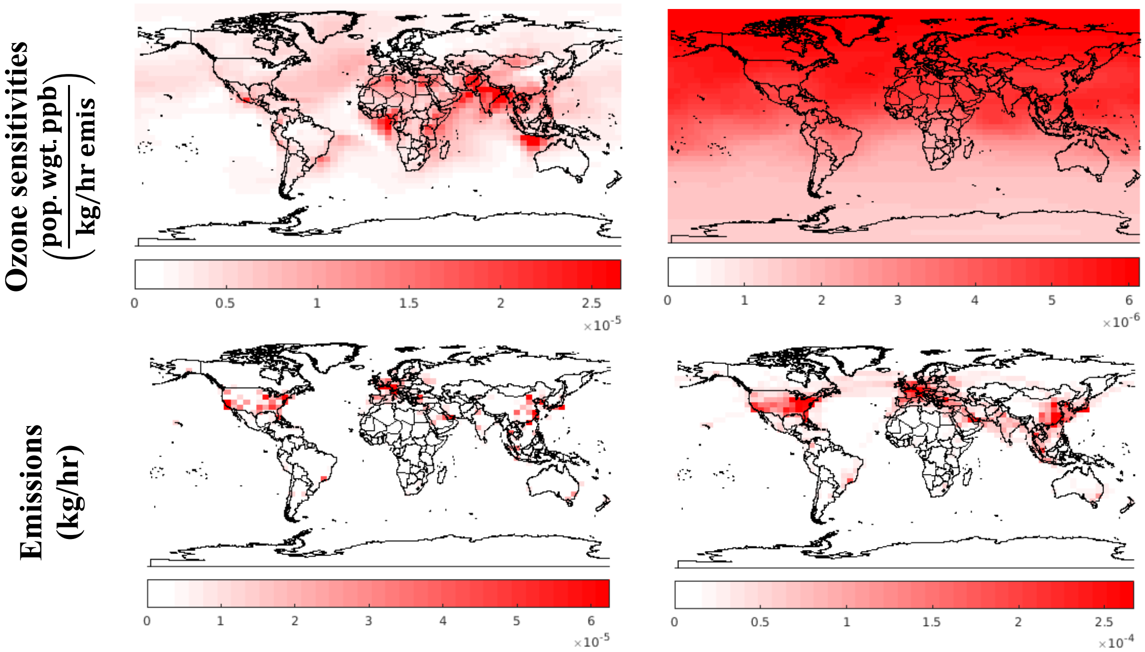


Figure 6: Global sensitivity to and aviation NOx emissions in 2015. Color scales differ between panels to allow geographical distributions to be more easily resolved. Sensitivities show the annual average response.

Multiplying the emissions matrix for each species emitted by aviation element-wise by the corresponding sensitivity matrix and summing the products (the Technical Guidance document contains further details on these operations) allows us to compute the total health impacts of aviation 2015 emissions in each region. We find that uncertainties in the health-response function yields a 95% confidence interval of (-49%, +50%).

In addition, previous MIT research found that aviation emissions result in ~16,000 premature mortalities annually due to impaired air quality (Yim et al. 2015; Eastham and Barrett 2016). When aiming to reduce these impacts and the impacts from climate change, decision makers often face trade-offs between different emission species or impacts in different times and locations. To inform rational decision-making, the sensitivity data computed for ASCENT 20 was combined with climate impact data from ASCENT 21. This enabled us to compute aviation's marginal climate and air quality impacts per tonne of species emitted, while accounting for the altitude and chemical composition of the emissions. Under ASCENT 20, global sensitivity data was used to determine air quality impacts. Uncertainty in chemistry transport modeling was incorporated using scaling factors based on prior literature. Uncertainty in climate, health impact, and economic factors was also quantified.

We found that air quality impacts account for 64% of the combined climate and air quality impacts, and that the majority of these impacts are associated with cruise-level NO_x emissions. A sensitivity study was also conducted to find the contribution of each of the uncertain Monte Carlo input variables to the observed output variance. We found uncertainty in the climate sensitivity and the DICE damage function to be the largest drivers in total output uncertainty.

A detailed description of the research approach, and results can be found in Grobler et al (2019). These findings were communicated to the FAA in a briefing.

Major accomplishments

We updated the GEOS-Chem adjoint model to produce maps of sensitivity of surface concentration of $PM_{2.5}$ and ozone to aviation emissions and delivered them to the FAA. These maps allow for rapid air quality assessment of large number of policy scenarios resulting in changes in aviation emissions. We also supported several applications of the updated tool.

Publications

Dedoussi, IC and Barrett, SRH (2015): US aviation air quality impacts and comparison with other sectors. 2015 Aircraft Noise and Emissions Reduction Symposium (ANERS), September 22-25, 2015, La Rochelle, France.

Grobler, Carla, Philip J. Wolfe, Kingshuk Dasadhikari, Irene C. Dedoussi, Florian Allroggen, Raymond L. Speth, Sebastian D. Eastham, et al. 2019. "Marginal Climate and Air Quality Costs of Aviation Emissions." Environmental Research Letters 14 (11): 114031. https://doi.org/10.1088/1748-9326/ab4942.

Outreach

Results were presented at the 2018 ASCENT Spring and Fall meetings.

Awards

Carla Grobler was awarded the 2020 Joseph Hartman award for her 2020 paper.

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasadhikari, MS student in the Department of Aeronautics and Astronautics at MIT

Task 2. Expand the air quality assessment tool to include nested geographic domains

Objective(s)

This task aims to: (1) 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; and (2) 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

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, we have increased the dimensionality of our analysis by providing alternative cost functions which take into account the needs of different stakeholders.

To this end, we have developed the receptor region for the Canadian portion of GEOS-Chem Adjoint's North American nested grid, including incorporation of the population map for Canada (Figure 7). 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.

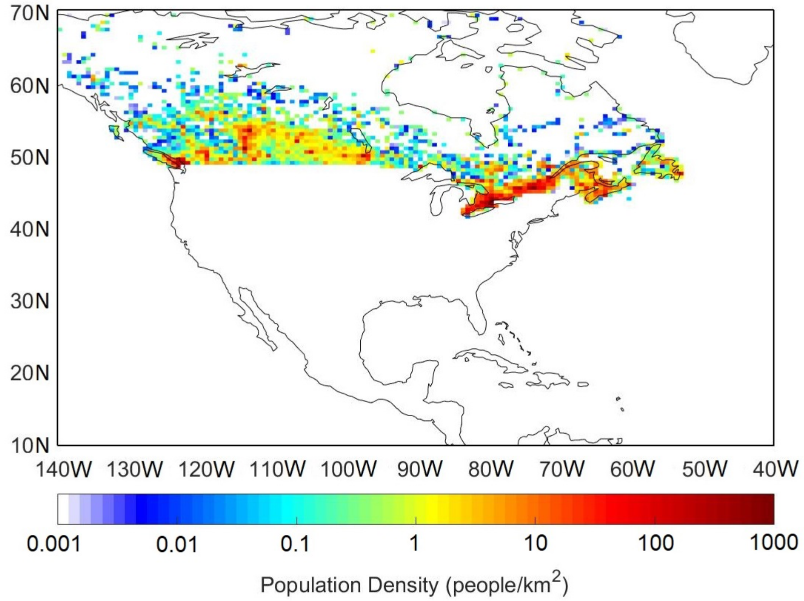


Figure 7: Population distribution used for calculation of sensitivity of Canadian air quality with respect to aviation emissions

In addition, given the global nature of aviation, much of our research to date has focused on global impacts using global models with global population maps used to define the receptor regions and weighting. However, our investigations using the North American nested domain have revealed that there are significant advantages to higher-resolution simulation over smaller domains, and these advantages are likely to be true for domains outside of North America. 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, Britter, and Waitz 2010; Eastham and Barrett 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, we have developed two additional nested domains for use with the GEOS-Chem adjoint. The first is the South-East Asia nested domain. This domain, modeled at a resolution of 0.5×0.667 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.

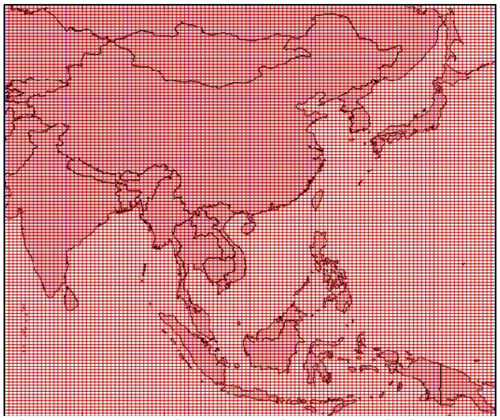


Figure 8: Southeast Asia nested domain

Example sensitivity maps to aviation NO$_x$ emissions for the nested Asia domain are shown in Figure 3. Beside committing work to capability extension, the project team conducted a validation of the tool by comparing the calculated health impacts attributable to aviation and due to exposure to PM$_{2.5}$ and ozone to the results obtained by modeling the impacts of aviation emissions on ground-level population exposure to PM$_{2.5}$ and ozone obtained from the forward model of GEOS-Chem. In both cases, the total health impacts were calculated using the gridded FAA AEDT-2015 aviation emissions. The comparisons between forward and adjoint results are presented in the Technical Guidance document delivered to the FAA along with the most up-to-date sensitivity data. The error between the impacts computed using the forward and adjoint methods vary from 1% to 31%, with the highest error observed for the MDA-8 O$_3$ impacts for the Canadian receptor region. These errors are within the expected bounds for adjoint-based results.

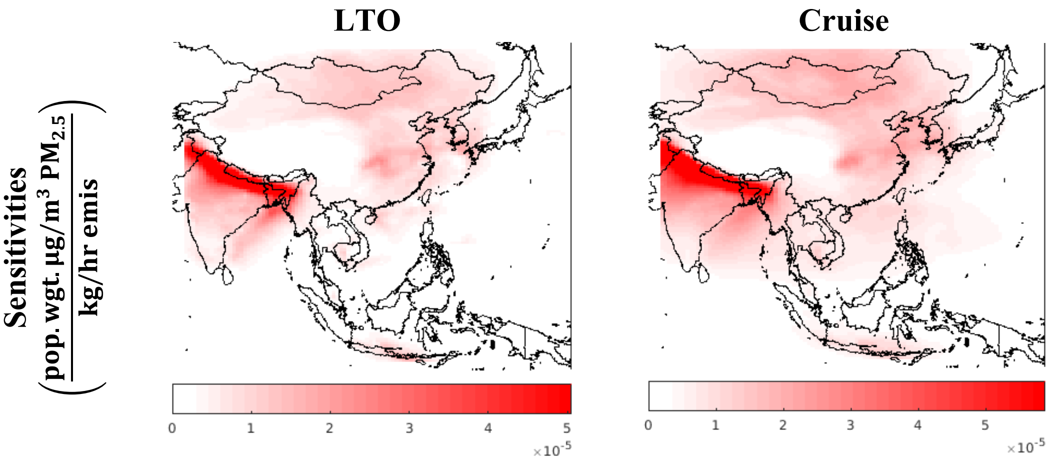


Figure 9: Example maps of the sensitivity of population-weighted PM2.5 concentrations to aviation NOx emissions during LTO (left) and at cruise altitude (right).

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's adjoint 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, we have acquired and implemented the most recent version of the EDGAR global anthropogenic emissions inventory (v4.3), 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, we generated an updated emissions map for Asia to cover the period 2010-2015. The impact of aviation on air quality throughout the region was quantified in a paper resulting from this project (Dasadhikari et al, 2019).

Publications

Dasadhikari, Kingshuk, Sebastian D. Eastham, Florian Allroggen, Raymond L. Speth, and Steven R. H. Barrett. 2019. "Evolution of Sectoral Emissions and Contributions to Mortality from Particulate Matter Exposure in the Asia-Pacific Region between 2010 and 2015." Atmospheric Environment 216 (November): 116916. https://doi.org/10.1016/j.atmosenv.2019.116916.

Outreach

We presented results at the ASCENT spring and fall meetings, and we presented the air quality impacts mechanism at an ECMWF seminar.

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

Task 3. Validate the rapid air quality assessment tool

Objective(s)

Compare results from the rapid air quality assessment tool to those from conventional modeling studies, and quantify sources of uncertainty.

Research approach

To ensure accuracy of the sensitivities computed using the adjoint tool, we compare aviation-attributable changes in $PM_{2.5}$ and ozone as estimated using adjoint sensitivities (post-multiplied by gridded FAA AEDT-2015 aviation emissions) compared to conventional forward modeling results. These later results were obtained by modelling ground-level PM2.5 and ozone distributions with AEDT-2015 aviation emissions turned on and off, and taking the difference. These comparisons are presented as bar plots in Figure 11. Error between impacts computed using the forward and adjoint approaches vary from 1% to 31%, with the highest error observed for the MDA-8 O3 impacts for the Canadian receptor region.

While the adjoint modelling method offers benefits of computational efficiency in policy analyses, it also has multiple inherent limitations, including some that are shared with the forward model, and some that are unique to the adjoint. Results from both models are subject to uncertainty. One contributor is uncertainty in background emissions, particularly in background (non-aviation) emissions of ammonia for evaluation of aviation-attributable $PM_{2.5}$ impacts, and in background emissions of NO_x and VOCs for evaluation of aviation-attributable ozone impacts. In order to quantify these components of uncertainty, a separate study was performed (Task 6) analyzing the contribution of background uncertainty in ammonia on aviation-attributable $PM_{2.5}$ health impacts as computed using the adjoint.

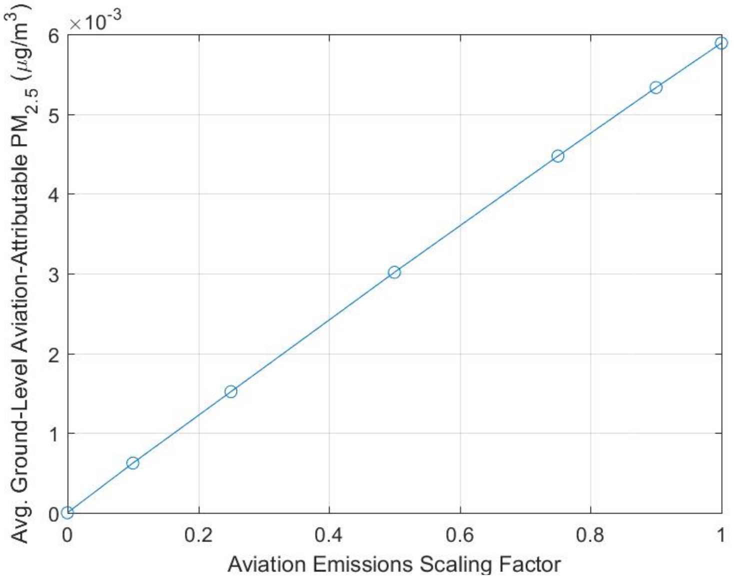


Figure 10: Linearity test for aviation-attributable ground-level $PM_{2.5}$

Uniquely, adjoint sensitivities only capture the linear gradient of the objective function (e.g. population exposure to $PM_{2.5}$) around whatever atmospheric state is described by the baseline simulation. It is therefore necessary to ensure that the response of the objective function is roughly linear across the range of scenarios of interest. For impacts due to aviation-attributable $PM_{2.5}$, this was tested by varying aircraft emissions (including both LTO and cruise emissions) by a scaling factor and checking the change in aviation-attributable ground-level concentration (non-weighted) of $PM_{2.5}$.Figure 10: Linearity test for aviation-attributable ground-level PM2.5 Figure 10 shows the variation of these parameters, confirming that aviation impacts remain within the linear regime. Therefore, the adjoint method is appropriate to quantify aviation-attributable $PM_{2.5}$ impacts.

Major accomplishments

We compared the results produced by the rapid air quality assessment tool developed in this project to a well-established chemistry-transport model and quantified the accuracy of the tool.

Publications

None

Outreach

Presented results at the ASCENT spring and fall meetings.

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

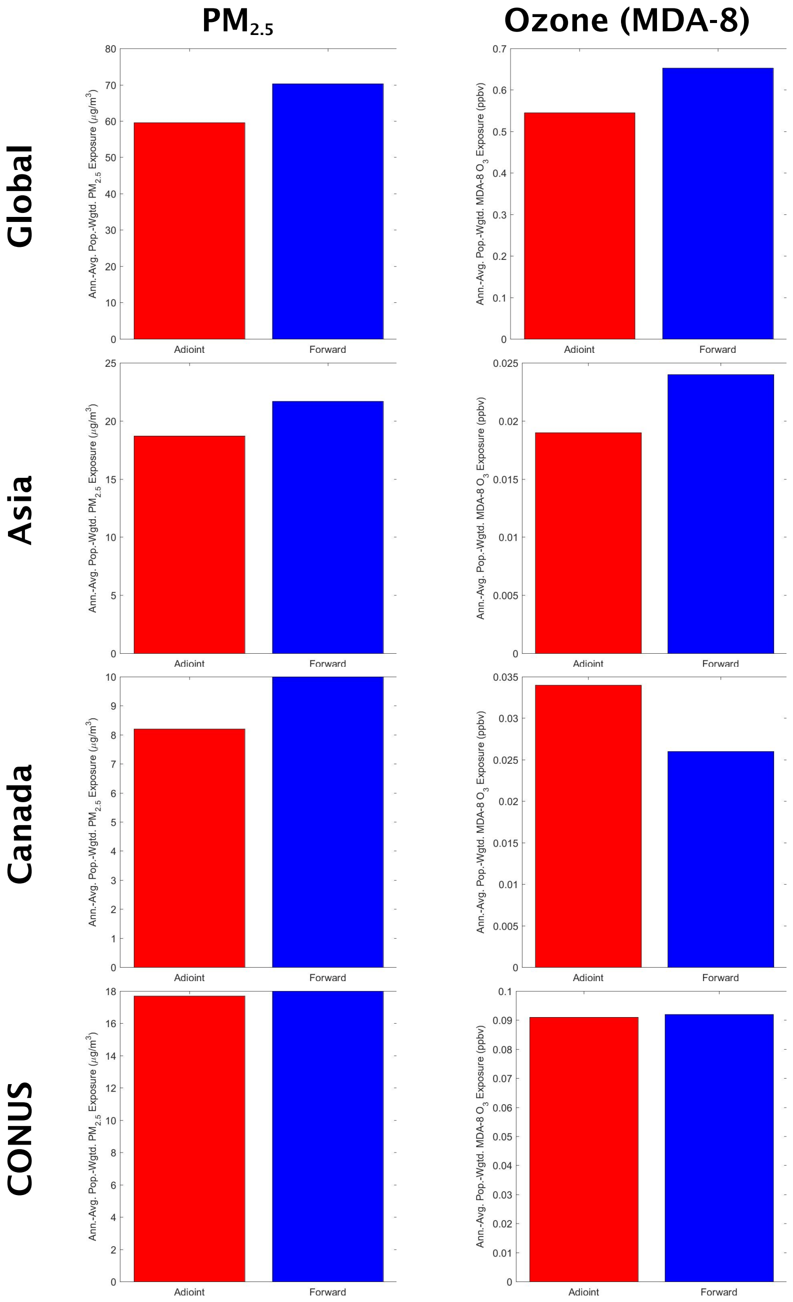


Figure 11. Comparison of aviation-attributable annual-average population-weighted exposure to PM2.5 and MDA-8 ozone, as computed from GEOS-Chem forward model and adjoint

Task 4. Operationalize the air quality assessment tool for internal use by FAA

Objective(s)

Operationalize the rapid air quality assessment tools and transition them to the FAA. The various model updates and the additions of the new nested domains were to be packaged and wrapped with a user-friendly MATLAB script and passed to the FAA with a brief guidance document, as previously performed for the North American domain.

Research approach

In the context of supporting the FAA in using the policy assessment tools, MIT organized and performed a series of trainings, one of which was on the adjoint air quality tool for the global and nested NA domains. The training consisted of two parts: an information session (performed remotely on Oct 27th 2015) and a hands-on training (performed at the FAA office on Oct 29th 2015). The information session aimed to present the motivation behind this (global and nested NA) tool, and to provide an overview of the application of the tool. It was aimed for people who are going to run or interpret the tool, and for people who are going to manage projects that involve the use of this adjoint tool. The broader capabilities and limitations of the tool and some of the future work aspects were also mentioned. This WebEx presentation has been recorded and transferred to the FAA in order to assist with future training later on and/or serve as a reference for how to use the tool. The hands-on training involved the application of the tool to a set of sample inputs, and the transfer of the tool (code and examples) to the FAA server/workstations.

In addition, the different model updates and the addition of the latest nested domains (namely Canada and Southeast Asia) have been packaged and wrapped in a MATLAB script to be delivered to the FAA along with the underlying data and supporting documentation on how the sensitivities were calculated and how to use them for practical health impacts calculations. This piece of software will be updated in the future as new domains become operational and as the air quality impacts assessment tool gets updated. Uncertainty analysis will also be included in this piece of software in the future. Please refer to the technical guidance document for further details on this part of this period of performance.

Major accomplishments

The rapid air quality assessment tool was operationalized and packaged in a user-friendly MATLAB script, with several in-person training sessions held. This enabled the FAA to conduct air quality impacts analysis using up-to-date outputs from the air quality assessment tool.

Publications

None

Outreach

Results were presented at the 2018 ASCENT Spring and Fall meetings.

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

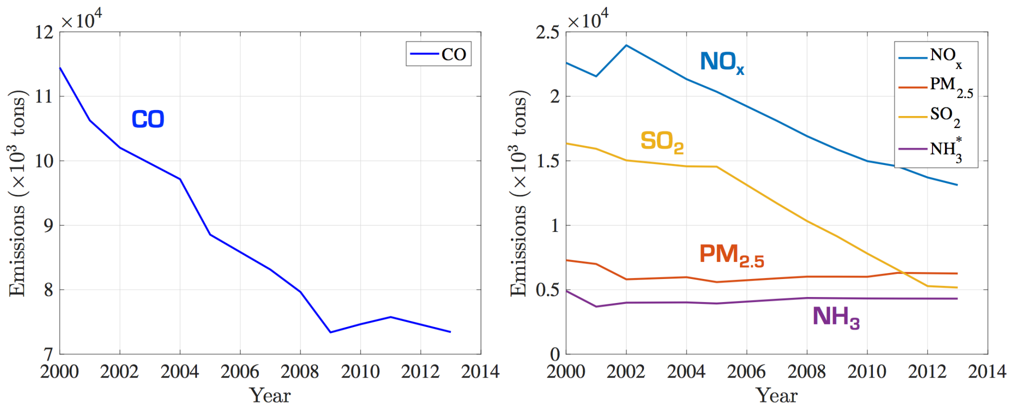
Task 5. Calculate and analyze second-order sensitivities

Objective(s)

Analyze the variation of the sensitivity of population exposure to $PM_{2.5}$ and ozone to aviation emissions over time.

Research approach

We investigated how the adjoint sensitivities depend on background concentrations of relevant chemical species (and therefore background emissions). This is of interest as there have been significant changes in anthropogenic emissions since 2000, as shown in Figure 12 for the US. The aim of this part of the project is to capture the impacts of the change in background emissions to the GEOS-Chem adjoint particulate matter ($PM_{2.5}$) sensitivity values. In order to calculate this impact, we calculated the sensitivities for two different years, specifically 2006 and 2011, taking into account changes in background emissions and meteorology. By comparing the 2011 sensitivities with the sensitivities of 2006, we were able to quantify the impacts that the changing atmospheric composition has on the atmospheric response to emissions (i.e. the adjoint sensitivities).



*NH3 in thousands of short tons

Figure 12: Anthropogenic emissions reductions in the US (US EPA 2015)

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. With the upgrade to version 35 of the adjoint, we were able to calculate sensitivities using meteorology generated by the current-generation GEOS-FP output from the GEOS-5 model. This allows us to re-calculate sensitivities on an ongoing basis, up to and including the current day. We estimate that changes in meteorology caused a 7% change in sensitivity between 2006 and 2011, compared to ~10% attributable to changes in population.

The major findings are presented in Figure 13 and Figure 14 below. We find that the sensitivity of $PM_{2.5}$ to NO_x emissions increased in some locations between 2006 and 2011, with the largest change in California. Sensitivities to SO_2 emissions instead decreased in most locations between 2006 and 2011, although there were some significant increases along the

East coast and in the Northwest. The sensitivity changes are the superposition of a variety of phenomena, including the changing emissions (in particular those of SO_2 and NO_x), meteorology, and population.

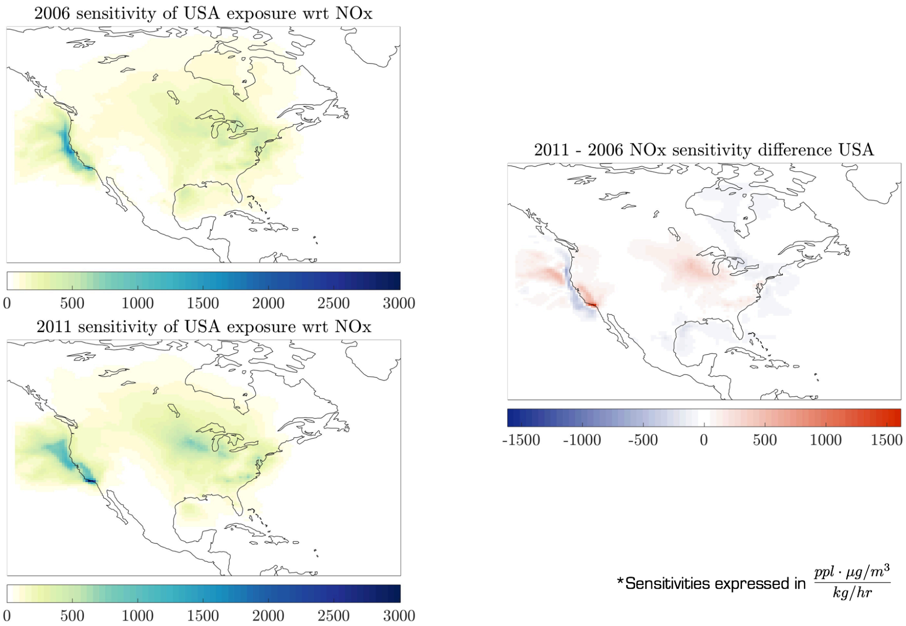


Figure 13: Sensitivity of US population exposure to $PM_{2.5}$ with respect to a unit of near-surface NOx emissions for 2006, 2011, and the difference between the two

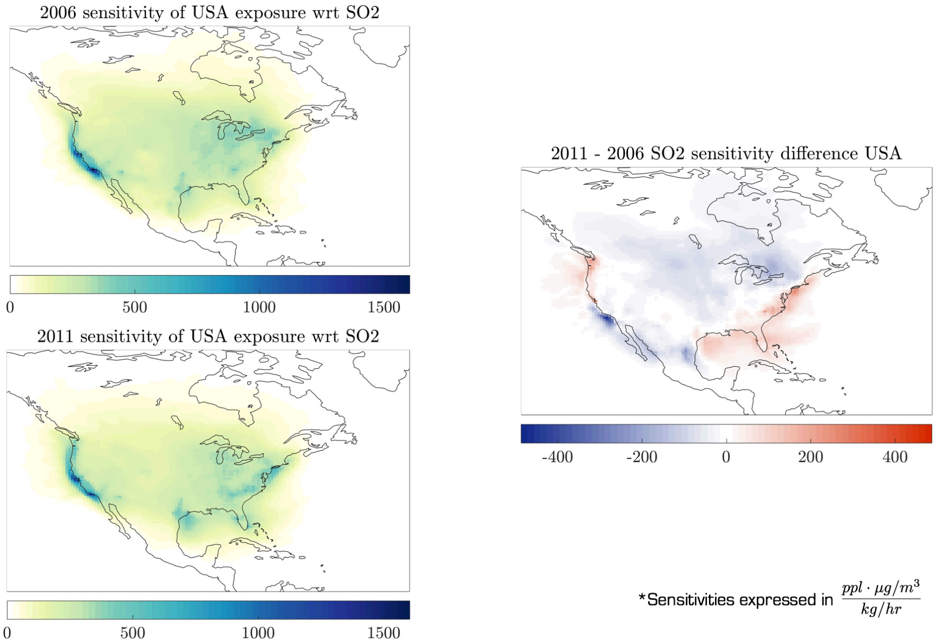


Figure 14: Sensitivity of US population exposure to $PM_{2.5}$ with respect to a unit of near-surface SO_2 emissions for 2006, 2011, and the difference between the two

Major accomplishments

The result of these task provides policymakers with important insights into the evolution in time of the emissions that matter the most. By comparing 2006 to 2011 sensitivities, we found that the importance of NO_x emissions for US population exposure to $PM_{2.5}$ increased over time, while that of SO_2 emissions decreased over time.

Publications

None

Outreach

We presented results at the ASCENT spring and fall meetings, and we presented the air quality impacts mechanism at an ECMWF seminar.

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

Task 6. Investigate the effect of changing ammonia emissions on aviation impacts

Objective(s)

This task aims to understand the relationship between changing ammonia emissions and aviation impacts on air quality.

Research approach

A key (and, as yet, unquantified) source of uncertainty 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 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.

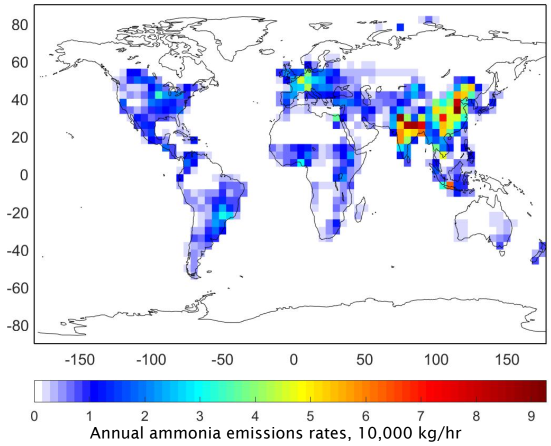


Figure 15: Baseline global ammonia emissions. Data are taken from the EDGAR v4.3.1 inventory.

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. We provide more details about this method and its application to project ASCENT 20 below. The global emissions that are currently used in the tool are plotted in Figure 15 at a resolution of 4°×5°. These emissions are taken from the EDGAR v4.3.1 inventory (Crippa et al. 2016), distributed as shown in Table 1.

Table 1: Baseline estimate of ammonia emissions by region.

Region	Emission Total (Tg/Year)
Global	55.06 (*100%*)
China	14.02 (*25.5%*)
Other Asia	17.81 (*32.3%*)
Europe	5.65 (*10.3%*)
USA	4.17 (*7.57%*)
Other North America	2.11 (*3.83%*)
Other	11.24 (*20.4%*)

A key task that was performed during this period of performance was to estimate from a literature review the uncertainty associated with these regional ammonia inventories. Although some studies suggest a low level of uncertainty in the overall global ammonia budget, with estimates ranging from 5 to 20% 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, 20) and ~50% for China (Zheng et al. 2012). The results are shown in Table 2. The column "Applied to" refers to the region to which the uncertainty was applied.

Table 2: Regionalized uncertainty in ammonia emissions.

Region	Relative uncertainty	Applied to	Source
Global	(−18.75 %, +18.75 %)	Other	(Beusen et al. 2008)
China	(−43 %, +50 %)	China, Other Asia	(Zheng et al. 2012)
Europe	(−30 %, +30 %)	Europe	(EMEP 2009, 2009)
USA	(−36 %, +36 %)	USA, Other NA	(Zhu et al. 2013, 2)

In order to compute the impact of these uncertainties in ammonia emissions on aviation-attributable health impacts, we first compute the first-order sensitivities of the desired health impacts to NH_3 emissions with and without aviation emissions. By multiplying the difference of these two matrices (whose values are expressed in units of $\frac{\mu g(PM_{2.5})/m^3}{kg(NH_3)/hr}$) by the uncertainty in ammonia emissions (in $\frac{kg\,(NH_3)}{hr}$), we compute, in each grid cell, the share of the uncertainty in the calculated total aviation-attributable impacts that can be traced back to uncertainties in ammonia emissions. The application of this method yielded the results shown in Table 3.

Table 3: Uncertainty in aviation impacts due to uncertainty in ammonia emissions.

Summary	
Aviation-attributable, population-weighted PM$_{2.5}$	59.6 ng/m^3 (*baseline*)
NH$_3$-driven uncertainty	(−24.0, +27.0) ng/m^3 *(−40.2%, +45.5%)*
Regional Contributions to NH$_3$-Driven Uncertainty	**China:** (−11.9, +13.8) ng/m^3 (*−43.9%, +51.1%*) **Other Asia:** (−6.6, +7.7) ng/m^3 (*−24.5%, +28.5%*) **Europe:** ± 4.0 ng/m^3 (*± 6.7%*) **USA:** ± 1.1 ng/m^3 (*± 1.8%*) **Other NA:** ± 0.1 ng/m^3 (*± 0.4%*) **Other:** ± 0.2 ng/m^3 (*± 0.7%*)

Major accomplishments

A full uncertainty quantification has estimated the share of the uncertainty in aviation-attributable health impacts that can be traced back to uncertainties in inventories of ammonia emissions.

Publications

None

Outreach

Results were presented at the 2018 ASCENT Fall meeting and 2019 Spring meeting.

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

Task 7. Support and assist the nvPM standard team (ASCENT 48) and the ICAO CAEP CO$_2$ standard (ASCENT 14)

Objective(s)

This part of our objectives consisted mainly in assisting the PM standard team and ensuring data consistency in their inputs such as gridded emissions data. We also provided them with support in the interpretation of their results. In addition, we applied the sensitivities we produced to the ICAO CAEP 10 CO$_2$ standard.

Research approach

We provided support 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 our efforts to update and improve the emissions data within the adjoint model. We will also assist the nvPM standard team in results interpretation and policy assessment using the tools described.

Additionally, the rapid air quality policy assessment tool was for the first time applied in the ICAO CAEP CO_2 standard work, where multiple scenarios were analyzed and compared. The ASCENT 20 team supported the ASCENT 14 team in interpreting the results and compiling the Information Paper that was presented at the CAEP meeting.

This global adjoint air quality tool, due to its source-oriented focus, as well as the minimal computational cost involved in applying the sensitivities to assess the impacts of emissions scenarios, was applied in the CO_2 standard policy assessment project (ASCENT 14), in order to quantify the air quality impacts of the proposed scenarios. Given that this was the first time that this tool was applied in a real-life policy, the interaction of the tool with upstream (emissions modeling) and downstream (monetization) processes had to be streamlined. The different process steps followed from emissions data to monetized scenario impacts are shown in the flow diagram below Figure 16. The gridded emissions provided by VOLPE had to be re-gridded into the GEOS-Chem global grid. The emissions preprocessor was thus developed to perform this task. The adjoint tool was also accompanied with some Monte Carlo simulations to estimate how the different sources of uncertainty (e.g. emissions uncertainties, CRF uncertainty, etc) propagate throughout the process.

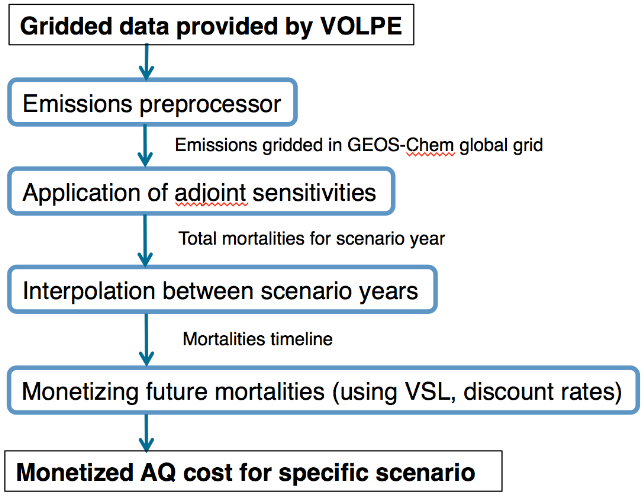


Figure 16: Process flow for scenario assessment

Major accomplishments

Contributed to the ICAO CAEP Information Paper on the cost-benefit analysis of the ICAO CO_2 stringency options and provided support to the ASCENT 48 team.

Publications

Brenner, M.; Yutko, B.; Wolfe, P.; Dedoussi. I. US cost-benefit analysis of ICAO CO_2 standard stringency options. ICAO CAEP Information paper to inform CO_2 standard work. 12/14/2015.

Outreach

We coordinated with the teams of ASCENT projects 48 and 14 and with stakeholders of the ICAO CAEP Information Paper on the cost-benefit analysis of the ICAO CO_2 stringency options

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

Task 8. Perform scoping of work for developing a multi-scale adjoint tool

Objective(s)

Perform scoping of work for developing a multi-scale adjoint tool that will enable the calculation of impacts from emissions occurring outside of the current nested domains, at the global scale. Perform comparison of aviation AQ impacts estimated using the global grid with the fine/nested grids' corresponding calculations.

Research approach

The development of a multiscale sensitivity analysis framework would combine the advantages of low-resolution global modeling for cruise sensitivity analysis with the advantages of high-resolution local modeling for resolving surface-level variations. Based on the work completed in this period of performance, a potential solution has been identified which would require to implement substantial modifications of the adjoint tool.

The proposed solution would involve re-engineering the adjoint to directly include sensitivity to changes in boundary conditions, supported by a finite-difference forward simulation to evaluate how the boundary conditions are affected by aviation. This effort would be supported by a multi-tier forward analysis to evaluate the difference in calculated impacts between the forward global, adjoint global, forward nested, and adjoint nested simulations.

Major accomplishments

Scoping work was conducted for developing a multi-scale adjoint tool that will enable the calculation of impacts from emissions occurring outside of the current nested domains, at the global scale. We determined that a tool developed using the approach above would be able to represent both the global-scale effects of changes in cruise altitude emissions and the local-scale effects of LTO emissions in a single, consistent tool. It would also yield unprecedented accuracy in estimating the effects of changes in cruise-altitude emissions on surface air quality in the US, Europe, and Asia.

Publications

None

Outreach

None

Awards

None

Student Involvement

Irene Dedoussi, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Guillaume Chossière, PhD candidate in the Department of Aeronautics and Astronautics at MIT
Kingshuk Dasidhakari, MS student in the Department of Aeronautics and Astronautics at MIT

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