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Data Assimilation Schemes in Colombian Geodynamics - Cooperative Research Plan for 2017 -2020 Between Universidad EAFIT and TUDelft

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Outline

- Introduction & Research relevance
 - Environmental Emergency (Contingency) 2016
 - Air Quality & Pollution
 - Air Quality Monitoring & Modeling (Valle de Aburrá)
- Theoretical framework
- Research Proposal

Environmental Emergency (a.k.a. Contingency)

Medellin, Mar-Apr 2016

Medellin, jueves 12 de febrero de 2016, 7:00 am



Medellin, miércoles 30 de marzo de 2016, 7:00 am



Environmental Emergency (a.k.a. Contingency)

Medellin - Mar 18-Apr 19, 2016

- $PM_{2.5} > 125 \mu\text{g}/\text{m}^3$
(WHO guidelines max. $25 \mu\text{g}/\text{m}^3$)
- Days without car & motorcycles
- Restricted truck (*volquetas*) movement
- Cease of outdoor activities
- Regional rush hour traffic restrictions (*pico y placa*)
- Free Metro



Source: El Colombiano, Medellín.

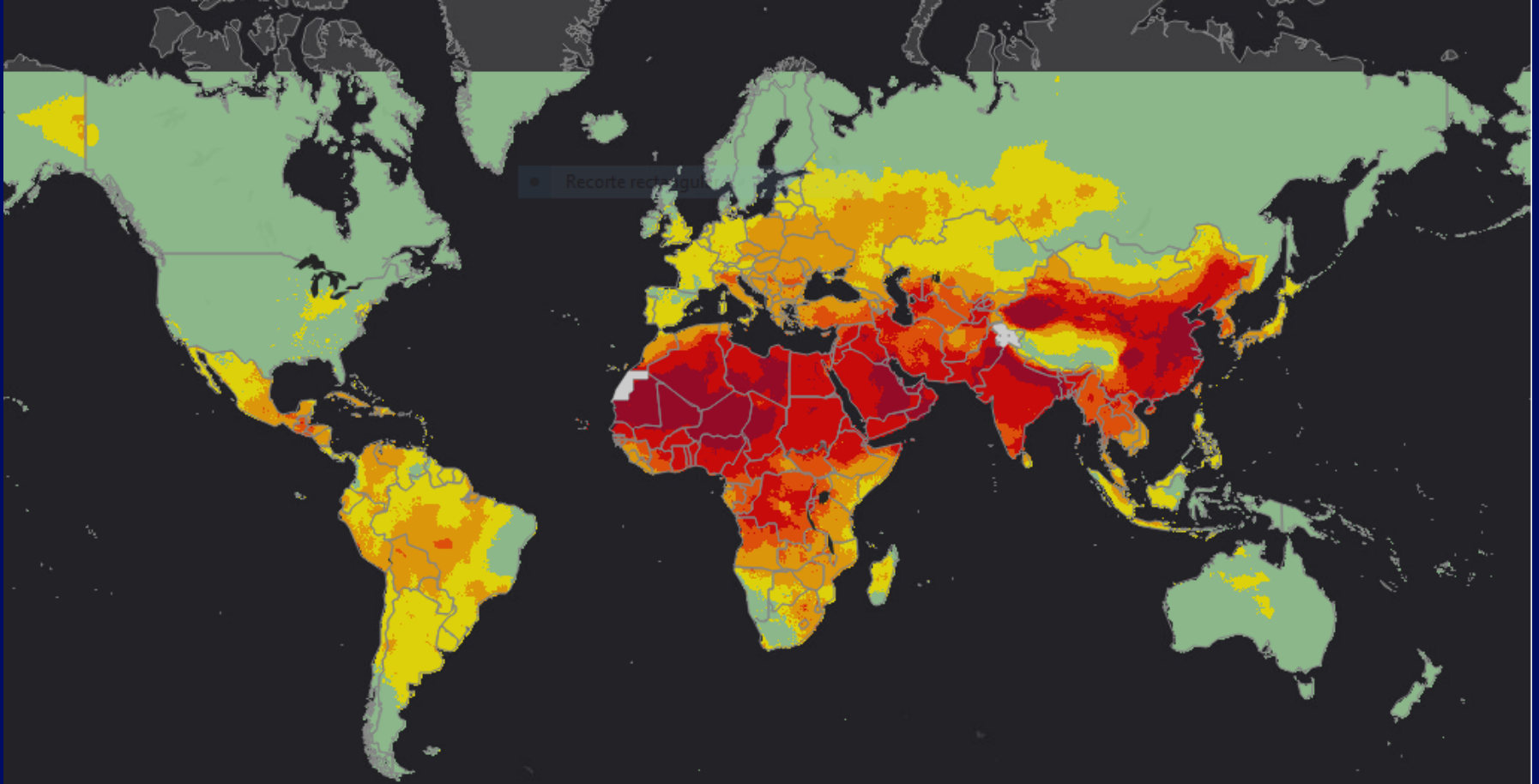
Health Impacts of Air Pollution

4th among the global killers.



Medellín, Colombia, on April 8, 2016 (AFP Photo/Raul Arboleda)

- 6.5×10^6 deaths worldwide
- ~4000 deaths Medellín
- Associated with:
 - heart disease
 - obstructive lung disease
 - cancer
- >90% world population at risk



WHO – Air Pollution (PM_{2.5,10}) Interactive Map

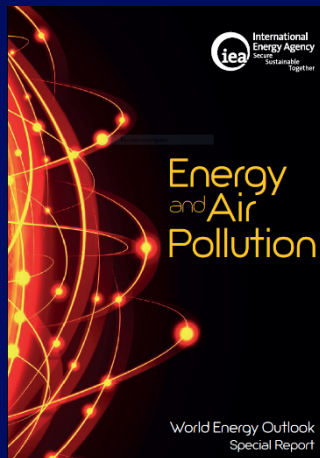
<http://maps.who.int/airpollution/>

Air Pollution

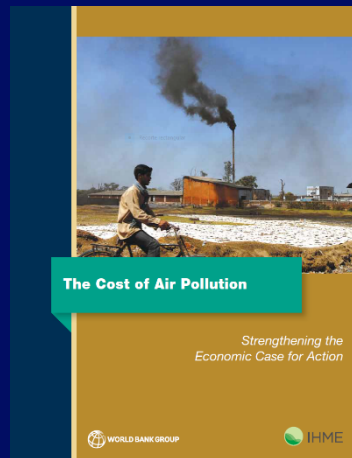
Issue of significant global concern

- Helsinki Protocol (1985) on the Reduction of Sulphur Emissions
- Oslo Protocol (1994) on Further Reduction of Sulphur Emissions
- 2015 World Health Assembly resolution to “address the adverse health effects of air pollution” (194 WHO member states)

International Energy Agency
June, 2016

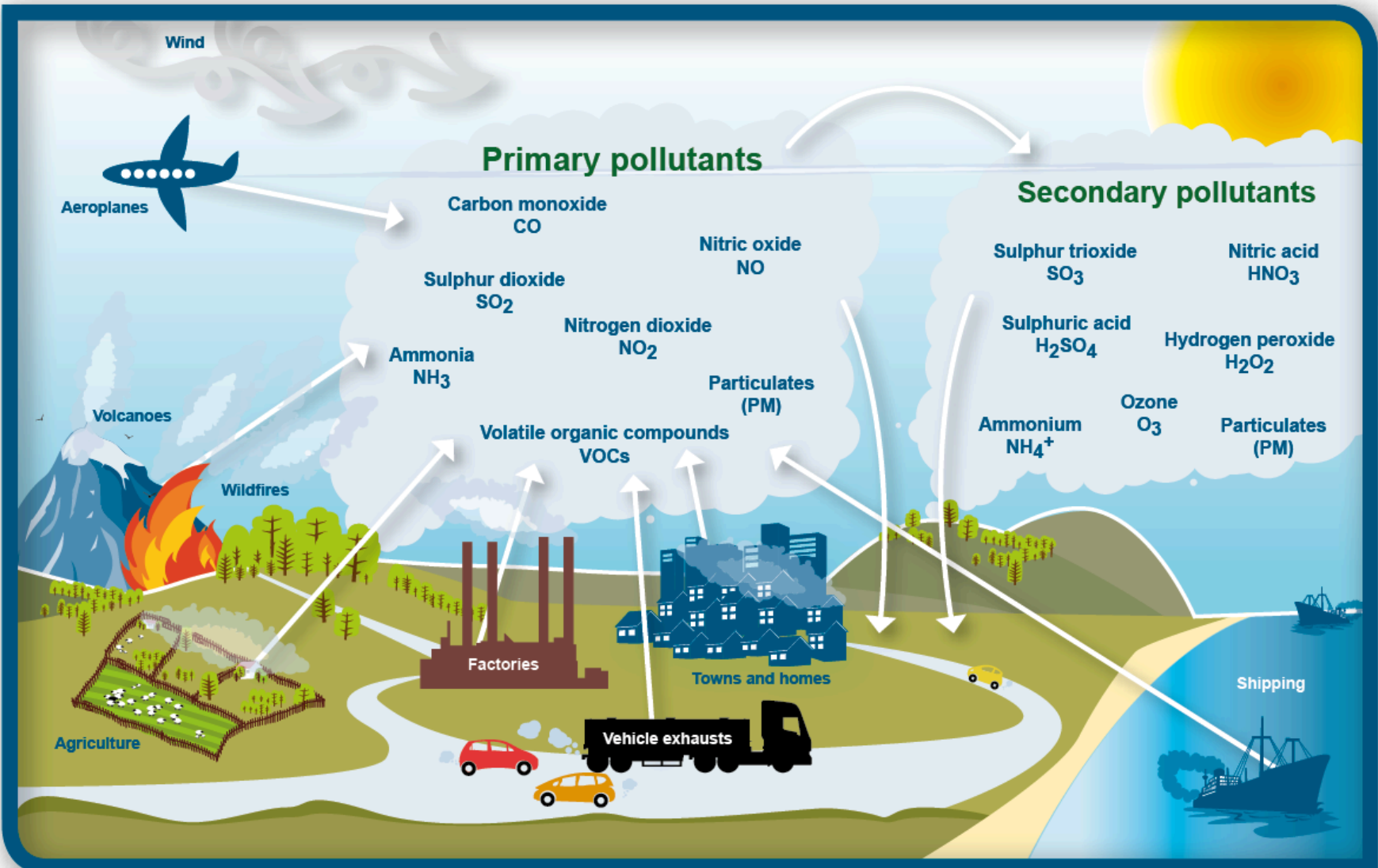


World Bank - IHME
September, 2016



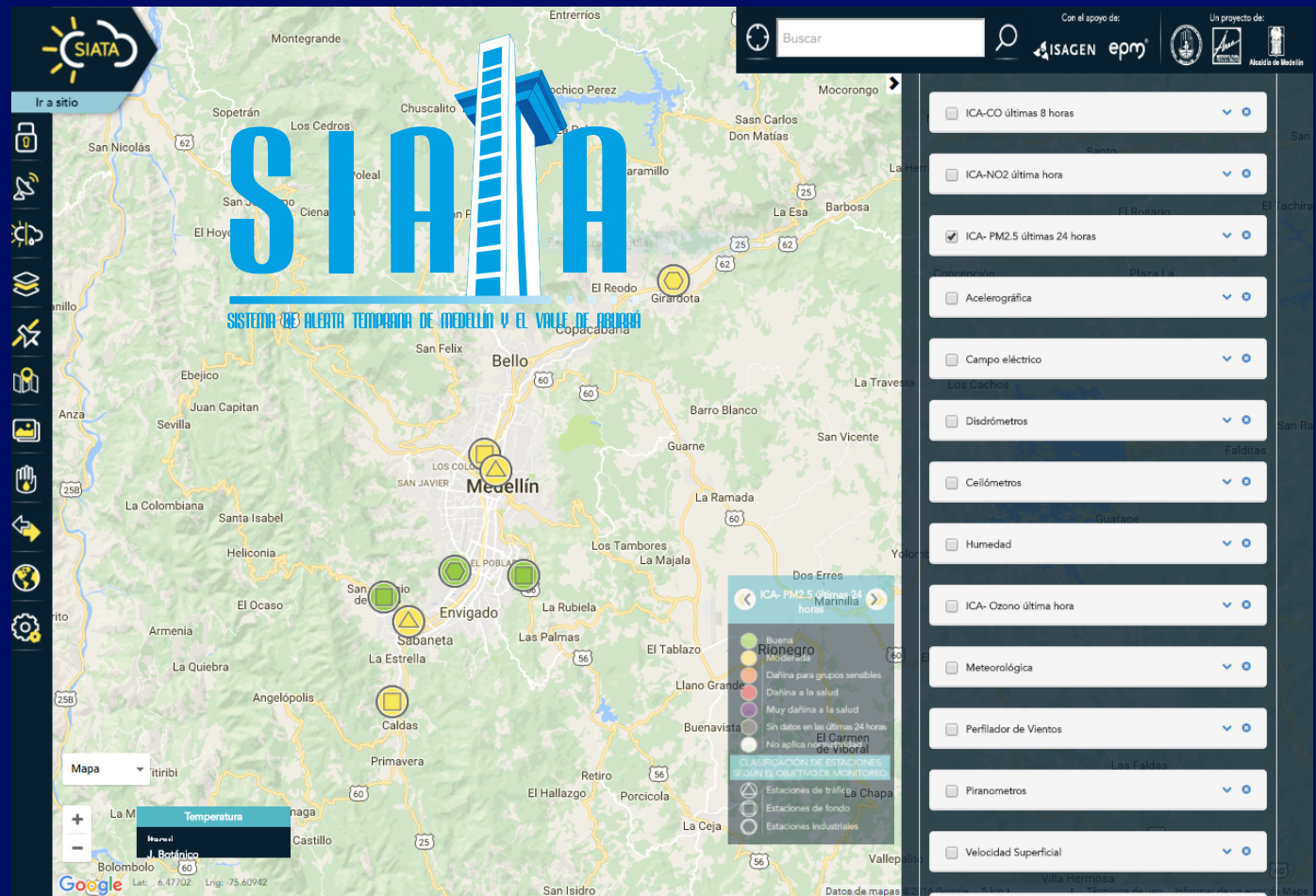
World Health Organization
September, 2016



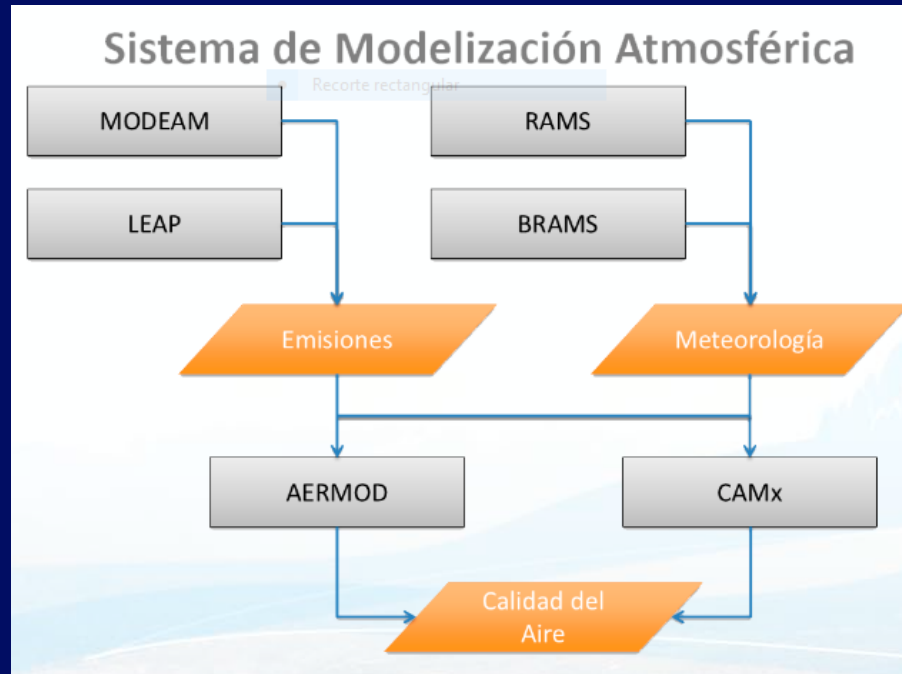


Source: Scotland's Environment, http://www.environment.scotland.gov.uk/media/26674/Sources-of-air-pollution_310314.png

Air Pollution Monitoring – Valle de Aburrá



Air Pollution Modeling – Valle de Aburrá



AERMOD

Local Air Quality Model

CAMx

Regional Air Quality Model

MODEAM, LEAP

Emissions Models

RAMS

Regional Modeling System

BRAMS

Regional Modeling System

Long-term goals:

To inform & motivate air quality-related public policy via...

Improved air quality models & forecasts



Causes



Emissions

Different pollutants



Chemical transformation



Formation

Impact of weather and topography



Dispersion and concentration

Exposure



Source: IEA adapted from (EEA, 2016).

Human exposure to air pollution models (e.g., EXPAND, EXPOLIS, INDAIR)



Theoretical framework

“The ensemble Kalman filter (EnKF) and its many variants have proven effective for data assimilation in large models, including those in atmospheric, oceanic, hydrologic, and petroleum reservoir systems. By bringing together technical experts, practitioners, researchers and students for presentations and informal exchange of information, we aim to share research results and suggest important challenges that have yet to be addressed”

...

[<http://www.iris.no/enkf/enkf-homepage>]



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Data assimilation relies on the use of an extension for high dimensional systems of the classical approach for filtering called the Kalman Filter.

$$\mathbf{x}_k = \mathcal{M}_{k,k-1}(\mathbf{x}_{k-1}) + \mathbf{u}_k$$
$$\mathbf{y}_k = \mathcal{H}_k(\mathbf{x}_k) + \mathbf{v}_k$$

$$\mathbf{x}_k \in \mathbb{R}^{m_x}$$

$$\mathbf{y}_k \in \mathbb{R}^{m_y}$$

$$\mathbf{u}_k \in \mathbb{R}^{m_x}$$

$$\mathbf{v}_k \in \mathbb{R}^{m_y}$$

$$\mathcal{M}_{k,k-1}: \mathbb{R}^{m_x} \rightarrow \mathbb{R}^{m_x}$$

$$\mathcal{H}_k: \mathbb{R}^{m_x} \rightarrow \mathbb{R}^{m_y}$$

[Evensen, 2009]

\mathbf{u}_k and \mathbf{v}_k are independent white noise

The EnKF is a modification that uses Monte Carlo approach to estimate the minimum variance solution to the state estimation problem.

At the analysis step in the EnKF, an ensemble of the system state, is generated with sample mean and covariance as the analysis state and error covariance matrix with the ensemble n typically much smaller than the dimension m_x in large scale applications.

$$\mathbf{X}_{k-1}^a = \{\mathbf{x}_{k-1,i}^a : i = 1, 2, \dots, n\}$$

By propagating the analysis ensemble through the transition operator, we obtain forecast ensemble at the next data assimilation cycle.

$$\mathbf{X}_k^f = \{\mathbf{x}_{k,i}^f : \mathbf{x}_{k,i}^f = \mathcal{M}_{k-1,k}(\mathbf{x}_{k-1,i}^a) + \mathbf{u}_{k,i}, i = 1, 2, \dots, n\}$$

When a new observation is available, the analysis step is used to compute the analysis ensemble from its forecast counterpart based on the sample covariance matrix of the forecast ensemble.

Two types of data assimilation:

- Related to the Ensemble Kalman filter for state estimation

$$\mathbf{x}_{k,i}^a = \mathbf{x}_{k,i}^f + \mathbf{K}_k [\mathbf{y}_{k,i}^s - \mathcal{H}_k(\mathbf{x}_{k,i}^f)], \quad \text{for } i = 1, 2, \dots, n,$$
$$\mathbf{K}_k = \hat{\mathbf{P}}_k^{xy} (\hat{\mathbf{P}}_k^{yy} + \mathbf{R}_k)^{-1},$$

$$\hat{\mathbf{S}}_k^f = \frac{1}{\sqrt{n-1}} [\mathbf{x}_{k,1}^f - \hat{\mathbf{x}}_k^f, \dots, \mathbf{x}_{k,n}^f - \hat{\mathbf{x}}_k^f],$$

$$\hat{\mathbf{S}}_k^{yy} = \frac{1}{\sqrt{n-1}} [\mathbf{y}_{k,1}^f - \hat{\mathbf{y}}_k^f, \dots, \mathbf{y}_{k,n}^f - \hat{\mathbf{y}}_k^f],$$

$$\mathbf{x}_{k,i}^a = \hat{\mathbf{x}}_k^a + \sqrt{n}(\mathbf{L}_k \mathbf{C}_k \boldsymbol{\Xi}_k)_i, \quad \text{for } i = 1, \dots, n$$

$$(\delta \mathbf{x}_{k,i})_j = (\hat{p}_{xy,k}^j / \hat{p}_{yy,k}^f) \delta y_{k,i}, \quad j = 1, \dots, m_x,$$

- Variational methods for the parameter estimation

$$X(t_{i+1}) = M_i X(t_i), \quad i = 1, \dots, m-1, \quad X(t_{i+1}) \in \mathfrak{R}^n$$

$$Y(t_i) = H(X(t_i)) + \eta(t_i),$$

$$H : \mathfrak{R}^n \rightarrow \mathfrak{R}^q$$

$$J(X_0) = \frac{1}{2} (X^b - X_0)^T B_0^{-1} (X^b - X_0) + \frac{1}{2} \sum_i (Y(t_i) - H(X(t_i)))^T R_i^{-1} (Y(t_i) - H(X(t_i))),$$

[Barbu 2010, Krymskaya, 2013, Sebacher, 2014, Altaf 2015, Fu et al, 2015, Lu et al, 2015, Krymskaya, 2013, Tijana et al, 2014, Verlaan and Sumihar, 2016]

Measuring the impact of observations (data) over the performance of a Data Assimilation Scheme in the enhancement of a model.

$$\begin{aligned} \Delta J(k, m) \approx & [(\mathbf{y}(k+m) - H\hat{\mathbf{x}}(k+m|k)) + (\mathbf{y}(k+m) - H\hat{\mathbf{x}}(k+m|k-1))]' \\ & \mathbf{R}(k+m)^{-1} \mathbf{D}(k+m|k-1) \mathbf{D}(k|k-1)' \\ & (\mathbf{D}(k|k-1) \mathbf{D}(k|k-1)' + \mathbf{R}(k))^{-1} (\mathbf{y}(k) - H\hat{\mathbf{x}}(k|k-1)) \end{aligned}$$

[Barbu 2010, Krymskaya, 2013, Sebacher, 2014, Altaf 2015, Fu et al, 2015, Lu et al, 2015, Krymskaya, 2013, Tijana et al, 2014, Verlaan and Sumihar, 2016]

During the last 3 years, the MahPhys group has been developing and improving the Data Assimilation schemes from at least three points of view, regarding the two types of data assimilation techniques: the variational methods, and sequential methods.

1. The reduced adjoint approach theoretical and idealized test cases (Altaf et al, 2013)
2. The quantification of the impact of data in reservoir modeling through observation sensitivity matrixes (Krymskaya, 2013)
3. Ensemble spurious correlations in Ensemble Kalman Filter (Fu et al, 2015- 2016) (Evans, 2009)
4. Observational spurious correlations solution in 4-d variational Data assimilation(Lu et al, 2015-2016)(Beney, 1982) (Jackson, 1991)
5. Conservation of mass and Preservation of positivity in physical meaning variables for Ensemble-Type kalman Filter Algorithms (Tijana et al, 2014) and The observation impact analysis methods for Storm Surge - TSBOI- MM algorithm (Verlaan and Sumihar, 2016)

Theoretical Questions

To analyze and/or quantify the impact of the proper selection of a data subset

Based in previous work of observation sensitivity matrix (Krymskaya et al, 2010) and its properties such as

- Structure: symmetry, scaling, positive (semi)definiteness
- Matrix norm
- Uncertainty measurement
- Evaluation with SVD and trace analysis

for the quantification of the impact in modeling.

Videos

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To answer the question: is it possible, under lineality and stationarity assumptions, to use the observation impact analysis methods developed by Verlaan and Sumihar, 2016 to improve the Data Assimilation Schemes over LOTOS-EUROS model forecasting?.

This will be held by studying the impact of the observations at the most recent analysis update under Ensemble based schemes in LOTOS EUROS model for volcanic ash.

$$\tilde{\mathbf{x}}(k|k-1) = \begin{bmatrix} \hat{\mathbf{x}}(k+m|k-1) \\ \hat{\mathbf{x}}(k|k-1) \end{bmatrix}$$

$$\begin{aligned} \tilde{H}_a &= [\mathbf{0} \ H] \\ \tilde{H}_v &= [H \ \mathbf{0}] \end{aligned}$$

$$\tilde{\mathbf{x}}(k|k) = \tilde{\mathbf{x}}(k|k-1) + \tilde{\mathbf{K}}_c \left(\mathbf{y}(k) - \tilde{H}_a \tilde{\mathbf{x}}(k|k-1) \right)$$

$$H \hat{\mathbf{x}}(k+m|k) = \tilde{H}_v \tilde{\mathbf{x}}(k|k-1) + \tilde{H}_v \tilde{\mathbf{K}}_c \left(\mathbf{y}(k) - \tilde{H}_a \tilde{\mathbf{x}}(k|k-1) \right)$$

The extension of the trj-4DVar (Lu et al, 2015) to bigger systems and mathematically feasible solutions to solve the modified cost function in a new or improved approach adjoint free. We find feasible to try a hybrid scheme for the ill conditioned problem in order to deal with reduced observational noise.

The use of a formal sensitivity analysis for the perturbation of the inputs to the two experience based modifications in cost function in the trj-4DVar (Lu et al, 2016 under review), specifically in the penalty term in order to develop a generalized method and probe the stability of the solution.

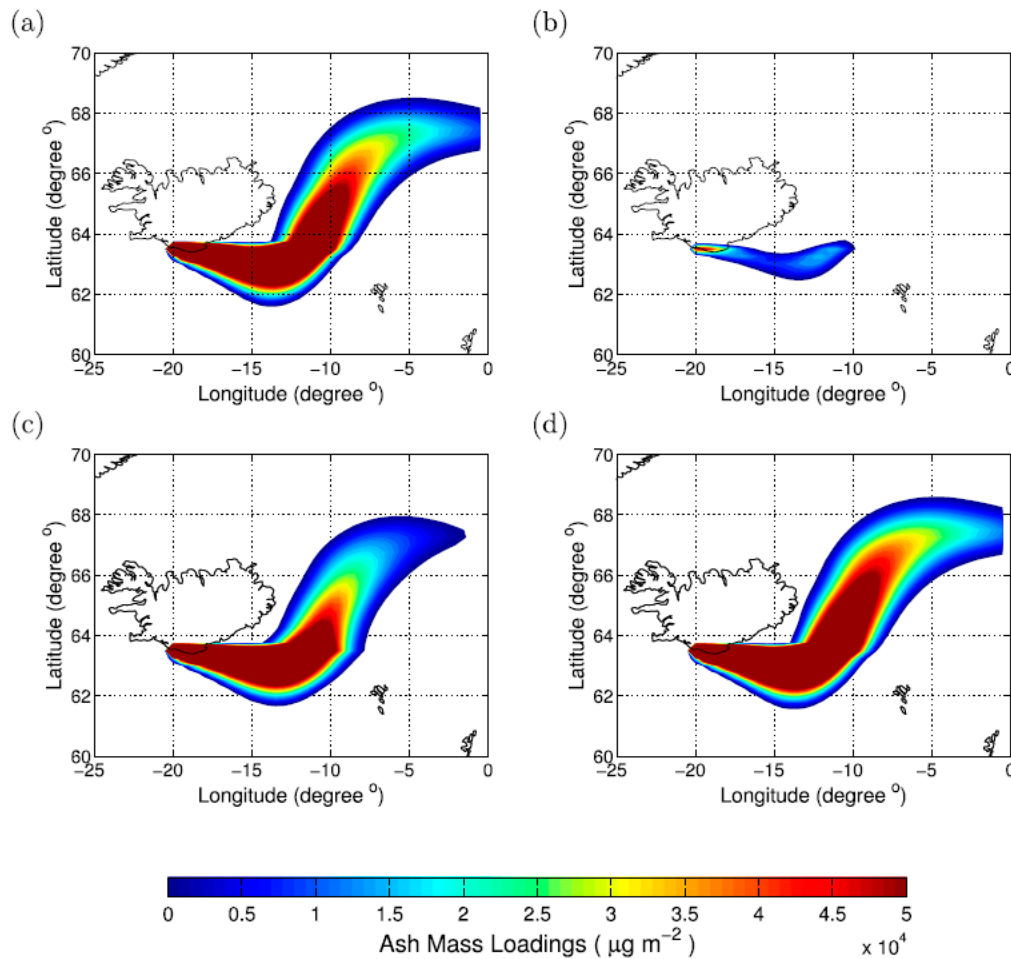


FIG. 5. Forecast of ash columns generated with emission rates of (a) the truth, (b) the background, (c) estimated through the standard 4D-Var method, and (d) estimated through the Trj4Dvar method at 1900 UTC 14 Apr 2010.

To develop further evidence and formalize the postulate of accuracy of the method for a physical-related window of assimilation, regarding the demonstrated accuracy in assimilation windows that does not compromise the constant concentration of particles in atmosphere (Lu et

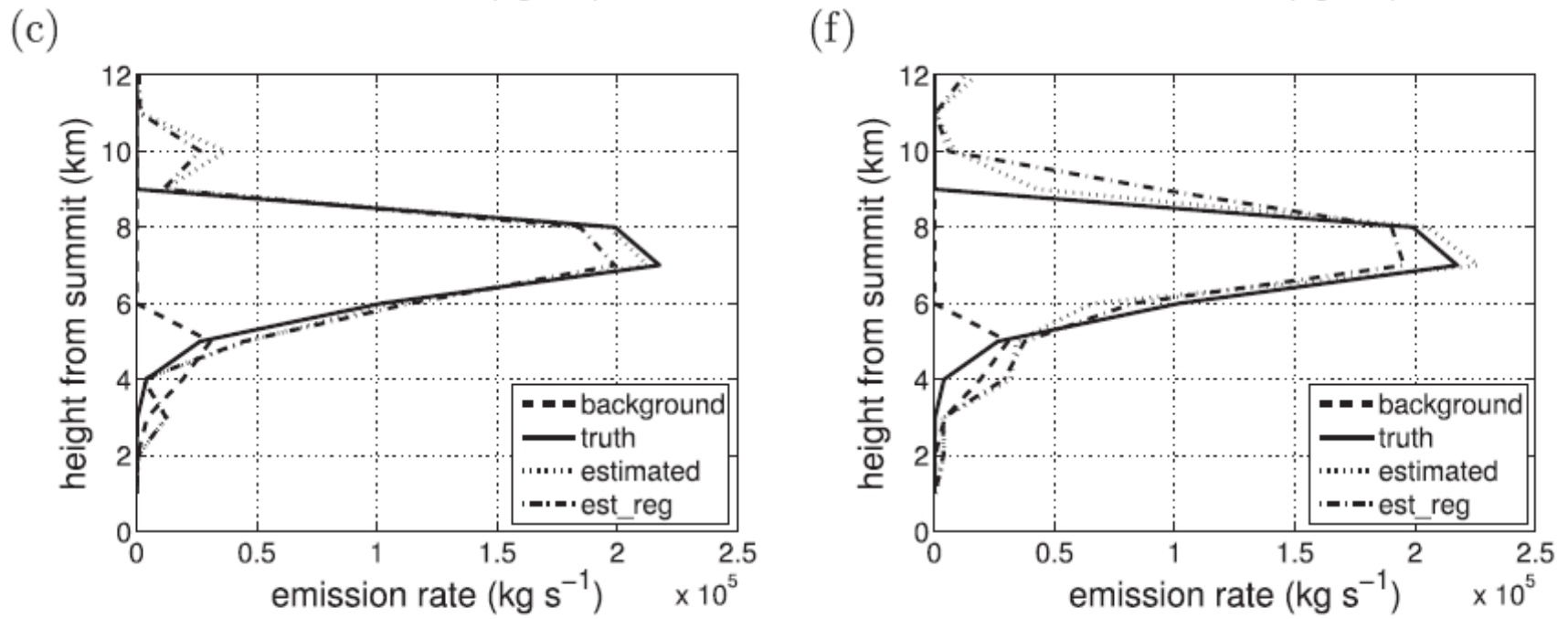


FIG. 9. Trj4DVar results of twin experiments with (a)–(c) 10% and (d)–(f) 50% observation noise and assimilation window of (a),(d) 1; (b),(e) 3; and (c),(f) 6 h.

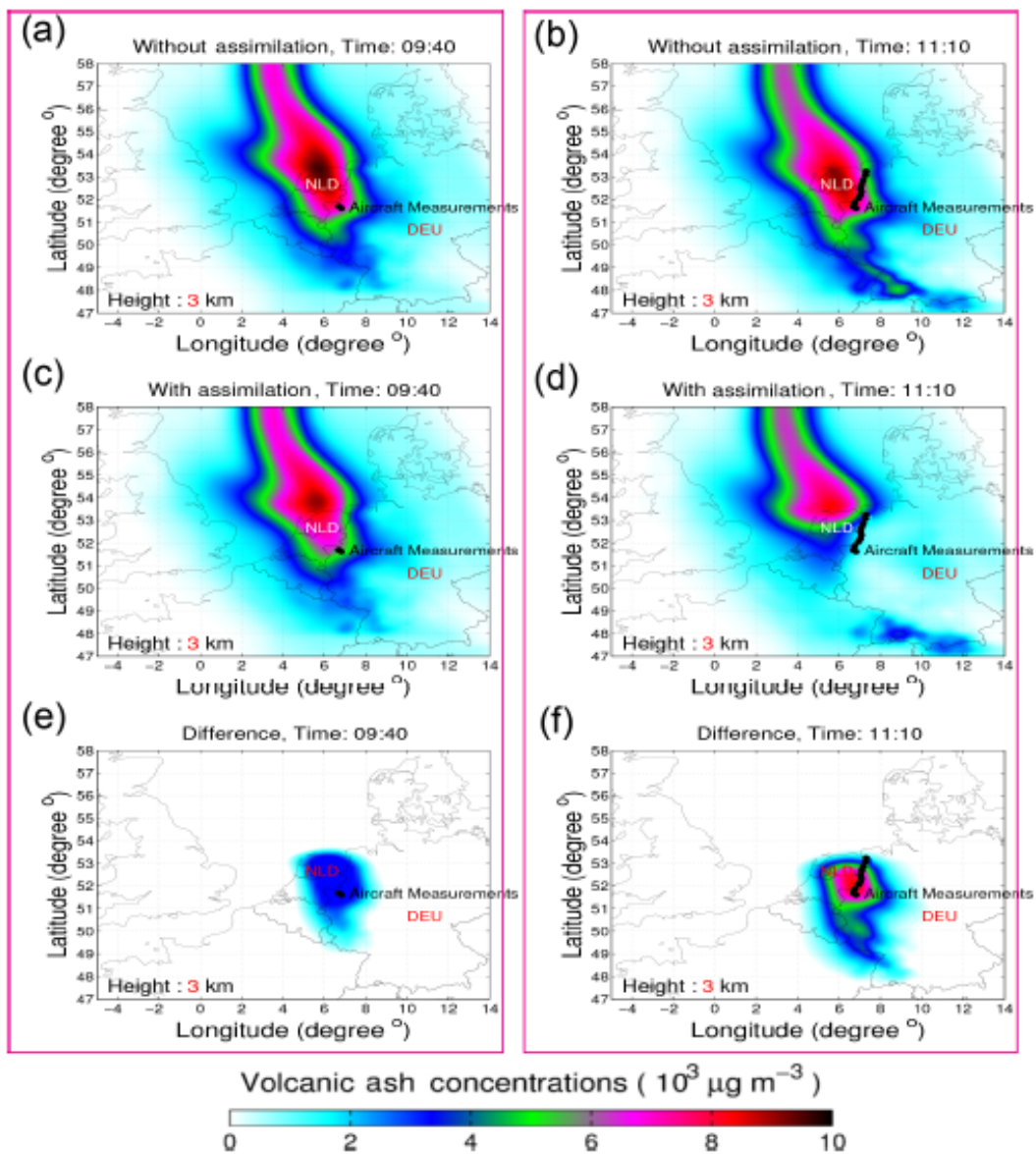


Figure 3. Comparison with and without assimilating aircraft in situ measurements on 18 May 2010. (a, b) Simulation results without assimilation at 09:40 and 11:10 UTC. (c, d), Simulation results with assimilation at 09:40 and 11:10 UTC. (e) Differences of (a, c). (f) Differences of (b, d). The differences are in absolute values which are obtained by numerically subtracting the values between (a, c), or (b, d). Panels (e, f) represent the areas where the assimilation has effect.

To merge both “spurious” approaches for “multiple observations” problems (variable localization).

Research Proposal

General Objective

“To start a research collaboration between both Mathematical Sciences Department at Universidad EAFIT and Applied Mathematical Department at TU Delft in order to develop and improve the Data Assimilation Schemes regarding the rigurocity and relevance of the theoretical and practical issues on the field, over complex dynamics such as environmental modeling.

This allows for the merging of the PhD programs and improves the capability of our departments to provide solutions to modeling issues worldwide.”

Specific Objectives

1. To start a joint research program for the development of Data Assimilation schemes.
2. To strengthen the research capabilities of the Systems and Control research line of the Mathematical Modeling research group through the formation of Doctoral students in Mathematical Engineering and Applied Mathematics programmes.
3. To improve the sequential methods for data assimilation.
4. To improve the variational methods for data assimilation.
5. To perform properly the mathematical analysis of the algorithms developed, related to insight, understanding, conditioning, deep performance and so on.
6. To contribute satisfactorily to the field of data assimilation through the development of new schemes from the solution of the particular problem related to air quality in Colombia.

Specific Objectives

7. To provide interdisciplinary work between the research groups of the School of Sciences at Universidad EAFIT.
8. To develop an approach for the Modelling of the Air Quality in Colombia through LOTOS-EUROS Model and learn on how the model behaves in different regions of the world.
9. To contribute to forecasting systems of Air Quality in Colombia using LOTOS-EUROS Model through Data Assimilation taking into account the need for more data provided by governmental agencies such as Area Metropolitana.
10. To analyze and evaluate the dynamics underlying the atmospheric behavior in Area Metropolitana, as the initial step in the development of a city-scale, pollution exposure risk model to explore the ecological and human health impact from the Biological Sciences framework.

Specific Objectives

11. To train two doctoral students under a joint scheme between the PhD in Mathematical Engineering (EAFIT) and Applied Mathematics (TUDELFT) programmes
12. To impact the programme of master in Applied Mathematics at Universidad EAFIT with research in Data Assimilation with applications to History matching.
13. To contribute to the international mobility of faculty and students for research

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