UNIVERSITY OF TECHNOLOGY, SYDNEY
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AIR POLLUTANT EMISSION AND PREDICTION WITH EXTENDED KALMAN FILTERING

by

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE

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Certificate of Authorship/Originality

I certify that the work in this thesis has not been previously submitted for a degree nor has it been submitted as a part of the requirements for other degree except as fully acknowledged within the text.

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Santanu Metia
ABSTRACT

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The major sources of air pollutants in New South Wales (NSW is a state on the east coast of Australia) are anthropogenic emissions and biomass burning emissions. Anthropogenic mega city emissions play an important role with respect to air pollution: a relatively large amount of pollutants is released in a small area potentially leading to nonlinear chemical processes, which may further aggravate air pollution. Highly populated cities in NSW are mainly located in coastal areas while bush fires on the other hand usually take place in the inland of NSW, a region with a relatively low population density.

In order to compare the impact of these two emission sources in NSW on a climatological time scale, The Air Pollution Model with Chemical Transport Model (TAPM-CTM) is used, which receives meteorological data, terrain data and emission data together with chemical processes. These emission data are generated by the Emissions Data Management System (EDMS v2.0). To improve the air quality modelling performance, uncertainties in association with the estimation must be handled properly. For this, the Extended Kalman Filter (EKF) together with its modifications are studied throughout this thesis.

The motivation for this work stems from recently growing research interest in environmental modelling and control. The challenging inverse problem has intrigued researchers in atmospheric science as well as sustainable engineering and technology. This work addresses the problem in air pollutant estimation by proposing the use of TAPM-CTM coupled with the Extended Fractional Kalman Filter (EFKF)
based on a Matérn covariance function to enhance the estimation accuracy and to smoothen the spatiotemporal correlation. Here, concentrations of air pollutants such as nitrogen oxide (NO), nitrogen dioxide (NO$_2$) and ozone (O$_3$) are predicted by TAPM-CTM in the airshed of Sydney and surrounding areas. For improvement of the emission inventory, and hence, the air quality prediction, the fractional order of the EFKF is tuned by using a Genetic Algorithm (GA).

Nonlinearity is further treated by using unscented transforms in the prediction step with an Unscented Kalman Filter (UKF) to preserve the stochastic characteristics of the nonlinear environmental system involved. A comparison with the conventional EKF and the UKF is included to indicate the UKF viability in air pollutant estimation.

Academic contributions of this thesis include investigation, application, design, and implementation of the EFKF and UKF for air pollution estimation. Discussions on theoretical aspects and implementation details of these extended Kalman filters for environmental data are included together with some recommendations.
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I would like to thank Dr. Hiep Duc who is an atmospheric scientist from the Office of Environment and Heritage (OEH) New South Wales. I appreciate his assistance with air quality modelling related theories and his valuable comments with respect to this research project. Also thanks to division team members of OEH for guiding and providing me with the valuable knowledge of air quality measurement methodologies from collection of the research dataset.

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Nomenclature and Notation

Throughout the thesis, the following nomenclatures and notations are used:

- AQI: Air Quality Index
- BIBO: Bounded Input Bounded Output
- CO: Carbon Monoxide
- CTM-DDS: Chemical Transport Model- Data Display System
- EDMS: Emissions Data Management System
- KF: Kalman Filter
- EKF: Extended Kalman Filter
- EFKF: Extended Fractional Kalman Filter
- EnKF: Ensemble Kalman Filter
- GA: Genetic Algorithm
- GP: Gaussian Process
- LTI: Linear Time Invariant
- MIMO: Multiple Input Multiple Output
- MSE: Mean Squared Error
- NO: Nitrogen Oxide
- NO$_2$: Nitrogen Dioxide
- NO$_X$: Generic term for the mono-nitrogen oxides NO and NO$_2$
- NSW: New South Wales
- O$_3$: Ozone
- OEH: Office of Environment and Heritage
- PM: Particulate Matter
- OMI: Ozone Monitoring Instrument
- SDE: Stochastic Differential Equation
- SO$_2$: Sulphur Dioxide
- TAPM-CTM: The Air Pollution Model with Chemical Transport Model
- UKF: Unscented Kalman Filter
- UT: Unscented Transform
- VOC: Volatile Organic Compounds
- $w(t)$: Gaussian white noise process $w(t) = df(t)/dt$
- $\mathbb{R}$: Field of real numbers
- $\mathbb{R}^n$: $n$-dimensional space
- $\mathbb{R}^{n \times m}$: Space of all matrices of $(n \times m)$-dimension
- $S_w(\omega)$: Spectral density
- $l$: Length scale
- $\sigma^2$: Magnitude hyper parameter
- $K_\nu$: Modified Bessel function
- $\nu$: Parameter controlling the smoothness of the process
- $\Gamma$: Gamma function
- $z$: Complex number
- $I_n$: Identity matrix of $(n \times n)$-dimension
- $\| \cdot \|$: Euclidean norm of a vector or spectral norm of a matrix
- $\forall$: For all