

# Master's Thesis

## Uncertainty Quantification of Atmospheric Chemistry Models

**Courses:** Mathematics, Computer Science, Atmospheric Chemistry and Physics

### Topic

Atmospheric chemistry models play an extremely important role both in climate science and in weather prediction. Typically, about 50 atmospheric species involved in more than 100 possible chemical reactions are considered. Chemical reactions can be modeled using ordinary differential equations for the concentration of the individual species. As parameters, they require the knowledge of reaction rate constants, which need to be measured. However, these measurements contain errors. More precisely, the reaction rate constants can be modeled as random variables. The research question for this thesis topic is how the uncertainties in the reaction rate constants influence model predictions.

### Task

To answer this question, methods from the field of Uncertainty Quantification should be applied. Several strategies are possible:

- Monte-Carlo, Quasi Monte-Carlo or Multi-level Monte-Carlo sampling techniques
- Sparse grid quadrature
- Sensitivity analysis using the adjoint method, and potentially algorithmic differentiation tools

The methods should be implemented in the existing atmospheric chemistry simulation model at the Institute of Meteorology and Climate Research (IMK-ASF). This code is actually used for weather and climate predictions, but can be run in a simplified setting which allows for tests.

Alternatively, it is also possible to look into the time integration that the code currently uses, and to try to come up with improvements. For example:

- Other time integration schemes
- Investigation of stability
- Investigation of linear and nonlinear solvers

The thesis will jointly be supervised with IMK-ASF.

### Contact

**Prof. Dr. Martin Frank**  
Faculty of Mathematics  
Steinbuch Centre for Computing  
[www.scc.kit.edu](http://www.scc.kit.edu)  
[martin.frank@kit.edu](mailto:martin.frank@kit.edu)

**Dr. Roland Ruhnke**  
Institute of Meteorology and Climate Research  
Atmospheric Trace gases and Remote Sensing  
[www.imk-asf.kit.edu](http://www.imk-asf.kit.edu)  
[roland.ruhnke@kit.edu](mailto:roland.ruhnke@kit.edu)