



Polluter group specific emission optimisation for regional air quality analyses using four-dimensional variational data assimilation

Pascal Martin Backes

Energie & Umwelt / Energy & Environment

Band / Volume 615

ISBN 978-3-95806-717-2

Forschungszentrum Jülich GmbH
Institut für Energie- und Klimaforschung (IEK)
Troposphäre (IEK-8)

Polluter group specific emission optimisation for regional air quality analyses using four-dimensional variational data assimilation

Pascal Martin Backes

Schriften des Forschungszentrums Jülich
Reihe Energie & Umwelt / Energy & Environment

Band / Volume 615

ISSN 1866-1793

ISBN 978-3-95806-717-2

Contents

| | |
|---|-------|
| Abstract | iii |
| Kurzzusammenfassung | v |
| List of Figures | ix |
| List of Tables | xviii |
| Acronyms | xix |
| 1. Introduction | 1 |
| 2. Data assimilation | 6 |
| 3. The atmospheric chemistry transport model EURAD-IM | 11 |
| 3.1. Forward model | 11 |
| 3.2. 4D-Var data assimilation system | 12 |
| 4. Theory on sector specific optimisation of emissions | 18 |
| 4.1. Theoretical basis | 18 |
| 4.2. Modification of the emission error correlation matrix | 20 |
| 4.3. Anisotropic correlation of emission correction factors along roads | 21 |
| 5. Model input | 27 |
| 5.1. Initial and boundary conditions | 27 |
| 5.2. Meteorological fields | 28 |
| 5.3. Emission data | 29 |
| 5.4. Ground observations in North Rhine-Westphalia | 38 |
| 6. Case studies based on identical twin experiments | 44 |
| 6.1. Experimental setup | 44 |
| 6.2. Emission corrections and cost reduction | 48 |
| 6.3. Impact of the anisotropic diffusion operator on the corrections of the road transport sector | 55 |
| 6.4. Conclusions of the identical twin experiments | 58 |
| 7. Simulation using ground station observations in North Rhine-Westphalia | 60 |
| 7.1. Configuration of the simulation | 60 |
| 7.2. Emission correction factors and gradients | 61 |

| | | |
|-----------|--|------------|
| 7.3. | Agreement between simulated and observed concentrations | 71 |
| 7.3.1. | NO ₂ and O ₃ | 71 |
| 7.3.2. | SO ₂ | 74 |
| 7.3.3. | Aerosols | 79 |
| 7.4. | Conclusions of the simulation using ground observations | 81 |
| 8. | Conclusion and outlook | 83 |
| | General acknowledgements | 86 |
| A. | Appendix: Supplements to the identical twin experiments | 88 |
| B. | Appendix: Supplements to the simulation using real observations | 90 |
| B.1. | Spatial distribution of emission corrections | 90 |
| B.2. | Initial value corrections of NO ₂ | 91 |
| B.3. | Time series of PM2.5 | 95 |
| B.4. | High emission corrections of the aviation sector | 96 |
| B.5. | Enhancement of agriculture II emissions | 98 |
| B.6. | Distinction between road transport and industrial emissions | 103 |
| | Bibliography | 107 |

Energie & Umwelt / Energy & Environment
Band / Volume 615
ISBN 978-3-95806-717-2

Mitglied der Helmholtz-Gemeinschaft

