Research Project #5

Influence of multiphase chemistry on tropospheric oxidants in a changing climate (ICE-3 & ICE-4)

In the troposphere ozone (O_3) is an important oxidant, pollutant, and short-lived climate forcer. Yet, despite decades of research global atmospheric models suffer from general overprediction when evaluated against observations [1]. Moreover, the recycling of nitrogen oxides (NO_x) is considered important for correctly predicting past and future O_3 trends [2]. Multiphase chemistry involving production and recycling of radicals and oxidants is extensive and believed to be crucial in the atmosphere. However, global models usually do not account for comprehensive chemistry across phases.

This project aims to unravel the multiphase chemistry with an impact on tropospheric O_3 starting with the quantification of the NO_x-recycling mechanisms. Of particular interest are the global budgets of reactive nitrogen species such as HONO and $ClNO_2$ Their chemistry involves aqueous-phase radical chemistry which in turn can be a driver of O_3 loss. In fact, high radical production in the aqueous phase is fueled by organic compounds and can boost ozone loss [3]. Finally, we will revisit the global budgets of O_3 for the recent past and warmer scenarios [4].

The project will be based on comprehensive observational datasets, such as aircraft missions [5], the TOAR database [6], and TROPOMI satellite retrievals [7]. The datasets will be worked out statistically using new tools as from machine learning. The datasets will be compared to global model simulations including advanced kinetic models for oxidation in the gas-phase, aerosols and cloud droplets [8]. Finally, the impact of future climate change on atmospheric chemistry and pollution will be assessed. Knowledge about these critical mechanisms is a key for assessing the risk of worsening air quality for ecosystem and human health.

Key Tasks in This PhD Project:

- Assess, organize and analyze large observational datasets with respect to ozone and reactive nitrogen species (aircraft, TOAR data base, TROPOMI)
- Develop and include chemical kinetic models in global model framework
- Run various model scenarios (including real world conditions and with a global temperature rise of +2K and +2.75K)
- Evaluate model simulation with observations
- Assess the global impact of including multiphase chemistry on tropospheric O_3 simulations and evaluate the impact of the results

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Troposphere (ICE-3), Director: Prof. Dr. Anke Nölscher https://www.fz-juelich.de/en/ice/ice-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Stratosphere (ICE-4), Director: Prof. Dr. Michaela I. Hegglin https://www.fz-juelich.de/en/ice/ice-4
Specific **requirements**	• M.Sc. in chemistry, physics, meteorology, environmental sciences or a related field • Experience in Earth System Modelling • Data analysis experience and/or programming knowledge • Excellent oral and written communication skills in English • Ability to communicate results clearly in presentations and in writing • Self-motivated, structured working style

	• Excellent cooperation and teamwork skills
For **project specific** questions please **contact**	Dr. Domenico Taraborrelli, ICE-3, d.taraborrelli@fz-juelich.de

[1] P. J. Young, V. Naik, A. M. Fiore, A. Gaudel, J. Guo, M. Y. Lin, J. L. Neu, D. D. Parrish, H. E. Rieder, J. L. Schnell, S. Tilmes, O. Wild, L. Zhang, J. Ziemke, J. Brandt, A. Delcloo, R. M. Doherty, C. Geels, M. I. Hegglin, L. Hu, U. Im, R. Kumar, A. Luhar, L. Murray, D. Plummer, J. Rodriguez, A. Saiz-Lopez, M. G. Schultz, M. T. Woodhouse, G. Zeng; Tropospheric Ozone Assessment Report: Assessment of global-scale model performance for global and regional ozone distributions, variability, and trends. *Elementa: Science of the Anthropocene* 1 January 2018; 6 10. doi: https://doi.org/10.1525/elementa.265

[2] Archibald, AT, Neu, JL, Elshorbany, Y, Cooper, OR, Young, PJ, Akiyoshi, H, Cox, RA, Coyle, M, Derwent, R, Deushi, M, Finco, A, Frost, GJ, Galbally, IE, Gerosa, G, Granier, C, Griffiths, PT, Hossaini, R, Hu, L, Jöckel, P, Josse, B, Lin, MY, Mertens, M, Morgenstern, O, Naja, M, Naik, V, Oltmans, S, Plummer, DA, Revell, LE, Saiz-Lopez, A, Saxena, P, Shin, YM, Shaahid, I, Shallcross, D, Tilmes, S, Trickl, T, Wallington, TJ, Wang, T, Worden, HM, Zeng, G. 2020. Tropospheric ozone assessment report: A critical review of changes in the tropospheric ozone burden and budget from 1850 to 2100. *Elem Sci Anth*. 8: 1. DOI: https://doi.org/10.1525/elementa.2020.034

[3] Rosanka, S., Sander, R., Franco, B., Wespes, C., Wahner, A., and Taraborrelli, D.: Oxidation of low-molecular-weight organic compounds in cloud droplets: global impact on tropospheric oxidants, Atmos. Chem. Phys., 21, 9909–9930, https://doi.org/10.5194/acp-21-9909-2021, 2021.

[4] Emmerichs, T., Taraborrelli, D., Shen, F. *et al.* Widespread reduction of ozone extremes in storylines of future climate. *npj Clean Air* **1**, 19 (2025). https://doi.org/10.1038/s44407-025-00019-4

[5] Weyland, B., Rosanka, S., Taraborrelli, D., Bohn, B., Zahn, A., Obersteiner, F., Förster, E., Mertens, M., Jöckel, P., Ziereis, H., Kaiser, K., Fischer, H., Crowley, J. N., Wang, N., Edtbauer, A., Williams, J., Andrés Hernández, M. D., Burrows, J. P., Kluge, F., Rotermund, M., Butz, A., and Pfeilsticker, K.: Airborne remote sensing of nitrous acid in the troposphere: potential sources of excess HONO, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-5085, 2025.

[6] https://toar-data.fz-juelich.de/

[7] Heue, K.-P., Loyola, D., Romahn, F., Zimmer, W., Chabrillat, S., Errera, Q., Ziemke, J., and Kramarova, N.: Tropospheric ozone retrieval by a combination of TROPOMI/S5P measurements with BASCOE assimilated data, Atmos. Meas. Tech., 15, 5563–5579, https://doi.org/10.5194/amt-15-5563-2022, 2022.

[8] Rosanka, S., Tost, H., Sander, R., Jöckel, P., Kerkweg, A., and Taraborrelli, D.: How non-equilibrium aerosol chemistry impacts particle acidity: the GMXe AERosol CHEMistry (GMXe–AERCHEM, v1.0) sub-submodel of MESSy, Geosci. Model Dev., 17, 2597–2615, https://doi.org/10.5194/gmd-17-2597-2024, 2024.