

New chemical schemes for atmospheric modelling : update of the methanol chemistry and reduced scheme

Olivia Venot (1), Thibault Cavalié (2), Roda Bounaceur (3), Pascal Tremblin (4), Michel Dobrijevic (2), Eric Hébrard (5), Benjamin Drummond (5) and Benjamin Charnay(6)

(1) Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), UMR CNRS 7583, Université Paris Est Créteil, Université de Paris), Créteil, France (olivia.venot@lisa.u-pec.fr), (2) Laboratoire d'Astrophysique de Bordeaux, Univ. Bordeaux, CNRS, B18N, allée Geoffroy Saint-Hilaire, Pessac 33615, France, (3) Laboratoire Réactions et Génie des Procédés, LRGP UMP 7274 CNRS, Université de Lorraine, 1 rue Grandville, BP 20401, F-54001 Nancy, France, (4) Maison de la Simulation, CEA, CNRS, Univ. Paris-Sud, UVSQ, Université Paris-Saclay, 91191 Gif-sur-Yvette, France, (5) Astrophysics Group, University of Exeter, EX4 4QL, Exeter, UK, (6) LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Univ. Paris Diderot, Sorbonne Paris Cité, 5 place Jules Janssen, 92195 Meudon, France

1 Introduction

Most of hot and warm exoplanets atmospheres have probably a disequilibrium composition because of the important out-of-equilibrium processes at play in these media (i.e. mixing and photodissociations). To analyse and understand spectroscopic observations of exoplanets, atmospheric models including chemical kinetics are mandatory. We will present in this talk two last developments concerning chemical schemes used for exoplanets atmospheres modelling.

2. Reduced Chemical Scheme

Atmospheric kinetic models in one dimension have been developed already [1, 2], but three-dimensional models including kinetics are still challenging because of the high computational time they would required. A solution would be to use a reduced chemical scheme instead of the very large detailed ones usually used in 1D models. In this view, we have developed a new scheme for warm hydrogen-dominated atmospheres. We have reduced the chemical scheme of [2], by a factor of 3 in terms of species and 5 in terms of reactions. This reduced scheme has been developed to reproduce the chemical abundances of current observable species: H_2O , CH_4 , CO , CO_2 , NH_3 and HCN . It has a large range of validity and give results very similar to the full scheme in most of cases, except for hot C-rich atmospheres. The reduced scheme allows for runs ~ 30 faster than with the full one in 1D. This new scheme has been published in [3].

3. Update on the Methanol Chemistry

The chemical scheme of [2] has been developed in close collaboration with experts in combustion and has been validated experimentally as a whole on large ranges of temperatures and pressures. However, this scheme can be improved. Motivated by the study of [4], who questioned the reliability of the kinetic data used by [2] for the reaction between methanol and hydrogen yielding to methyl radical and water ($\text{H} + \text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$), we have entirely revisited the sub-mechanism for methanol combustion of [2]'s scheme.

In this talk, we will present these two chemical schemes and their impact on the 1D model results of various objects, such as GJ 1214b, GJ436b, Uranus, Neptune ...

Acknowledgements

O.V. and T.C. thanks the CNRS/INSU Programme National de Planétologie (PNP) for funding support and acknowledge support from the CNES. PT acknowledges support from the European Research Council (grant no. 757858 - ATMO). BD and EH acknowledge support from the STFC Consolidated Grant ST/R000395/1.

References

- [1] Moses, J. I., Visscher, C., Fortney, J. J., et al., The Astrophysical Journal, 737, 15, 2011
- [2] Venot, O., Hébrard, E., Agúndez, M., et al., Astronomy & Astrophysics, 546, A43, 2012
- [3] Venot, O., Bounaceur, R., Dobrijevic, M., et al., Astronomy & Astrophysics, 624, A58, 2019
- [4] Moses, J. I., Philosophical Transactions of the Royal Society of London, Series A, 372, 20130073, 2014