An intercomparison of 1D chemical kinetics codes for exoplanet atmospheres

ISSI International Team Proposal 2018

Abstract

As the upcoming launch of the James Webb Space Telescope (JWST) will provide a step-change in the quality of observations of exoplanet atmospheres, we propose to perform an intercomparison study of the 1D chemical kinetics codes that will be used to interpret those observations. Recent observations and results from theoretical works suggest that 3D processes are key in shaping the structure (temperature and circulation) and composition of real exoplanet atmospheres. Modelling the gas-phase chemistry of these atmospheres with 3D models is on the horizon, however one of the main challenges to overcome is the high computational cost of the chemistry calculations. Therefore, 1D codes are vital in the development and validation of reduced chemical networks and chemical relaxation schemes that provide the required efficiency gains to make 3D modelling of exoplanet atmospheres computationally feasible. A significant number of 1D chemical kinetics codes have now been applied to hot exoplanet atmospheres in the literature. However a detailed intercomparison of these models has never been performed. Variation in the output from these models can result from differences in the model discretisation, numerical methods, physics schemes (e.g. transport and radiative transfer) as well as the choice of chemical network and other model inputs. As the quality of observations continues to increase it is becoming more crucial to quantify, understand and, ultimately, reduce this model variation. This project will bring together many experts in the field and also, importantly, seven of the currently published codes in the literature. *We propose to perform, for the first time, a detailed intercomparison study of 1D chemical kinetics codes applied to exoplanet atmospheres.* We will investigate the differences that are introduced by the choice of numerous model inputs (including the chemical network) but mainly by the codes themselves, by performing simulations with identical model input. The project will identify the most important sources of variation in model output, providing a clear focus for future developments. The improvements to theoretical tools that will follow this project are vital for keeping pace with advances in observational techniques and facilities.

Research domain: planetary sciences

1 Scientific justification

Over the past few decades the detection and characterisation of exoplanets and their atmospheres has grown rapidly [e.g. Sing et al., 2016]. Hot Jupiters (Jovian-mass planets on very close-in orbits around their host stars) have been the dominant focus of observational and theoretical studies of exoplanet atmospheres to date as they offer the best opportunities for observational characterisation with current and future instruments. Using a variety of ground-based [e.g. Nikolov et al., 2016] and space-based telescopes [e.g. Kreidberg et al., 2014, Wakeford et al., 2018] various chemical species have been successfully detected. Due to the limited spectral coverage of current instruments these detections have largely been limited to water (H_2O) and the alkali species (e.g. Na, K). However, upcoming instruments, such as the James Webb Space Telescope (JWST), will both improve the precision and make accessible a wider range of wavelengths that will allow for the detection of chemical species that absorb in the mid-infrared, such as methane (CH_4), carbon monoxide (CO), carbon dioxide (CO_2) and ammonia (NH_3).

The step-change in observations promised by new instruments can only be fully exploited with a concurrent development and improvement of the theoretical tools used to interpret those observations. To date one-dimensional (1D) models that either assume local chemical equilibrium or include the effects of chemical disequilibrium, via a chemical kinetics approach, have been the workhorse for such studies. The latter, the chemical kinetics codes, usually include the effects of vertical transport, due to parameterised vertical motions of the atmosphere, and photochemical dissociations, due to irradiation from the planets' host star. Many studies [e.g. Moses et al., 2011, Venot et al., 2012, Agúndez et al., 2014b, Zahnle and Marley, 2014, Hu et al., 2015, Drummond et al., 2016, Rimmer and Helling, 2016] have shown that these processes are expected to drive the gas-phase chemistry away from local chemical equilibrium, with consequences for the simulated observables.

Observations [e.g. Knutson et al., 2012, Louden and Wheatley, 2015] and theory [e.g. Showman et al., 2009, Amundsen et al., 2016] suggest that horizontal transport is at least as important as vertical transport in the atmospheres of hot exoplanets, requiring the use of multi-dimensional chemical modelling [Cooper and Showman, 2006, Agúndez et al., 2014a, Drummond et al., 2018]. However, due to the high computational expense, chemical modelling with 3D models has been

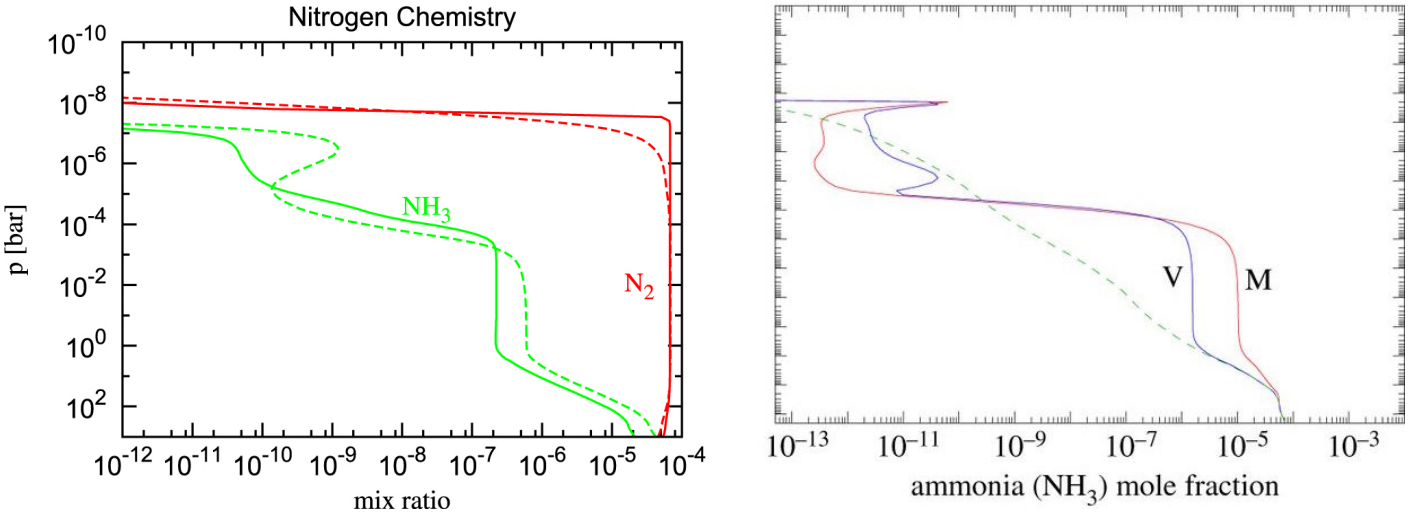

Figure 1: Examples of previous bilateral model comparisons. Left: abundance profiles of ammonia and nitrogen comparing KINETICS [Moses et al., 2011] with ARGO [Rimmer and Helling, 2016]. Right: abundance profiles of ammonia comparing KINETICS [Moses et al., 2011] with the Venot Model [Venot et al., 2012]. Figures taken from [Rimmer and Helling, 2016] and [Moses , 2014].

strictly limited. Therefore, alternative methods such as the use of reduced chemical networks [Dobrijevic et al., 2011] and chemical relaxation schemes [Cooper and Showman, 2006, Tsai et al., 2017a] are likely required to overcome this difficulty. A reduced chemical network relies on removing chemical species and reactions while maintaining accurate results for a subset of species of interest. The chemical relaxation method is effectively a parameterisation of the chemical kinetics method that involves the estimation of a chemical timescale from a full chemical network. Both options result in increased computational efficiency but both also depend on verification and validation with 1D chemical kinetics codes.

A fundamental input of a chemical kinetics code is a chemical network: a list of chemical reactions with associated rate coefficients. It is well understood that the choice of chemical network, and the reactions and rate coefficients contained within, determine the rate at which chemical species are interconverted within the model and, therefore, the end result. There are several instances of bilateral comparisons between different kinetics codes, with each code using a different chemical network, that find significant variations in the steady-state abundances [Venot et al., 2012, Rimmer and Helling, 2016, Tsai et al., 2017b, see Fig. 1]. However, in this case it is difficult to separate differences that are due to the choice of chemical network from those that are due to the kinetics code itself.

We propose to perform the first detailed intercomparison study of seven chemical kinetics codes applied to hot exoplanet atmospheres, focusing on differences that result from the codes, as opposed to differences due to the model inputs. We will achieve this by designing a set of experiments to test the main components of the models while using identical inputs, including the chemical network. Such a detailed model intercomparison has been performed for models of brown dwarf atmospheres [Helling et al., 2008] but not yet for the irradiated atmospheres of exoplanets, where photochemistry is much more significant. We will consider differences due to:

- Numerical methods (e.g. solution of the continuity equation)
- Model discretisation (e.g. vertical grid, resolution of UV irradiation)
- Physics schemes (e.g. vertical diffusion, radiative transfer)
- Model parameters and choices (e.g. convergence criteria, initial conditions, boundary conditions).

A detailed intercomparison of the available chemical networks, though highly complementary to this proposal, warrants a dedicated project. The members of this team were either involved in development of, or have access to, the following chemical kinetics codes:

“Agúndez Model”	Agúndez et al., *A&A*, 2014
ARGO	Rimmer and Helling, *ApJS*, 2016
ATMO	Tremblin et al., *ApJL*, 2015
“Kasting Model”	Kopparapu et al., *ApJ*, 2012
KINETICS	Moses et al., *ApJ*, 2011
“Venot Model”	Venot et al., *A&A*, 2012
VULCAN (Open-source)	Tsai et al., *ApJS*, 2017

This set of seven codes represents almost of all of the currently published codes in the literature.

The project will be comprised of two sets of experiments: the “core” experiments and the “secondary” experiments. The exact design of the core experiments will discussed and agreed upon during the first meeting, but they will be a broad test of the most fundamental aspects of the codes; e.g. the numerical solver, the vertical mixing scheme and the photochemistry scheme. The secondary set of experiments will be designed in response to the results of the core experiments. For instance, if the core experiments suggest that most of the variation is introduced when photochemistry is included then the secondary experiments will be designed to test this element in more detail; for example, to test whether the main difference results from a different method of calculating the radiative transfer or from discretisation of the vertical grid, amongst other possibilities.

This project brings together world-leading experts in the field of chemical modelling of exoplanet atmospheres along with seven chemical kinetics codes. The results of this model intercomparison study will quantify the variation in model output, for a given chemical network, that will inform the confidence of theoretical predictions in future model-observation comparisons. It will also indentify the most important model components that determine the final model result, that will allow for a more targeted approach for future model developments and improvements.

2 Expected output

The project will identify and quantify the main causes of variation in the output of 1D chemical kinetics codes. This knowledge will guide future model developments and improvements, and inform future studies that compare theoretical predictions with observations. It will also provide the possibility to detect unknown “bugs” leading to more accurate and stable codes.

We expect this project to produce one or two peer-reviewed publications. A paper presenting the results of a model intercomparison study with a large number of codes is likely to gain a significant number of citations. There is also potential for a paper reviewing the theory and methods involved with chemical kinetics codes.

3 Added value of ISSI

Any model intercomparison study will, by necessity, involve lengthy discussion of many fine details. This is difficult to achieve through email or time-limited video conferences, particularly with $\sim$16 participants from 12 institutions and 6 countries. The format of the ISSI Team project is highly suited to our proposal as it will guarantee large amounts of time (two one-week meetings) for face-to-face discussions of ideas, to agree on experimental design and discuss and understand results. The increased face-to-face interaction, that is uniquely offered by the ISSI Team project format, will greatly enhance the collaborative nature of the work and will lead to a more robust set of experiments, results and publications.

4 List of team members - 16 (inc. 2 external) from 6 countries

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* External members - not expected to attend meetings

5 Schedule

This project will involve two one-week meetings spaced 6-12 months apart.

First meeting:

- Presentations by participants on kinetics codes and major results
- Discuss and decide on a set of "core" experiments, including model inputs
- Discuss and agree on a standard format for model output
- Discuss and agree on a format for making the experiment setup, model inputs and ouputs openly available (i.e. via a team website)
- Discuss the option to write a review paper on methods in chemical kinetics codes
- Allocated time for work on setting up "core" experiments

Second meeting:

- Present and discuss results from “core” experiments
- Design a set of “secondary” experiments
- Discuss format and content for publication of results
- Allocated time for work on setting up “secondary” experiments

After second meeting:

- Collate results from “secondary” experiments
- Write and submit an article presenting our results to a peer-reviewed journal

6 Requested facilities and financial support

We request the use of a meeting room for 15 people with an internet connection, a visual projector and video-conferencing facilities. We also request per diem living expenses for each team member while attending the meetings in Bern.

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