ISSI Team proposal: Intercomparison of 1D photochemical models of Titan atmosphere

Abstract

We propose a series of three workshops to proceed to the first inter-comparison of existing 1D models of photochemistry in Titan’s atmosphere. The team regroups the responsible and/or developers of major models used to interpret data from the Cassini mission, and to understand coupled dynamic and complex chemistry processes occurring in the dense nitrogen-methane atmosphere of Titan. The aim of the three meetings will be first to compare and overcome present discrepancies between the independent codes developed by the participants, in order to detect, discuss and develop the most relevant possible evolutions for future Titan 1D modelling.

1 Scientific justification

The Cassini mission reveals daily that the chemical complexity of Titan’s atmosphere is beyond our expectations (Waite et al., 2005, 2007). This atmosphere is composed mainly of nitrogen, with a few percents of methane. Irradiation of this mixture with solar UV, energetic electrons and cosmic rays drives a very rich and complex chemistry, leading to the formation of aerosols which eventually precipitate on Titan’s surface. Heavy positive and negative ions are also observed by Cassini in the ionosphere.

This constitutes a very challenging system for modelers. Many physico-chemical processes are involved: radiative transfer, photo-dissociation, electron impact, radical- and ion-neutral chemistry, recombinations, heterogeneous chemistry, soot formation micro-physics, turbulent transport... Several groups over the world have developed independently models of the photochemistry of Titan (Yung et al., 1984; Toublanc et al., 1995; Lara et al., 1996; Banaszkiewicz et al., 2000b; Cravens et al., 2004; Wilson and Atreya, 2004; Lebonnois, 2005; Hébrard et al., 2007; De La Haye et al., 2007; Vuitton et al., 2007; Lavvas et al., 2008). The codes implementing the models are complex and rely on different levels of numerical and algorithmic approximations, such as space/time discretization for chemistry-transport. Moreover, all physico-chemical processes are described by empirical parameters. At this stage, there is no consensus on the various input parameters, and it becomes increasingly difficult to compare outputs from different models, as they increase their sophistication level to cope with observations.

Many interesting new results have been obtained with 1D models. These models are the first level of approximation, and if we really understand up to what level of confidence we can use them, then they may still be very useful. Due to unrealistic computer times, 2D or 3D models cannot be presently pushed to the same level of sophistication in chemistry modeling. A standard, validated, 1D code would have a great added value for the planning of future missions (TANDEM) and for the integration in a planetary virtual observatory (IDIS - EuroPlaNet). It is thus of paramount importance to gather experts of the existing codes and proceed to an inter-comparison.

Similar comparisons in other scientific fields did not go without surprise (Rickert, 1995; Bowen et al., 2003, 2006; Röllig et al., 2007; Rubiano et al., 2007). They show that it is sometimes very difficult to get a set of codes to produce identical quantitative predictions, even when these codes implement similar models.

Before addressing code validation with regard to observed data, we will proceed to code verification.

Verification. Given identical sets of inputs, all codes should provide identical outputs. Common inputs are: Kv profile, T,p,n structure, list of compounds, photodissociation cross-sections, solar flux
at top of atmosphere, list of reactions, condensation vapor pressures, boundary fluxes... We propose to compare the codes at three levels:

1. identical conditions, where each code runs with it’s own parameters set, for specified conditions;
2. identical parameters sets, where all codes have to be tuned in order to implement the same model;
3. extreme parameters sets, where it is checked that codes remain stable in extreme conditions.

Discrepancies will have to be elucidated and reduced as much as possible.

**Validation.** This inter-comparison will also be a necessary step to estimate explicitly the importance of various physico-chemical processes on model predictions, as compared to observations (effect of ions on neutral densities, effect of eddy diffusion coefficient - Kv - profile...). Among these codes, one major aspect is the incorporation of ion-neutral chemistry, or limitation to neutral chemistry. This aspect has been shown to be significant in the determination of the neutral abundances (Banaszkiewicz et al., 2000a; Wilson and Atreya, 2004). For the codes that do have this possibility, separate simulations will be run with and without ions. The runs without ions will allow a full inter-comparison between all models, while the runs with ions will demonstrate the influence of this component in Titan’s chemistry.

2 Expected Outputs

Scientific outputs, in terms of code verification and validation, have been exposed in the previous section. This original experience will provide, without any doubt, matter for methodological papers in planetary sciences journals, and notably for a review of the existing codes and models.

3 Added value by ISSI

ISSI provides a unique infrastructure for gathering researchers in planetary sciences.

4 List of confirmed members

**Participants responsible for the development of a model of Titan atmospheric chemistry:**

- T. Cravens, Dept of Physics & Astronomy, University of Kansas, USA.
- V. De La Haye & J. H. Waite, Southwest Research Institute, San Antonio, Texas, USA.
- M. Dobrijevic, Laboratoire d’Astrophysique de Bordeaux, France.
- L. M. Lara, Instituto de Astrofísica de Andalucía - CSICL. Spain.
- S. Lebonnois, Laboratoire de Météorologie Dynamique du CNRS, France.
- I. Vardavas, Department of Physics, University of Crete, Greece.

**Specialists of Titan’s atmosphere and chemistry are also volunteer to the team:**

- I. Müller-Wodarg, Space and Atmospheric Physics Group, Imperial College, UK.
- N. Carrasco & E. Hébrard, Service d’Aéronomie du CNRS, France.

**Young scientists:**

- M. Papadopoulos, Department of Physics, University of Crete, Greece.
- J. Bell, University of Michigan, USA.
Team leader:

▷ P. Pernot, Laboratoire de Chimie Physique, Orsay, France

External members. A few other persons, working on additional models, have expressed their interest to this project, without being able to commit. This is particularly the case for some American colleagues, detracted by the involved travel costs. It will be possible to make the standard parameters sets defined by the experts available to the interested persons, who could contribute the outputs of their models to the inter-comparison, without attending the ISSI meetings. Video-conferences could be used to involve these people.

5 Schedule of the project

The project will be covered by three meetings over 18 months, with enough time between meetings to enable team members to run the required reference simulations. In order to minimize the costs for our colleagues from overseas, the meetings will be held as close as possible to major European planetology meetings (EPSC, EGU...).

First meeting. Elaboration of the framework for the inter-comparison and cross-validation of the codes.

1. presentation of the status of knowledge on Titan’s chemistry;
2. detailed presentations of the codes in order to design a list of capabilities;
3. definition of standard sets of inputs (solar radiation, magnetosphere effects, localizations, chemistry database, transport parameters...) related to present and expected future missions; the sets will be designed to test and ascertain the effect of the various physico-chemical processes;
4. definition of a common data model, specially for data outputs on which the comparison will be based. A common data model for inputs, enabling inter-operability of models, would also be a plus.

Second meeting. Between the meetings, the staffs will have run the benchmark tests and returned the results data files to a web storage platform.

1. comparison of the raw outputs;
2. presentation and analysis of the results by participants;
3. comparison of outputs and elucidation of possible discrepancies;
4. discussion of the influence of the different input parameters, based on each participant’s experience with his own code, and on the comparison of outputs;
5. definition of potential nominal and extreme inputs sets, in order to cross-validate the codes over a large range of atypical conditions.

Third meeting.

1. comparison of outputs for potential nominal inputs sets, by comparing obtained abundances to observations (and elucidation of possible discrepancies);
2. comparison of the outputs for extreme cases and elucidation of possible discrepancies;
3. definition of the framework and content of a publication of these results.
6 Facilities and financial support requested from ISSI

The workshops would benefit from a reunion room for 15 persons, with a video projector, internet connections and a video-conference equipment. No additional support, beyond the standard financial support defined by ISSI is asked for.

7 Coordinates of all participants

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References


