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A Vapor Pressure Database for Modeling Planetary Atmospheres

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Abstract

Atmospheric modeling involving the condensation process, such as in photochemical or microphysical models, requires knowledge of the vapor pressure of the condensing species as a function of temperature. Additionally latent heat values, which can be related to the vapor pressure through the Clausius-Clapeyron equation, are important when modeling energy transport processes. Online reference sites such as the NIST Chemistry WebBook contain formulations of the vapor pressure for many species found in the planetary atmospheres of our solar system. However the NIST equations most often report data for the liquid phase, whereas at the colder temperatures in outer solar system, these species would condense as ices. There have been some works in the literature that compile lists of vapor pressure equations and data points for sublimation, but an online database allowing the user to perform calculations or create plots over a desired temperature range is lacking.

1. Introduction

Understanding the validity of vapor pressure and latent heat equations for a given temperature range is of great importance to a variety of researchers across the planetary science community. Applications include photochemical modeling, microphysical modeling, energy balance models, general circulation models, planetesimal formation models, and interpreting spacecraft observations.

Ices are prevalent in the outer solar system and have been detected at the surface of many planetary bodies. The prevalence of methane (CH4) in outer planet atmospheres leads to an abundance of hydrocarbons created through photochemistry. The molecular nitrogen composition, particularly on Titan and Pluto, also results in creation of a number of nitrile species. Thus, modeling the condensation process in the outer solar system requires knowledge of vapor pressure and latent heat values as a function of temperature, often well below the triple point of the various (hydrocarbon and nitrile) species present in these planetary atmospheres.

The National Institute of Standards and Technology (NIST) Chemistry WebBook (Linstrom and Mallard: /http://webbook.nist.gov/chemistry/) provides the most complete online database of vapor pressure, latent heat, and triple point temperature/pressure values. [4] is an example, containing temperature relations for the vapor pressures of nine hydrocarbons anticipated to condense in Neptune's atmosphere. [1] has been widely cited by the modeling community. They give both liquid and ice forms of the vapor pressure equations for a dozen species, including the alpha and beta phases of some ices (e.g., N2, CO). [2] more recently conducted an extensive study of sublimation vapor pressure lab data in order to evaluate the measurements for low temperatures and construct a polynomial fit (similar in form to Brown and Ziegler's equation)

While the works cited above have proved extremely useful, they do have their limitations, particularly with reference to the outer planet atmospheres in our solar system – the NIST database primarily due to a lack of data for low temperatures and Fray and Schmitt due to gaps in the number of species where suitable equations could be derived and (as with [1]) the computational expense of their equation. What would be most useful for the research community would be the ability to graphically compare all reference equations for a given species across any desired temperature range. Such a task is currently being undertaken by developing the software tools described below.

2. Vapor Pressure Modules

A number of Fortran 90 modules will be written so that these equations can be called directly from existing code. Each reference equation is coded into a separate function, named with the condensing species and the specific reference name (e.g. nist, author's name). The complete citation and temperature range (if available) cited from the original source is listed. A wrapper function (e.g., vapor_press_CH4) is then used to access the specific reference equation for a given species, providing an input argument of phase and reference ID. There is a similar looking latent_heat_CH4 wrapper function with calls to the collected latent heat equations.

Each condensing species is self-contained in its own 'database' module. All module names take the same form, database_formula, where formula is the molecular formula of the condensing species, e.g. CH4, C2H6, C2H2, etc. Within each module, the vapor pressure and latent heat functions all follow the same naming convention as well, for ease of use.

The Fortran modules will be designed such that they can be compiled/run on their own or called from an existing model. Fortran was chosen as many of the models listed in Sec. 1 have this language as their heritage, and also a Fortran compiler is typically available on the systems of most researchers. Additionally, Fortran code can be called from C, Python, and IDL. The modules will be tested on both Linux and Windows platforms and have currently been compiled using both gfortran and ifort with no problems.

Additionally, a similar set of functions will be coded in Python. These functions also take temperature as an input argument, as well as a string for pressure units for the output value. A reference string is given, similarly to the Fortran functions. If the string is simply 'ref' the function will print a list of available references and their temperature range instead of calculating the vapor pressure or latent heat. The Python dictionary tool allows for the creation of a simple plotting program, where all relevant equations can be accessed simply by giving the species' chemical formula. The vapor pressure module uses only the Python numpy package; the pylab package is used in the plotting module. Python was chosen as it is freely available and is becoming increasingly used within the research community - both by modelers and non-modelers to visualize their data.

3. Summary

Instructions for compiling and running the Fortran and Python modules will also be provided in the submission to NASA's GitHub. In addition to a separate instructions file, the Python module also contains a help function. The vapor pressure and latent heat calculation functions for all species are contained in a single file (module) for the Python code. There will also be separate python programs for generating the vapor pressure comparison curves and latent heat curves over a user-supplied range of temperatures. The Fortran code will be a set of separate files (modules) for each species along with a global module file to supply relevant constants (e.g. universal gas constant and unit conversions). To further provide for a wide variety of uses, numerical tables of vapor pressure and latent heat values over a range of temperatures will be generated for all species and submitted to NASA's GitHub.

Initial work on equations relevant to icy species in the Outer Planet atmospheres will be presented here. Future work will include species relevant to exoplanet atmospheres.

Acknowledgements

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References

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