EPSC Abstracts
Vol. 13, EPSC-DPS2019-1276-1, 2019
EPSC-DPS Joint Meeting 2019

EPSC
EPSC-DPS Joint Meeting 2019
15–20 September 2019 | Geneva, Switzerland

A database of vapor pressure equations for modeling cloud condensation in the atmospheres of the outer solar system

Erika Barth

Southwest Research Institute, Boulder, Colorado, USA (ebarth@boulder.swri.edu)

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 ChemistryWebBook 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

The photochemistry of methane and nitrogen molecules present in the atmospheres of the outer solar system creates a number of hydrocarbon and nitrile trace species that can affect the physical and optical properties of these atmospheres. In order to determine if these species might condense and grow as atmospheric particles, the vapor pressure must be known as a function of the relevant atmospheric temperatures, often well below the triple points of the various species.

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.

2. Vapor Pressure Modules

Fortran 90 modules have been 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 (Fig. 1). 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.

```
!````````````````````````````````````````````````````````````````````````````
function vapor_press_CH4(Tz, phase, ref_id)

!+ Use phase and reference input value to choose vapor pressure function

!~ ELB 05/26/2014

implicit none

!== Arguments:
integer, intent(IN) :: ref_id
real(fk), intent(IN) :: Tz ! Temperature point [K]
character(len=3) :: phase

!== Local declarations
real(fk) :: vp
real(fk) :: vapor_press_CH4

!== Executable statements:

  if( phase == 'sub' ) then ! Call functions for ice-phase equations

    if( ref_id == 1 ) then ! Moses et al. (1992) - ice phase
      vp = vaporp_eqn_CH4_moses_ice(Tz)
    elseif( ref_id == 2 ) then ! Fray & Schmitt (2009)
      vp = vaporp_eqn_CH4_fs(Tz)
    elseif( ref_id == 3 ) then ! Brown & Ziegler (1980)
      vp = vaporp_eqn_CH4_bz_ice(Tz)
    else
      write(*,*) 'Invalid reference for CH4 vapor pressure (ice)'
      stop
    endif

  else ! Liquid-phase equations

    if( ref_id == 1 ) then ! Antoine eqn. from NIST
      vp = vaporp_eqn_CH4_nist(Tz)
    elseif( ref_id == 2 ) then ! Moses et al. (1992) - liquid phase
      vp = vaporp_eqn_CH4_moses_liq(Tz)
    elseif( ref_id == 3 ) then ! Brown & Ziegler (1980)
      vp = vaporp_eqn_CH4_bz_liq(Tz)
    elseif( ref_id == 4 ) then ! Reid et al. (1987)
      vp = vaporp_eqn_CH4_reid(Tz)
    else
      write(*,*) 'Invalid reference for CH4 vapor pressure (liq)'
      stop
    endif

  endif

  vapor_press_CH4 = vp

end function vapor_press_CH4
```

Figure 1: Methane database wrapper function for calculation of vapor pressure as a function of temperature.

The Fortran modules are designed such that they can be compiled/run on their own or called from an existing model. Fortran was chosen as many models 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 are tested on both Linux and Windows platforms and have currently been compiled using both gfortran and ifort with no problems.

A similar set of functions have been 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.

The Fortran and Python modules, as well as instructions for compiling and running, will be available on NASA's GitHub. In addition to a separate instructions file, the Python module also contains a help function. 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 consists of 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.

Acknowledgements

This work is funded by the NASA PDART program.

References

[1] Brown, G.N. andW.T. Ziegler: Vapor pressure and heats of vaporization and sublimation of liquids and solids of interest in cryogenics below 1-atm pressure, Adv. Cryogen. Eng. Vol. 75, pp. 662-670, 1980.

[2] Fray, N. and B. Schmitt: Sublimation of ices of astrophysical interest: A bibliographic review, Planet. Space Sci., Vol. 57, pp. 2053-2080, 2009.

[3] P.J. Linstrom and W.G. Mallard, Eds., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, http://webbook.nist.gov.

[4] Moses, J. I., M. Allen, and Y. L. Yung. Hydrocarbon nucleation and aerosol formation in Neptune's atmosphere. Icarus 99, 318–346, 1992.