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# **iapws Documentation**

***Release 0.1.1***

**M. Skocic**

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## GETTING STARTED

### 1.1 iapw

## Modern Fortran IAPWS

*ipaws* is a Fortran library providing the formulas for computing light and heavy water properties. It also provides a API for the C language. The formulations are taken from <http://iapws.org>. A shared and a static library *libiapws* are compiled (f2008+) with the Fortran and C headers. The static and shared libraries can be installed in order to be included in Fortran or C programs.

The compilation was tested on Linux (Debian), MacOS and Windows.

Sources: <https://github.com/MilanSkocic/iapws>

#### 1.1.1 How to install

Create build directory

```
$ mkdir build
$ cd build
```

Generate a makefile

- On Unix-like OS:

```
cmake -G "Unix Makefiles" -S .. -DCMAKE_BUILD_TYPE=release -DCMAKE_INSTALL_PREFIX=/
↳path/to/folder
```

- On windows with MSYS2:

```
cmake -G "Unix Makefiles" -S .. -DCMAKE_BUILD_TYPE=release -DCMAKE_INSTALL_PREFIX=/
↳path/to/folder
```

- On windows with ifort and msvc:

```
cmake -G "NMake Makefiles" -S .. -DCMAKE_BUILD_TYPE=release -DCMAKE_INSTALL_PREFIX=/
↳path/to/folder
```

Build

```
cmake --build .
```

Run tests

```
ctest
```

Install

```
cmake --install .
```

## 1.1.2 Dependencies

```
gcc>=4.6 or msvc>=14  
gfortran>=4.6 or ifort>=18  
cmake>=3.10
```

## 1.1.3 License

GNU General Public License v3 (GPLv3)

# 1.2 pyiapws

Python wrapper around the [Fortran iapws library](#). Follow the [installation instructions](#). for compiling and installing the library.

For now,the wrapper must be compiled on Linux, windows and MacOS platforms after installing the iapws library using the compiler that was used to compile your python interpreter.

## 1.2.1 How to install

```
pip install pyiapws
```

## 1.2.2 Dependencies

```
numpy>=1.21
```

## 1.2.3 License

GNU General Public License v3 (GPLv3)

# 1.3 Examples

## 1.3.1 Example in Fortran

```
program example_in_f  
  use iso_fortran_env  
  use iapws  
  implicit none
```

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```

real(real64) :: kh, kd
character(len=5) :: gas = "O2"
character(len=5) :: solvent = "H2O"
real(real64) :: T = 25.0d0

kh = iapws_kh(T, gas, solvent)
print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F10.4)", "Gas=", gas, "T=", T,
↪ "C", "kh=", kh

kd = iapws_kd(T, gas, solvent)
print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F15.4)", "Gas=", gas, "T=", T,
↪ "C", "kh=", kd

end program

```

### 1.3.2 Example in C

```

#include <string.h>
#include <stdio.h>
#include "iapws.h"

int main(int argc, char **argv){

    double T = 25.0; /* in C*/
    char *gas = "O2";
    char *solvent = "H2O";
    double kh, kd;

    if(argc > 1 ){
        printf("%s\n", argv[1]);
    }

    kh = iapws_capi_kh(T, gas, solvent, strlen(gas), strlen(solvent));
    printf("Gas=%s\tT=%fC\tkh=%+10.4f\n", gas, T, kh);

    kd = iapws_capi_kd(T, gas, solvent, strlen(gas), strlen(solvent));
    printf("Gas=%s\tT=%fC\tkd=%+15.4f\n", gas, T, kd);

    return 0;
}

```

### 1.3.3 Example in Python

```

r"""Example in python"""
import numpy as np
import pyiapws

T = 25.0
pyiapws.kh(T, "O2", "H2O")
pyiapws.kd(T, "O2", "H2O")

```





## IAPWS - THEORETICAL BACKGROUND

### 2.1 IAPWS G7-04

The computation is based on the parameters provided by the IAPWS 2004 [1].

#### 2.1.1 Henry Contant: $k_H$

The Henry constant  $k_H$  is defined as shown in equation Eq.2.1.1.  $k_H$  is expressed in MPa.

$$k_H = \lim_{x_2 \rightarrow 0} f_2/x_2 \quad (2.1.1)$$

- $f_2$ : liquid-phase fugacity
- $x_2$ : mole fraction of the solute

The Henry's constant  $k_H$  is given as a function of temperature by:

$$\ln \left( \frac{k_H}{p_1^*} \right) = A/T_R + \frac{B \cdot \tau^{0.355}}{T_R} + C \cdot T_R^{-0.41} \cdot \exp \tau \quad (2.1.2)$$

- $\tau = 1 - T_R$
- $T_R = T/T_{c1}$
- $T_{c1}$ : critical temperature of the solvent as recommended by IAPWS [2]
- $p_1^*$  is the vapor pressure of the solvent at the temperature of interest and is calculated from the correlation of Wagner and Pruss for  $H_2O$  [3] and from the correlation of Harvey and Lemmon for  $D_2O$  [4].

Both equations have the form:

$$\ln (p_1^*/p_{c1}) = T_R^{-1} \sum_{i=1}^n a_i \tau^{b_i} \quad (2.1.3)$$

- $n$  is 6 for  $H_2O$  and 5 for  $D_2O$
- $p_{c1}$  is the critical pressure of the solvent recommended by IAPWS [2]

#### 2.1.2 Vapor-Liquid Distribution Constant: $k_D$

The liquid-vapor distribution constant  $k_D$  is defined as shown in equation Eq.2.1.4.  $K_D$  is adimensional.

$$k_D = \lim_{x_2 \rightarrow 0} y_2/x_2 \quad (2.1.4)$$

- $x_2$ : mole fraction of the solute
- $y_2$  is the vapor-phase solute mole fraction in equilibrium with the liquid

The vapor-liquid distribution constant  $k_D$  is given as a function of temperature by:

$$\ln K_D = qF + f(\tau) + (F + G\tau^{2/3} + H\tau) \exp\left(\frac{273.15 - T(K)}{100}\right) \quad (2.1.5)$$

- $q$  : -0.023767 for  $H_2O$  and -0.024552 for  $D_2O$ .
- $f(\tau)$  [3] for  $H_2O$  and [5] for  $D_2O$ .

In both cases,  $f(\tau)$  has the following form:

$$f(\tau) = \sum_{i=1}^n c_i \cdot \tau^{d_i} \quad (2.1.6)$$

- $n$  is 6 for  $H_2O$  and 4 for  $D_2O$

### 2.1.3 Molar fractions

$$\begin{aligned} x_2 &= \frac{f_2}{k_H} \\ \frac{x_2}{f_2} &= \frac{1}{k_H} \\ y_2 &= \frac{k_D}{k_H} \cdot f_2 \\ \frac{y_2}{f_2} &= \frac{k_D}{k_H} \end{aligned} \quad (2.1.7)$$

## RELEASE NOTES

### 3.1 iapws 0.1.1 Release Note

#### 3.1.1 Summary

- Logo creation
- Error handling in python wrapper for arrays with rank greater than 1
- Tests in python wrapper for expected failures with rank-n arrays

#### 3.1.2 Download

iapws

pyiapws

#### 3.1.3 Contributors

Milan Skocic

#### 3.1.4 Commits

Full Changelog: <https://github.com/MilanSkocic/pyiapws/compare/0.1.0...0.1.1>

### 3.2 iapws 0.1.0 Release Note

#### 3.2.1 Changes

- Implementation of kH and kD from IAPWS G7-04 in fortran + C API
- Python wrapper for kH and kD.
- Documentation with sphinx.

### 3.2.2 Download

iapws

pyiapws

### 3.2.3 Contributors

Milan Skocic

### 3.2.4 Commits

Full Changelog: <https://github.com/MilanSkocic/pyiapws/compare/...0.1.0>

## AUTOGENERATED DOCUMENTATION

### 4.1 iapws

namespace **iapws**

Main module for IAPWS computations.

#### Functions

**pure real(real64) function, public iapws\_kh (t, gas, solvent)**

Compute the henry constant for a given temperature and gas in solvent.

##### Parameters

- **T** – [in] Temperature in °C.
- **gas** – [in] Gas.
- **solvent** – [in] Solvents: H2O or D2O. Default is H2O.

##### Returns

kh Henry constant. NaN if gas not found.

**pure real(real64) function, public iapws\_kd (t, gas, solvent)**

Compute the vapor-liquid constant for a given temperature and gas in solvent.

##### Parameters

- **T** – [in] Temperature in °C.
- **gas** – [in] Gas.
- **solvent** – [in] Solvents: H2O or D2O. Default is H2O.

##### Returns

kd Vapor-liquid constant. NaN if gas not found.

namespace **iapws\_capi**

C API for the IAPWS module.

## Functions

`real(c_double) function, public iapws_capi_kh (t, gas, solvent, size_gas, size_solvent)`

Compute the henry constant for a given temperature and gas in solvent.

### Parameters

- **T** – [in] Temperature in °C.
- **gas** – [in] Gas.
- **solvent** – [in] Solvents: H2O or D2O. Default is H2O.
- **size\_gas** – [in] Length of the string gas.
- **size\_solvent** – [in] Length of the string gas.

### Returns

kh Henry constant. NaN if gas not found.

`real(c_double) function, public iapws_capi_kd (t, gas, solvent, size_gas, size_solvent)`

Compute the vapor-liquid constant for a given temperature and gas in solvent.

### Parameters

- **T** – [in] Temperature in °C.
- **gas** – [in] Gas.
- **solvent** – [in] Solvents: H2O or D2O. Default is H2O.
- **size\_gas** – [in] Length of the string gas.
- **size\_solvent** – [in] Length of the string gas.

### Returns

kd Vapor-Liquid constant. NaN if gas not found.

## 4.2 pyipaws

IAPWS computations.

`pyiapws.iapws.kd(temperature: int | float | ndarray[Any, dtype[ScalarType]], gas: str, solvent: str) → float | ndarray[Any, dtype[ScalarType]]`

Compute the vapor-liquid distribution constant for the gas and solvent at temperature.

### Parameters

- temperature: int, float or array-like.**  
Temperature in °C.
- gas: str**  
Desired gas.
- solvent: str**  
Desired solvent: H2O or D2O.

### Returns

- kd: float or array-like**  
Liquid-Vapor distribution constant.

```
pyiapws.iapws.kh(temperature: int | float | ndarray[Any, dtype[ScalarType]], gas: str, solvent: str) → float |  
ndarray[Any, dtype[ScalarType]]
```

Compute the Henry constant for the gas and solvent at temperature.

#### Parameters

**temperature: int, float or array-like.**

Temperature in °C.

**gas: str**

Desired gas.

**solvent: str**

Desired solvent: H2O or D2O.

#### Returns

**kh: float or array-like**

Henry constant.





## INDICES AND TABLES

- `genindex`
- `modindex`
- `search`



## BIBLIOGRAPHY

- [1] IAPWS. Guideline on the Henry's Constant and Vapor-Liquid Distribution Constant for Gases in  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  at High Temperatures. Technical Report G7-04, IAPWS, Kyoto, Japan, 2004.
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- [5] R. Fernandez-Prini, J.L. Alvarez, and A.H. Harvey. Henry's Constants and Vapor–Liquid Distribution Constants for Gaseous Solutes in  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  at High Temperatures. *Journal of Physical Chemistry Reference Data*, 32(2):903–916, 2003.



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