# IAPWS

0.1

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# Chapter 1

# Introduction

`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.

Links:

- Sources: `https://github.com/MilanSkocic/iapws`.
- Online documentation: `https://milanskocic.github.io/iapws/iapws/index.html`.
- PDF documentation: `https://milanskocic.github.io/iapws/iapws/refman.pdf`.
- Python wrapper: `https://milanskocic.github.io/iapws/pyiapws/index.html`.

## 1.1 Installation

See the file `INSTALL`.

## 1.2 Dependencies

See the file `REQUIREMENTS`.

## 1.3 License information

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# Chapter 2

# IAPWS G7-04

The computation is based on the parameters provided by the IAPWS 2004 [2] : $k_H = \lim_{x_2 \to 0} f_2/x_2$.

where $f_2$ and $x_2$ are, respectively, the liquid-phase fugacity and mole fraction of the solute.

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

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

$$\tau = 1 - T_R$$

$$T_R = T/T_{c1}$$

- $T_{c1}$ is the critical temperature of the solvent as recommended by IAPWS [3] (647.096 for H2O and 643.847 K for D2O) and $p_1^*$ is the vapor pressure of the solvent at the temperature of interest.
- $p_1^*$ is calculated from the correlation of Wagner and Pruss for H2O [4] and from the correlation of Harvey and Lemmon for D2O [1].

Both equations have the form $\ln(p_1^*/p_{c1}) = T_R^{-1} \sum_{i=1}^{n} a_i \tau^{b_i}$ where the number of terms n is 6 for H2O and 5 for D2O , $p_{c1}$ is the critical pressure of the solvent recommended by IAPWS [3] (22.064 MPa for H2O and 21.671 MPa for D2O)

The Henry's constant : $k_H$ has a dimension of pressure expressed here in GPa-1.

# Chapter 3

# Installation

## 3.1 Create build directory

- mkdir build
- cd build

## 3.2 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`

## 3.3 Build either with cmake

```
cmake --build .
```

## 3.4 Run tests

```
ctest
```

## 3.5 Install

```
cmake --install .
```

# Chapter 4

# license

```
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```

# Chapter 5

# requirements

gcc>=10.0

gfortran>=10.0

cmake>=3.10

# Chapter 6

# Modules Index

## 6.1 Modules List

Here is a list of all documented modules with brief descriptions:

# Chapter 7

# File Index

## 7.1 File List

Here is a list of all documented files with brief descriptions:

# Chapter 8

# Module Documentation

## 8.1 iapws Module Reference

Main module for IAPWS computations.

### Functions/Subroutines

- pure real(real64) function, public iapws_kh (t, gas, solvent)

  *Compute the henry constant for a given temperature and gas in solvent.*
- pure real(real64) function, public iapws_kd (t, gas, solvent)

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

### 8.1.1 Detailed Description

Main module for IAPWS computations.

### 8.1.2 Function/Subroutine Documentation

#### 8.1.2.1 iapws_kd()

```
pure real(real64) function, public iapws::iapws_kd (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas,
            character(len=*), intent(in) solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in ℃. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |

**Returns**

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

#### 8.1.2.2 iapws_kh()

```
pure real(real64) function, public iapws::iapws_kh (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas,
            character(len=*), intent(in) solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in ℃. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |

**Returns**

kh Henry constant in mole fraction per GPa. NaN if gas not found.

## 8.2 iapws_capi Module Reference

C API for the IAPWS module.

### Functions/Subroutines

- 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.*
- 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.*

### 8.2.1 Detailed Description

C API for the IAPWS module.

### 8.2.2 Function/Subroutine Documentation

#### 8.2.2.1 iapws_capi_kd()

```
real(c_double) function, public iapws_capi::iapws_capi_kd (
             real(c_double), value t,
             type(c_ptr), intent(in), value gas,
             type(c_ptr), intent(in), value solvent,
             integer(c_int), intent(in), value size_gas,
             integer(c_int), intent(in), value size_solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in ℃. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |
| in | *size_gas* | Length of the string gas. |
| in | *size_solvent* | Length of the string gas. |

**Returns**

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

#### 8.2.2.2 iapws_capi_kh()

```
real(c_double) function, public iapws_capi::iapws_capi_kh (
             real(c_double), value t,
             type(c_ptr), intent(in), value gas,
             type(c_ptr), intent(in), value solvent,
             integer(c_int), intent(in), value size_gas,
             integer(c_int), intent(in), value size_solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in ℃. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |
| in | *size_gas* | Length of the string gas. |
| in | *size_solvent* | Length of the string gas. |

**Returns**

kh Henry constant in mole fraction per GPa. NaN if gas not found.

## 8.3 iapwsg704 Module Reference

Module for IAPWS G7-04.

### Functions/Subroutines

- pure real(real64) function, public iapwsg704_kh_water (t, gas)

  *Compute the henry constant for a given temperature and gas in water.*
- pure real(real64) function, public iapwsg704_kh_heavywater (t, gas)

  *Compute the henry constant for a given temperature and gas in heavywater.*
- pure real(real64) function, public iapwsg704_kd_water (t, gas)

  *Compute the kd constant for a given temperature and gas in water.*
- pure real(real64) function, public iapwsg704_kd_heavywater (t, gas)

  *Compute the kd constant for a given temperature and gas in heavywater.*

### Variables

- real(real64), dimension(6, 2), parameter **iapwsg704_aibi_water** = reshape([-7.85951783d0, 1.84408259d0, -11.78664970d0, 22.68074110d0, -15.96187190d0, 1.80122502d0,1.000d0, 1.500d0, 3.000d0, 3.500d0, 4.000d0, 7.500d0], [6,2])

  *ai and bi coefficients for water*

### 8.3.1 Detailed Description

Module for IAPWS G7-04.

### 8.3.2 Function/Subroutine Documentation

#### 8.3.2.1 iapwsg704_kd_heavywater()

```
pure real(real64) function, public iapwsg704::iapwsg704_kd_heavywater (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas )
```

Compute the kd constant for a given temperature and gas in heavywater.

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in °C. |
| in | *gas* | Gas. |

**Returns**

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

#### 8.3.2.2 iapwsg704_kd_water()

```
pure real(real64) function, public iapwsg704::iapwsg704_kd_water (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas )
```

Compute the kd constant for a given temperature and gas in water.

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in °C. |
| in | *gas* | Gas. |

**Returns**

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

#### 8.3.2.3 iapwsg704_kh_heavywater()

```
pure real(real64) function, public iapwsg704::iapwsg704_kh_heavywater (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in °C. |
| in | *gas* | Gas. |

**Returns**

kh Henry constant in mole fraction per GPa. NaN if gas not found.

#### 8.3.2.4 iapwsg704_kh_water()

```
pure real(real64) function, public iapwsg704::iapwsg704_kh_water (
            real(real64), intent(in) t,
            character(len=*), intent(in) gas )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in ℃. |
| in | *gas* | Gas. |

**Returns**

kh Henry constant in mole fraction per GPa. NaN if gas not found.

# Chapter 9

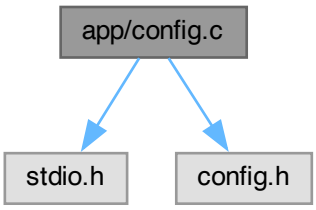
# File Documentation

## 9.1 app/config.c File Reference

Provides the configuration of the iapws library.

```
#include <stdio.h>
#include "config.h"
```

Include dependency graph for config.c:




### Functions

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

  *Prints the configuration for the iapws library.*

### 9.1.1 Detailed Description

Provides the configuration of the iapws library.

## 9.2 src/iapws.f90 File Reference

Main module for IAPWS.

### Modules

- module iapws

  *Main module for IAPWS computations.*

### Functions/Subroutines

- pure real(real64) function, public iapws::iapws_kh (t, gas, solvent)

  *Compute the henry constant for a given temperature and gas in solvent.*
- pure real(real64) function, public iapws::iapws_kd (t, gas, solvent)

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

#### 9.2.1 Detailed Description

Main module for IAPWS.

## 9.3 src/iapws.h File Reference

C header for the IAPWS libary.

### Functions

- double iapws_capi_kh (double T, char ∗gas, char ∗solvent, int size_gas, int size_solvent)

  *Compute the henry constant for a given temperature and gas in solvent.*
- double iapws_capi_kd (double T, char ∗gas, char ∗solvent, int size_gas, int size_solvent)

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

#### 9.3.1 Detailed Description

C header for the IAPWS libary.

#### 9.3.2 Function Documentation

##### 9.3.2.1 iapws_capi_kd()

```
double iapws_capi_kd (
            double T,
            char * gas,
            char * solvent,
            int size_gas,
            int size_solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in °C. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |
| in | *size_gas* | Length of gas string |
| in | *size_solvent* | Length of solvent string |

**Returns**

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

#### 9.3.2.2 iapws_capi_kh()

```
double iapws_capi_kh (
            double T,
            char * gas,
            char * solvent,
            int size_gas,
            int size_solvent )
```

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

**Parameters**

| | | |
|---|---|---|
| in | *T* | Temperature in °C. |
| in | *gas* | Gas. |
| in | *solvent* | Solvents: H2O or D2O. Default is H2O. |
| in | *size_gas* | Length of gas string |
| in | *size_solvent* | Length of solvent string |

**Returns**

kh Henry constant in mole fraction per GPa. NaN if gas not found.

**Examples**

example_in_c.c.

## 9.4 iapws.h

Go to the documentation of this file.

```
00001
00007 #ifndef IAPWS_H
00008 #define IAPWS_H
00009
00019 extern double iapws_capi_kh(double T, char *gas, char *solvent, int size_gas, int size_solvent);
00020
00030 extern double iapws_capi_kd(double T, char *gas, char *solvent, int size_gas, int size_solvent);
00031
00032 #endif
```

## 9.5 src/iapws_capi.f90 File Reference

C API for the IAPWS module.

### Modules

- module iapws_capi

  *C API for the IAPWS module.*

### Functions/Subroutines

- real(c_double) function, public iapws_capi::iapws_capi_kh (t, gas, solvent, size_gas, size_solvent)

  *Compute the henry constant for a given temperature and gas in solvent.*
- real(c_double) function, public iapws_capi::iapws_capi_kd (t, gas, solvent, size_gas, size_solvent)

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

### 9.5.1 Detailed Description

C API for the IAPWS module.

## 9.6 src/iapwsG704.f90 File Reference

Module for IAPWS G7_04.

### Modules

- module iapwsg704

  *Module for IAPWS G7-04.*

### Functions/Subroutines

- pure real(real64) function, public iapwsg704::iapwsg704_kh_water (t, gas)

  *Compute the henry constant for a given temperature and gas in water.*
- pure real(real64) function, public iapwsg704::iapwsg704_kh_heavywater (t, gas)

  *Compute the henry constant for a given temperature and gas in heavywater.*
- pure real(real64) function, public iapwsg704::iapwsg704_kd_water (t, gas)

  *Compute the kd constant for a given temperature and gas in water.*
- pure real(real64) function, public iapwsg704::iapwsg704_kd_heavywater (t, gas)

  *Compute the kd constant for a given temperature and gas in heavywater.*

### Variables

- real(real64), dimension(6, 2), parameter **iapwsg704::iapwsg704_aibi_water** = reshape([-7.85951783d0, 1.84408259d0, -11.78664970d0, 22.68074110d0, -15.96187190d0, 1.80122502d0,1.000d0, 1.500d0, 3.↩ 000d0, 3.500d0, 4.000d0, 7.500d0], [6,2])

  *ai and bi coefficients for water*

### 9.6.1 Detailed Description

Module for IAPWS G7_04.

# Chapter 10

# Example Documentation

## 10.1 example_in_f.f90

```
00001 program example_in_f
00002     use iso_fortran_env
00003     use iapws
00004     implicit none
00005     real(real64) :: kh, Scm3, Sppm
00006     integer(int32) :: status
00007     character(len=5) :: gas = "O2"
00008     character(len=5) :: solvent = "H2O"
00009     real(real64) :: T = 25.0d0
00010
00011     kh = iapws_kh(t, gas, solvent)
00012     print "(A10, X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F10.4)", "Gas=", gas, "T=", t, "C", "kh=", kh
00013
00014 end program
```

## 10.2 example_in_c.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;

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

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

    return 0;
}
```

# Bibliography


[1] Allan H. Harvey and Eric W. Lemmon. Correlation for the Vapor Pressure of Heavy Water From the Triple Point to the Critical Point. *Journal of Physical and Chemical Reference Data*, 31(1):173–181, March 2002. 3

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[3] IAPWS. Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. Technical Report R7-97, Lucerne, Switzerland, 2007. 3

[4] Wolfgang Wagner and A. Pruss. International Equations for the Saturation Properties of Ordinary Water Substance. Revised According to the International Temperature Scale of 1990. Addendum to J. Phys. Chem. Ref. Data 16, 893 (1987). *Journal of Physical and Chemical Reference Data*, 22(3):783–787, May 1993. 3

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