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

See the file `LICENSE` for information on the history of this software, terms & conditions for usage, and a DISCLAIMER OF ALL WARRANTIES.

Chapter 2

iapws 0.1.0 Release Note

2.1 Changes

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

2.2 Download

```
iapws releases
```

2.3 Contributors

Milan Skocic

2.4 Commits

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

Chapter 3

IAPWS G7-04

The computation is based on the parameters provided by the IAPWS 2004 [3].

3.1 Henry Contant: kh

$$k_H = \lim_{x_2 \to 0} f_2 / x_2$$

- 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:

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

- $\tau = 1 - T_R$
- $T_R = T/T_{c1}$
- T_{c1}: critical temperature of the solvent as recommended by IAPWS [4] (647.096 for H2O and 643.847 K for D2O)
- 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 H2O [5] and from the correlation of Harvey and Lemmon for D2O [2].

Both equations have the form:

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

- n is 6 for H2O and 5 for D2O
- p_{c1} is the critical pressure of the solvent recommended by IAPWS [4] (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.

3.2 Vapor-Liquid Distribution Constant: kd

$$k_D = \lim_{x_2 \to 0} y_2/x_2$$

- 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:

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

- q : -0.023767 for H2O and -0.024552 for D2O.
- $f(\tau)$ [5] for H2O and [1] for D2O.

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

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

- n is 6 for H2O and 4 for D2O

3.3 Molar fractions

$$x_2 = \frac{1}{k_H}$$
$$y_2 = \frac{k_D}{k_H}$$

Chapter 4

Installation

4.1 Create build directory

- mkdir build
- cd build

4.2 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`

4.3 Build either with cmake

```
cmake --build .
```

4.4 Run tests

```
ctest
```

4.5 Install

```
cmake --install .
```

Chapter 5

license

```
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Chapter 6

requirements

gcc>=10.0

gfortran>=10.0

cmake>=3.10

Chapter 7

Modules Index

7.1 Modules List

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

Chapter 8

File Index

8.1 File List

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

Chapter 9

Module Documentation

9.1 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.

9.1.1 Detailed Description

Main module for IAPWS computations.

9.1.2 Function/Subroutine Documentation

9.1.2.1 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.

9.1.2.2 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.

9.2 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.

9.2.1 Detailed Description

C API for the IAPWS module.

9.2.2 Function/Subroutine Documentation

9.2.2.1 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_size_t), intent(in), value size_gas,
             integer(c_size_t), 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.

9.2.2.2 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_size_t), intent(in), value size_gas,
             integer(c_size_t), 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.

9.3 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

9.3.1 Detailed Description

Module for IAPWS G7-04.

9.3.2 Function/Subroutine Documentation

9.3.2.1 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.

9.3.2.2 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.

9.3.2.3 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.

9.3.2.4 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 10

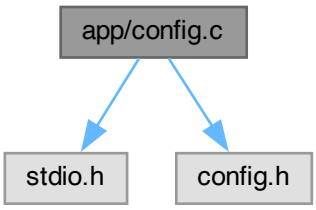
File Documentation

10.1 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.

10.1.1 Detailed Description

Provides the configuration of the iapws library.

10.2 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.

10.2.1 Detailed Description

Main module for IAPWS.

10.3 src/iapws.h File Reference

C header for the IAPWS libary.

Functions

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

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

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

10.3.1 Detailed Description

C header for the IAPWS libary.

10.3.2 Function Documentation

10.3.2.1 iapws_capi_kd()

```
double iapws_capi_kd (
            double T,
            char * gas,
            char * solvent,
            size_t size_gas,
            size_t 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 gas string
in	*size_solvent*	Length of solvent string

Returns

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

Examples

example_in_c.c.

10.3.2.2 iapws_capi_kh()

```
double iapws_capi_kh (
            double T,
            char * gas,
            char * solvent,
            size_t size_gas,
            size_t 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 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.

10.4 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, size_t size_gas, size_t size_solvent);
00020
00030 extern double iapws_capi_kd(double T, char *gas, char *solvent, size_t size_gas, size_t size_solvent);
00031
00032 #endif
```

10.5 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.

10.5.1 Detailed Description

C API for the IAPWS module.

10.6 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

10.6.1 Detailed Description

Module for IAPWS G7_04.

Chapter 11

Example Documentation

11.1 example_in_f.f90

```
00001 program example_in_f
00002     use iso_fortran_env
00003     use iapws
00004     implicit none
00005     real(real64) :: kh, kd
00006     character(len=5) :: gas = "O2"
00007     character(len=5) :: solvent = "H2O"
00008     real(real64) :: T = 25.0d0
00009
00010     kh = iapws_kh(t, gas, solvent)
00011     print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F10.4)", "Gas=", gas, "T=", t, "C", "kh=", kh
00012
00013     kd = iapws_kd(t, gas, solvent)
00014     print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F15.4)", "Gas=", gas, "T=", t, "C", "kh=", kd
00015
00016 end program
```

11.2 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, 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;
}
```

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