IAPWS

0.1

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Chapter 1

Introduction

ipaws is a (Modern) 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, Windows.

The sources are available are available on github. The online documentation is available here. A pdf version of the documentation can be found here.

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

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 IAPWS1997 (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 and from the correlation of Harvey and Lemmon for D2O.

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 IAPWS1997 (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 bars:

$$x_2[\text{mole fraction per bar}] = \frac{1}{k_H}$$

$$S[ppm.bar^{-1}] = \frac{x_2 \cdot M_{gas}}{M_s} \cdot 10^6$$

$$S[cm^3.kg^{-1}.bar^{-1}] = \frac{x_2 \cdot V_m}{M_s}$$

See also

Guideline on the Henry's Constant and Vapor-Liquid Distribution Constant for Gases in H2O and D2O at High Temperatures », IAPWS, Kyoto, Japan, G7-04, 2004

Revised Release on the IAPWS Industrial Formulation 1997 for the thermodynamic Properties of Water and Steam, IAPWS, Lucerne Switzerland R7-97, 2012.

W. Wagner et 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, vol. 22, n°3, p. 783-787, mai 1993. https://doi.org/10.1063/1.555926

A. H. Harvey et E. 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, vol. 31, n°1, p. 173-181, mars 2002 https://doi.org/10.1063/1.1430231

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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```

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If the program does terminal interaction, make it output a short notice like this when it starts in an interactive mode:

```
<program>  Copyright (C) <year>  <name of author>
This program comes with ABSOLUTELY NO WARRANTY; for details type 'show w'.
This is free software, and you are welcome to redistribute it
under certain conditions; type 'show c' for details.
```

The hypothetical commands 'show w' and 'show c' should show the appropriate parts of the General Public License. Of course, your program's commands might be different; for a GUI interface, you would use an "about box".

You should also get your employer (if you work as a programmer) or school, if any, to sign a "copyright disclaimer" for the program, if necessary. For more information on this, and how to apply and follow the GNU GPL, see https://www.gnu.org/licenses/.

The GNU General Public License does not permit incorporating your program into proprietary programs. If your program is a subroutine library, you may consider it more useful to permit linking proprietary applications with the library. If this is what you want to do, use the GNU Lesser General Public License instead of this License. But first, please read https://www.gnu.org/licenses/why-not-lgpl.html.

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_scm3 (T, gas, solvent)

  Compute the solubility for a given temperature and gas in solvent.
- pure real(real64) function, public iapws_sppm (T, gas, solvent)

  Compute the solubility for a given temperature and gas in solvent.
- pure subroutine, public iapws_kh_vs_t (T, gas, solvent, kh)

  Compute the henry constant for different temperatures 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_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 °C.
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.

8.1.2.2 iapws_kh_vs_t()

```
pure subroutine, public iapws::iapws_kh_vs_t (
             real(real64), dimension(:), intent(in) T,
             character(len=*), intent(in) gas,
             character(len=*), intent(in) solvent,
             real(real64), dimension(:), intent(out) kh )
```

Compute the henry constant for different temperatures and gas in solvent.

Parameters

in	*T*	rank-1 array of temperatures in °C.
in	*gas*	Gas.
in	*solvent*	Solvents: H2O or D2O. Default is H2O.
out	*kh*	rank-1 array of Henry constants in mole fraction per GPa. NaN if gas not found.

8.1.2.3 iapws_scm3()

```
pure real(real64) function, public iapws::iapws_scm3 (
             real(real64), intent(in) T,
             character(len=*), intent(in) gas,
             character(len=*), intent(in) solvent )
```

Compute the solubility 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.

Returns

Scm3 Solubility constant in cm3.kg-1.bar-1. NaN if gas not found.

8.1.2.4 iapws_sppm()

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

Compute the solubility 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.

Returns

Sppm Solubility constant in ppm. 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_scm3 (T, gas, solvent, size_gas, size_solvent)
  Compute the solubility constant for a given temperature and gas in solvent.
- real(c_double) function, public iapws_capi_sppm (T, gas, solvent, size_gas, size_solvent)
  Compute the solubility 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_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 °C.
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 constante in mole fraction per GPa. NaN if gas not found.

8.2.2.2 iapws_capi_scm3()

```
real(c_double) function, public iapws_capi::iapws_capi_scm3 (
             real(c_double), intent(in), 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 solubility 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 the string gas.
in	*size_solvent*	Length of the string gas.

Returns

Scm3 Solubility constant in cm3.kg-1.bar-1. NaN if gas not found.

8.2.2.3 iapws_capi_sppm()

```
real(c_double) function, public iapws_capi::iapws_capi_sppm (
             real(c_double), intent(in), 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 solubility 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

Sppm Solubility constant in ppm. NaN if gas not found.

8.3 iapws_g7_04 Module Reference

Module for IAPWS G7-04.

Functions/Subroutines

- pure real(real64) function, public iapws_g7_04_kh_water (T, gas)

  Compute the henry constante for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04_kh_heavywater (T, gas)

  Compute the henry constante for a given temperature and gas in heavywater.
- pure real(real64) function, public iapws_g7_04_scm3_water (T, gas)

  Compute the solubility for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04_scm3_heavywater (T, gas)

  Compute the solubility for a given temperature and gas in heavywater.
- pure real(real64) function, public iapws_g7_04_sppm_water (T, gas)

  Compute the solubility for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04_sppm_heavywater (T, gas)

  Compute the solubility for a given temperature and gas in heavywater.

8.3.1 Detailed Description

Module for IAPWS G7-04.

8.3.2 Function/Subroutine Documentation

8.3.2.1 iapws_g7_04_kh_heavywater()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_kh_heavywater (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

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

Parameters

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

Returns

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

8.3.2.2 iapws_g7_04_kh_water()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_kh_water (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

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

Parameters

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

Returns

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

8.3.2.3 iapws_g7_04_scm3_heavywater()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_scm3_heavywater (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

Compute the solubility for a given temperature and gas in heavywater.

Parameters

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

Returns

Scm3 Solubility constant in cm3.kg-1.bar-1. NaN if gas not found.

8.3.2.4 iapws_g7_04_scm3_water()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_scm3_water (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

Compute the solubility for a given temperature and gas in water.

Parameters

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

Returns

Scm3 Solubility constant in cm3.kg-1.bar-1. NaN if gas not found.

8.3.2.5 iapws_g7_04_sppm_heavywater()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_sppm_heavywater (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

Compute the solubility for a given temperature and gas in heavywater.

Parameters

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

Returns

Sppm Solubility constant in ppm. NaN if gas not found.

8.3.2.6 iapws_g7_04_sppm_water()

```
pure real(real64) function, public iapws_g7_04::iapws_g7_04_sppm_water (
            real(real64), intent(in) T,
            character(len=*), intent(in) gas )
```

Compute the solubility for a given temperature and gas in water.

Parameters

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

Returns

Sppm Solubility constant in ppm. NaN if gas not found.

Chapter 9

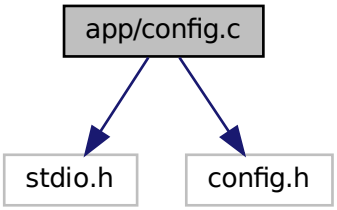
File Documentation

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_scm3 (T, gas, solvent)

  Compute the solubility for a given temperature and gas in solvent.
- pure real(real64) function, public iapws::iapws_sppm (T, gas, solvent)

  Compute the solubility for a given temperature and gas in solvent.
- pure subroutine, public iapws::iapws_kh_vs_t (T, gas, solvent, kh)

  Compute the henry constant for different temperatures 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 constante for a given temperature and gas in solvent.
- double iapws_capi_scm3 (double T, char ∗gas, char ∗solvent, int size_gas, int size_solvent)

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

  Compute the solubility 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_kh()

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

Compute the henry constante 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 constante in mole fraction per GPa. NaN if gas not found.

Examples

example_in_c.c.

9.3.2.2 iapws_capi_scm3()

```
double iapws_capi_scm3 (
            double T,
            char * gas,
            char * solvent,
            int size_gas,
            int size_solvent )
```

Compute the solubility 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

Scm3 Solubility constant in cm3.kg-1.bar-1. Nan if gas not found.

Examples

example_in_c.c.

9.3.2.3 iapws_capi_sppm()

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

Compute the solubility 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

Sppm Solubility constant in ppm. Nan if gas not found.

Examples

example_in_c.c.

9.4 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_scm3 (T, gas, solvent, size_gas, size_solvent)
  Compute the solubility constant for a given temperature and gas in solvent.
- real(c_double) function, public iapws_capi::iapws_capi_sppm (T, gas, solvent, size_gas, size_solvent)
  Compute the solubility constant for a given temperature and gas in solvent.

9.4.1 Detailed Description

C API for the IAPWS module.

9.5 src/iapws_G7_04.f90 File Reference

Module for IAPWS G7_04.

Modules

- module iapws_g7_04

  Module for IAPWS G7-04.

Functions/Subroutines

- pure real(real64) function, public iapws_g7_04::iapws_g7_04_kh_water (T, gas)

  Compute the henry constante for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04::iapws_g7_04_kh_heavywater (T, gas)

  Compute the henry constante for a given temperature and gas in heavywater.
- pure real(real64) function, public iapws_g7_04::iapws_g7_04_scm3_water (T, gas)

  Compute the solubility for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04::iapws_g7_04_scm3_heavywater (T, gas)

  Compute the solubility for a given temperature and gas in heavywater.
- pure real(real64) function, public iapws_g7_04::iapws_g7_04_sppm_water (T, gas)

  Compute the solubility for a given temperature and gas in water.
- pure real(real64) function, public iapws_g7_04::iapws_g7_04_sppm_heavywater (T, gas)

  Compute the solubility for a given temperature and gas in heavywater.

9.5.1 Detailed Description

Module for IAPWS G7_04.

Chapter 10

Example Documentation

10.1 example_in_f.f90

```
1 program example_in_f
2     use iso_fortran_env
3     use iapws
4     implicit none
5     real(real64) :: kh, Scm3, Sppm
6     integer(int32) :: status
7     character(len=5) :: gas = "O2"
8     character(len=5) :: solvent = "H2O"
9     real(real64) :: T = 25.0d0
10
11     kh = iapws_kh(t, gas, solvent)
12     print "(A10, X, A10, X, A2, F10.1, A, 4X, A3, SP, F10.4)", "Gas=", gas, "T=", t, "C", "kh=", kh
13     scm3 = iapws_scm3(t, gas, solvent)
14     print "(A10, X, A10, X, A2, F10.1, A, 4X, A3, SP, F10.4, A20)", "Gas=", gas, "T=", t, "C", "kh=",
       scm3, " cm3.kg-1.bar-1"
15     sppm = iapws_sppm(t, gas, solvent)
16     print "(A10, X, A10, X, A2, F10.1, A, 4X, A3, SP, F10.4, A20)", "Gas=", gas, "T=", t, "C", "kh=",
       sppm, " ppm.bar-1"
17
18 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, Scm3, Sppm;

    if(argc > 1 ){
        printf("%s\n", argv[1]);
    }
    kh = iapws_capi_kh(T, gas, solvent, strlen(gas), strlen(solvent));
    Scm3 = iapws_capi_scm3(T, gas, solvent, strlen(gas), strlen(solvent));
    Sppm = iapws_capi_sppm(T, gas, solvent, strlen(gas), strlen(solvent));
    printf("Gas=%s\tT=%f°C\tkh=%+10.4f\n", gas, T, kh);
    printf("Gas=%s\tT=%f°C\tS=%+10.4f cm3.kg-1.bar-1\n", gas, T, Scm3);
    printf("Gas=%s\tT=%f°C\tS=%+10.4f ppm.bar-1\n", gas, T, Sppm);

    return 0;
}
```

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