iapws Documentation

Release 0.2.0

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CONTENTS:

CHAPTER

ONE

GETTING STARTED

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

1.1 iapw

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 formulas are taken from http://iapws.org.

1.1.1 How to install

A Makefile is provided which uses fpm for building the library with additional options:

- compile the source generator and generate the sources
- copy needed sources into the python wrapper folder
- build a shared library
- install the C headers
- uninstall the library and headers

On windows, msys2 needs to be installed and use the mingw64 or mingw32 terminals.

On Darwin, the gcc toolchain needs to be installed.

Build: the configuration file will set all the environmental variables necessary for the compilation

```
source configuration
make
```

Run tests

```
fpm test
```

Install

```
make install
```

Uninstall

```
make uninstall
```

If building the python wrapper is needed:

```
cd pywrapper
python setup.py bdist_wheel
```

1.1.2 Dependencies

```
gcc>=9.0
gfortran>=9.0
fpm>=0.7
```

1.1.3 License

GNU General Public License v3 (GPLv3)

1.2 pyiapws

Python wrapper around the Fortran iapws library. The Fortran library does not need to be installed, the python wrapper embeds all needed dependencies. On linux, you might have to install *libgfortran* if it is not distributed with your linux distribution.

1.2.1 How to install

```
pip install pyiapws
```

1.2.2 Dependencies

```

```

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_g704
    implicit none
    integer(int32) :: i, ngas
    real(real64) :: T(1), kh(1), kd(1)
    character(len=2) :: gas = "O2"
    integer(int32) :: heavywater = 0
    type(iapws_g704_gas_t), pointer :: gases_list(:)
    character(len=:), pointer :: gases_str
```

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```
    ! Compute kh and kd in H2O
    T(1) = 25.0d0
    call iapws_g704_kh(T, gas, heavywater, kh)
    print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F10.4)", "Gas=", gas, "T=", T,
↪ "C", "kh=", kh

    call iapws_g704_kd(T, gas, heavywater, kd)
    print "(A10, 1X, A10, 1X, A2, F10.1, A, 4X, A3, SP, F15.4)", "Gas=", gas, "T=", T,
↪ "C", "kh=", kd

    ! Get and print available gases
    heavywater = 0
    ngas = iapws_g704_ngases(heavywater)
    gases_list => null()
    gases_list => iapws_g704_gases(heavywater)
    gases_str => iapws_g704_gases2(heavywater)
    print *, "Gases in H2O: ", ngas
    print *, gases_str
    do i=1, ngas
        print *, gases_list(i)%gas
    enddo

    heavywater = 1
    ngas = iapws_g704_ngases(heavywater)
    gases_list => null()
    gases_list => iapws_g704_gases(heavywater)
    gases_str => iapws_g704_gases2(heavywater)
    print *, "Gases in D2O: ", ngas
    print *, gases_str
    do i=1, ngas
        print *, gases_list(i)%gas
    enddo

end program
```

1.3.2 Example in C

```
#include <string.h>
#include <stdio.h>
#include "iapws_g704.h"

int main(void){

    double T = 25.0; /* in C*/
    char *gas = "O2";
    double kh, kd;
    char **gases_list;
    char *gases_str;
    int ngas;
    int i;
    int heavywater = 0;

    /* Compute kh and kd in H2O*/
```

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```
    iapws_g704_capi_kh(&T, gas, heavywater, &kh, strlen(gas), 1);
    printf("Gas=%s\tT=%fC\tkh=%+10.4f\n", gas, T, kh);

    iapws_g704_capi_kd(&T, gas, heavywater, &kd, strlen(gas), 1);
    printf("Gas=%s\tT=%fC\tkd=%+15.4f\n", gas, T, kd);

    /* Get and print the available gases */
    ngas = iapws_g704_capi_ngases(heavywater);
    gases_list = iapws_g704_capi_gases(heavywater);
    gases_str = iapws_g704_capi_gases2(heavywater);
    printf("Gases in H2O: %d\n", ngas);
    printf("%s\n", gases_str);
    for(i=0; i<ngas; i++){
        printf("%s\n", gases_list[i]);
    }

    heavywater = 1;
    ngas = iapws_g704_capi_ngases(heavywater);
    gases_list = iapws_g704_capi_gases(heavywater);
    gases_str = iapws_g704_capi_gases2(heavywater);
    printf("Gases in D2O: %d\n", ngas);
    printf("%s\n", gases_str);
    for(i=0; i<ngas; i++){
        printf("%s\n", gases_list[i]);
    }

    return 0;
}
```

1.3.3 Example in Python

```
r"""Example in python"""
import array
import pyiapws

gas  = "O2"
T = array.array("d", (25.0,))

# Compute kh and kd in H2O
heavywater = False
m = pyiapws.g704.kh(T, "O2", heavywater)
k = array.array("d", m)
print(f"Gas={gas}\tT={T[0]}C\tkh={k[0]:+10.4f}\n")

m = pyiapws.g704.kd(T, "O2", heavywater)
k = array.array("d", m)
print(f"Gas={gas}\tT={T[0]}C\tkh={k[0]:+10.4f}\n")

# Get and print the available gases
heavywater = False
gases_list = pyiapws.g704.gases(heavywater)
gases_str = pyiapws.g704.gases2(heavywater)
ngas = pyiapws.g704.ngases(heavywater)
print(f"Gases in H2O: {ngas:}")
```

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```
print(gases_str)
for gas in gases_list:
    print(gas)

heavywater = True
gases_list = pyiapws.g704.gases(heavywater)
gases_str = pyiapws.g704.gases2(heavywater)
ngas = pyiapws.g704.ngases(heavywater)
print(f"Gases in D2O: {ngas:}")
print(gases_str)
for gas in gases_list:
    print(gas)
```

CHAPTER

TWO

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: kh

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

$$k_H = \lim_{x_2 \to 0} f_2/x_2 \tag{2.1.1}$$

- 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:

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

- $\tau = 1 - T_R$
- $T_R = T/T_{c1}$
- 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:

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

- 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: kd

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

$$k_D = \lim_{x_2 \to 0} y_2/x_2 \tag{2.1.4}$$

- 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:

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

- 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:

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

- n is 6 for H_2O and 4 for D_2O

2.1.3 Molar fractions

The molar fractions x_2 and y_2 can be expressed from the equations Eq.2.1.1 and Eq.2.1.4 as shown in Eq.2.1.7.

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

By fixing f_2 at 1.0 it comes that the molar fractions x_2 and y_2 are then expressed per unit of pressure as shown in equation Eq.2.1.8 .

$$\begin{aligned} x_2 &= \frac{1}{k_H} \\ y_2 &= \frac{k_D}{k_H} \end{aligned} \tag{2.1.8}$$

The molar fractions can be converted to solubilties in ppm or cm3/kg as shown in equation Eq.2.1.9 by considering dilute solutions. X is the considered gas and the solvent is either H_2O or D_2O.

$$\begin{aligned} S_X[mg.kg^{-1}.bar^{-1}] &= x_2[bar^{-1}] \cdot \frac{M_X[g.mol^{-1}]}{M_{solvent}[g.mol^{-1}]} \cdot 10^6 \\ S_X[cm3.kg^{-1}.bar^{-1}] &= \frac{S_X[mg.kg^{-1}.bar^{-1}]}{M_X[g.mol^{-1}]} \cdot V_m[mol.L^{-1}] \end{aligned} \tag{2.1.9}$$

Available gases

kh and kd can be computed for the following gases:

- in water: He, Ne, Ar, Kr, Xe, H2, N2, O2, CO, CO2, H2S, CH4, C2H6, SF6
- in heavywater: He, Ne, Ar, Kr, Xe, D2, CH4

Plots

The evolution of kh in H_2O and D_2O, between 0°C and 360°C, are shown in figures Fig. 2.1.1 and Fig. 2.1.2.

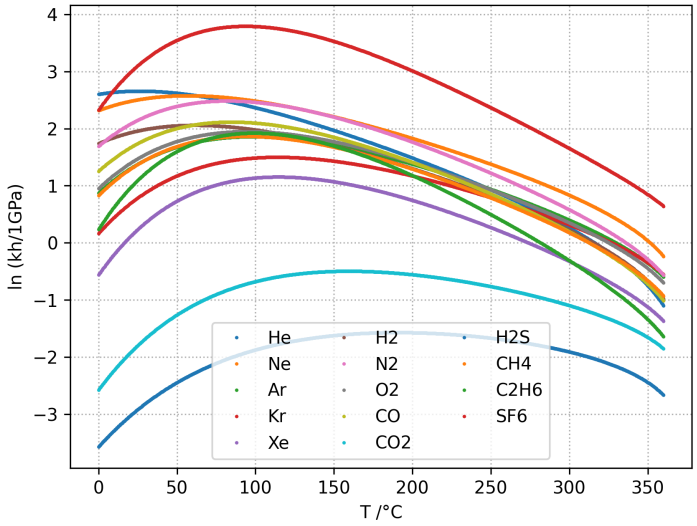

Fig. 2.1.1: kh in H2O

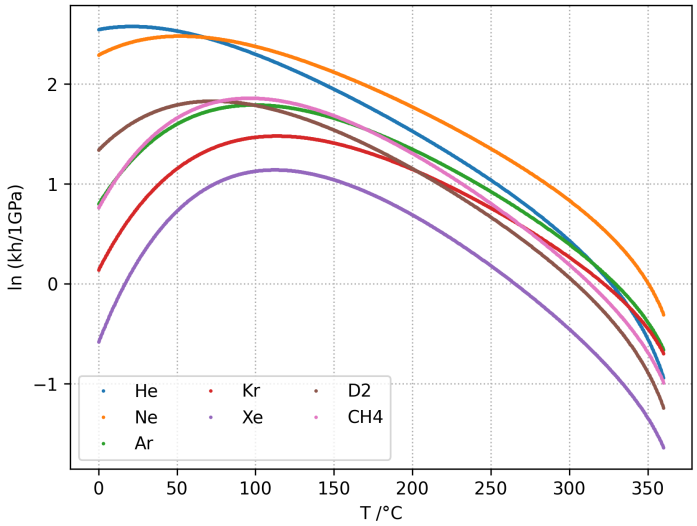

Fig. 2.1.2: kh in D2O

The evolution of kd in H_2O and D_2O, between 0°C and 360°C, are shown in figures Fig. 2.1.3 and Fig. 2.1.4.

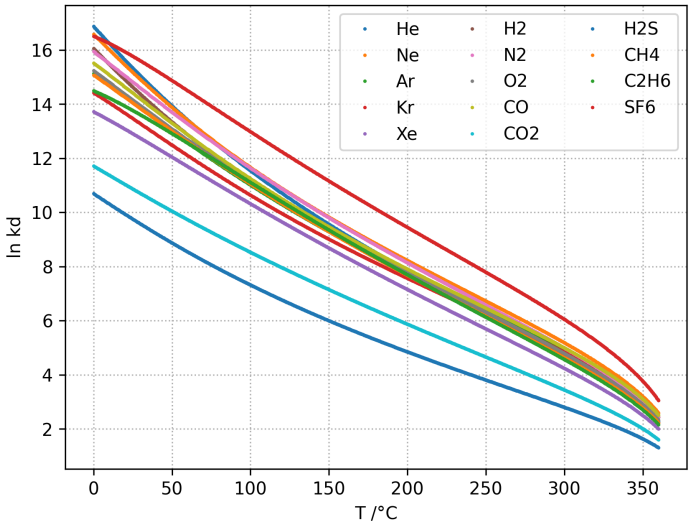

Fig. 2.1.3: kh in H2O

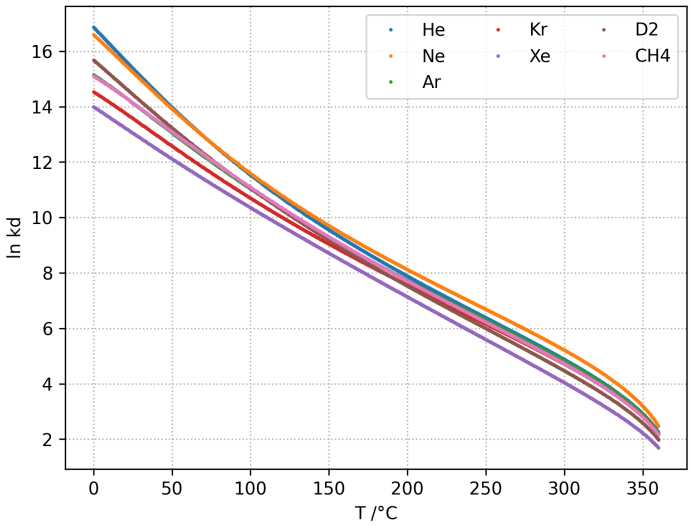

Fig. 2.1.4: kd in D2O

CHAPTER

THREE

RELEASE NOTES

3.1 iapws 0.2.0 Release Note

3.1.1 Summary

- New structure with modules corresponding to the IAPWS papers.
- Compatible with fpm.
- fpm module naming convention.
- **API break for iapws_g704_kh and iapws_g704_kd functions:**
  - only 1d-arrays as inputs in Fortran and C API.
  - only objects with buffer protocol as inputs in python wrapper.
  - python wrappers return memoryviews.
- **New functions:**
  - providing the number of gases in H2O and D2O.
  - providing the available of gases in H2O and D2O as list of strings.
  - providing the available of gases in H2O and D2O as a unique string.
- Cleanup old app code not needed anymore.
- Fix memory allocation in pywrapper.
- Completed tests.
- **Documentation improvements:**
  - Add conversion equations from molar fractions to solubilities.
  - Add plots for visualizing kh and kd.

3.1.2 Download

iapws

pyiapws

3.1.3 Contributors

Milan Skocic

3.1.4 Commits

Full Changelog: https://github.com/MilanSkocic/pyiapws/compare/0.1.1...0.2.0

3.2 iapws 0.1.1 Release Note

3.2.1 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

3.2.2 Download

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3.2.3 Contributors

Milan Skocic

3.2.4 Commits

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

3.3 iapws 0.1.0 Release Note

3.3.1 Changes

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

3.3.2 Download

iapws

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3.3.3 Contributors

Milan Skocic

3.3.4 Commits

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

CHAPTER

FOUR

API

4.1 iapws

4.1.1 Fortran

- *iapws.f90*: Main module for the whole library.

```
module iapws_g704
    !! Module for IAPWS G7-04
    use iso_fortran_env
    use ieee_arithmetic
    implicit none
    private

integer(int32), parameter :: lengas = 5
integer(int32), parameter :: ngas_H2O = 14
integer(int32), parameter :: ngas_D2O = 7

type :: iapws_g704_gas_t
    !! Derived type containing a allocatable string for representing a gas.
    character(len=:), allocatable :: gas !! Gas
end type
type(iapws_g704_gas_t), allocatable, target :: f_gases(:)
character(len=:), allocatable, target :: f_gases_str

!> Absolute temperature in KELVIN
real(real64), parameter ::  T_KELVIN = 273.15d0

!! Parameters from IAPWS G7-04
!> critical temperature of water in K
real(real64), parameter ::  Tc1_H2O = 647.096d0
!> critical pressure of the water in K
real(real64), parameter ::  pc1_H2O = 22.064d0
!> critical temperature of heavy water MPa
real(real64), parameter ::  Tc1_D2O = 643.847d0
!> critical pressure of heavywater MPa
real(real64), parameter ::  pc1_D2O = 21.671d0

!> solvent coefficient for kd in water
real(real64), parameter :: q_H2O = -0.023767d0
!> solvent coefficient for kd in heavywater
real(real64), parameter :: q_D2O = -0.024552d0

!! ABC coefficients for gases in water.
```

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```
type :: abc_t
    character(len=lengas) :: gas
    real(real64) :: A
    real(real64) :: B
    real(real64) :: C
end type

type :: efgh_t
    character(len=lengas) :: gas
    real(real64) :: E
    real(real64) :: F
    real(real64) :: G
    real(real64) :: H
end type

!> ai and bi coefficients for water
real(real64), dimension(6, 2), parameter :: aibi_H2O = 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 heavywater
real(real64), dimension(5, 2), parameter :: aibi_D2O = reshape([&
-7.8966570d0, 24.7330800d0, -27.8112800d0,  9.3559130d0, -9.2200830d0, &
1.00d0, 1.89d0, 2.00d0, 3.00d0, 3.60d0], [5, 2])

!> ABC constants water.
type(abc_t), dimension(ngas_H2O), parameter :: abc_H2O = &
    [abc_t("He", -3.52839d0, 7.12983d0, 4.47770d0),&
     abc_t("Ne", -3.18301d0, 5.31448d0, 5.43774d0),&
     abc_t("Ar", -8.40954d0, 4.29587d0, 10.52779d0),&
     abc_t("Kr", -8.97358d0, 3.61508d0, 11.29963d0),&
     abc_t("Xe", -14.21635d0, 4.00041d0, 15.60999d0),&
     abc_t("H2", -4.73284d0, 6.08954d0, 6.06066d0),&
     abc_t("N2", -9.67578d0, 4.72162d0, 11.70585d0),&
     abc_t("O2", -9.44833d0, 4.43822d0, 11.42005d0),&
     abc_t("CO", -10.52862d0, 5.13259d0, 12.01421d0),&
     abc_t("CO2", -8.55445d0, 4.01195d0, 9.52345d0),&
     abc_t("H2S", -4.51499d0, 5.23538d0, 4.42126d0),&
     abc_t("CH4", -10.44708d0, 4.66491d0, 12.12986d0),&
     abc_t("C2H6", -19.67563d0, 4.51222d0, 20.62567d0),&
     abc_t("SF6", -16.56118d0, 2.15289d0, 20.35440d0)]

!> ABC constants for heavywater
type(abc_t), dimension(ngas_D2O), parameter :: abc_D2O = &
    [abc_t("He", -0.72643d0, 7.02134d0, 2.04433d0),&
     abc_t("Ne", -0.91999d0, 5.65327d0, 3.17247d0),&
     abc_t("Ar", -7.17725d0, 4.48177d0, 9.31509d0),&
     abc_t("Kr", -8.47059d0, 3.91580d0, 10.69433d0),&
     abc_t("Xe", -14.46485d0, 4.42330d0, 15.60919d0),&
     abc_t("D2", -5.33843d0, 6.15723d0, 6.53046d0),&
     abc_t("CH4", -10.01915d0, 4.73368d0, 11.75711d0)]

!> ci and di coefficients for water
real(real64), dimension(6, 2), parameter :: cidi_H2O = reshape([&
1.99274064d0, 1.09965342d0, -0.510839303d0, -1.75493479d0, -45.5170352d0, -6.
```

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```
↪7469445d5,&
1.0d0/3.0d0, 2.0d0/3.0d0, 5.0d0/3.0d0, 16.0d0/3.0d0, 43.0d0/3.0d0, 110.0d0/3.0d0], [6,
↪2])

!> ci and di coefficients for heavywater
real(real64), dimension(4, 2), parameter :: cidi_D2O = reshape([&
2.7072d0, 0.58662d0, -1.3069d0, -45.663d0, &
0.374d0, 1.45d0, 2.6d0, 12.3d0], [4,2])

!> EFGH constants for water
type(efgh_t), dimension(ngas_H2O), parameter :: efgh_H2O = &
[efgh_t("He", 2267.4082d0, -2.9616d0, -3.2604d0, 7.8819d0),&
 efgh_t("Ne", 2507.3022d0, -38.6955d0, 110.3992d0, -71.9096d0),&
 efgh_t("Ar", 2310.5463d0, -46.7034d0, 160.4066d0, -118.3043d0),&
 efgh_t("Kr", 2276.9722d0, -61.1494d0, 214.0117d0, -159.0407d0),&
 efgh_t("Xe", 2022.8375d0, 16.7913d0, -61.2401d0, 41.9236d0),&
 efgh_t("H2", 2286.4159d0, 11.3397d0, -70.7279d0, 63.0631d0),&
 efgh_t("N2", 2388.8777d0, -14.9593d0, 42.0179d0, -29.4396d0),&
 efgh_t("O2", 2305.0674d0, -11.3240d0, 25.3224d0, -15.6449d0),&
 efgh_t("CO", 2346.2291d0, -57.6317d0, 204.5324d0, -152.6377d0),&
 efgh_t("CO2", 1672.9376d0, 28.1751d0, -112.4619d0, 85.3807d0),&
 efgh_t("H2S", 1319.1205d0, 14.1571d0, -46.8361d0, 33.2266d0),&
 efgh_t("CH4", 2215.6977d0, -0.1089d0, -6.6240d0, 4.6789d0),&
 efgh_t("C2H6", 2143.8121d0, 6.8859d0, -12.6084d0, 0.0d0),&
 efgh_t("SF6", 2871.7265d0, -66.7556d0, 229.7191d0, -172.7400d0)]

 !> EFGH constants for heavywater
type(efgh_t), dimension(ngas_D2O), parameter :: efgh_D2O = &
[efgh_t("He", 2293.2474d0, -54.7707d0, 194.2924d0, -142.1257), &
 efgh_t("Ne", 2439.6677d0, -93.4934d0, 330.7783d0, -243.0100d0),&
 efgh_t("Ar", 2269.2352d0, -53.6321d0, 191.8421d0, -143.7659d0),&
 efgh_t("Kr", 2250.3857d0, -42.0835d0, 140.7656d0, -102.7592d0),&
 efgh_t("Xe", 2038.3656d0, 68.1228d0, -271.3390d0, 207.7984d0),&
 efgh_t("D2", 2141.3214d0, -1.9696d0, 1.6136d0, 0.0d0),&
 efgh_t("CH4", 2216.0181d0, -40.7666d0, 152.5778d0, -117.7430d0)]

public :: iapws_g704_gas_t
public :: iapws_g704_kh, iapws_g704_kd
public :: iapws_g704_ngases
public :: iapws_g704_gases, iapws_g704_gases2

contains

!> @brief Find the index of the gas in the ABC table.
!! @param[in] gas Gas.
!! @param[in] abc ABC table.
pure function findgas_abc(gas, abc)result(value)
    implicit none
    !! arguments
    character(len=*), intent(in) :: gas
    type(abc_t), dimension(:), intent(in) :: abc
    !! returns
    integer(int32) :: value
    !! local variables
    integer(int32) :: i
```

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```
    value = 0

    do i=1, size(abc)
        if(trim(gas) .eq. abc(i)%gas)then
            value = i
            exit
        endif
    end do
end function

!> @brief Find the index of the gas in the ABC table.
!! @param[in] gas Gas.
!! @param[in] efgh ABC table.
pure function findgas_efgh(gas, efgh)result(value)
    implicit none
    !! arguments
    character(len=*), intent(in) :: gas
    type(efgh_t), dimension(:), intent(in) :: efgh
    !! returns
    integer(int32) :: value
    !! local variables
    integer(int32) :: i

    value = 0

    do i=1, size(efgh)
        if(trim(gas) .eq. efgh(i)%gas)then
            value = i
            exit
        endif
    end do
end function

pure elemental function f_p1star_H2O(T)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau = 1 - Tr
    value = exp(1/(Tr) * sum(aibi_H2O(:,1)*tau**(aibi_H2O(:,2)))) * pc1_H2O
end function

pure elemental function f_p1star_D2O(T)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
```

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```
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau = 1 - Tr
    value = exp(1/(Tr) * sum(aibi_D2O(:,1)*tau**(aibi_D2O(:,2)))) * pc1_D2O
end function

pure elemental function f_kh_p1star_H2O(T, abc)result(value)
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau = 1 - Tr
    value = exp(abc%A/Tr + abc%B*(tau**0.355d0)/Tr + abc%C*exp(tau)*Tr**(-0.41d0))
end function

pure elemental function f_kh_p1star_D2O(T, abc)result(value)
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau = 1 - Tr
    value = exp(abc%A/Tr + abc%B*(tau**0.355d0)/Tr + abc%C*exp(tau)*Tr**(-0.41d0))
end function

pure elemental function ft_H2O(tau)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: tau
    !! return
    real(real64) :: value
    value = sum(cidi_H2O(:,1) * tau**(cidi_H2O(:,2)))
end function

pure elemental function ft_D2O(tau)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: tau
    !! return
    real(real64) :: value
    value = sum(cidi_D2O(:,1) * tau**(cidi_D2O(:,2)))
end function

pure elemental function f_kh_H2O(T, abc)result(value)
```

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```
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! returns
    real(real64) :: value
    value = f_kh_p1star_H2O(T, abc) * f_p1star_H2O(T)
end function

pure elemental function f_kh_D2O(T, abc)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! returns
    real(real64) :: value
    value = f_kh_p1star_D2O(T, abc) * f_p1star_D2O(T)
end function

pure elemental function f_kd_H2O(T, efgh) result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(efgh_t), intent(in) :: efgh
    !! returns
    real(real64) :: value
    !! local variables
    real(real64) :: Tr
    real(real64) :: tau
    real(real64) :: p1
    real(real64) :: p2
    real(real64) :: p3
    real(real64) :: p4

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau  = 1-Tr

    p1 = q_H2O*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_H2O(tau)
    p3 = (efgh%F + efgh%G*tau**(2.0d0/3.0d0) + efgh%H*tau)
    p4 = exp(-T/100.0d0)

    value = exp(p1 + p2 + p3 * p4)

end function

pure elemental function f_kd_D2O(T, efgh) result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(efgh_t), intent(in) :: efgh
    !! returns
    real(real64) :: value
    !! local variables
    real(real64) :: Tr
    real(real64) :: tau
```

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```
    real(real64) :: p1
    real(real64) :: p2
    real(real64) :: p3
    real(real64) :: p4

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau  = 1-Tr

    p1 = q_D2O*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_D2O(tau)
    p3 = (efgh%F + efgh%G*tau**(2.0d0/3.0d0) + efgh%H*tau)
    p4 = exp(-T/100.0d0)

    value = exp(p1 + p2 + p3 * p4)

end function

pure subroutine iapws_g704_kh(T, gas, heavywater, k)
    !! Compute the henry constant for a given temperature.
    implicit none

    ! arguments
    real(real64), intent(in) :: T(:)
        !! Temperature in °C.
    character(len=*), intent(in) :: gas
        !! Gas.
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    real(real64), intent(out) :: k(:)
        !! Henry constant. Filled with NaNs if gas not found.

    ! variables
    integer(int32) :: i

    if(heavywater > 0)then
        i = findgas_abc(gas, abc_D2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k =  f_kh_D2O(T, abc_D2O(i))
        endif
    else
        i = findgas_abc(gas, abc_H2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k = f_kh_H2O(T, abc_H2O(i))
        endif
    endif

end subroutine

pure subroutine iapws_g704_kd(T, gas, heavywater, k)
    !! Compute the vapor-liquid constant for a given temperature.
    implicit none
```

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```
    ! arguments
    real(real64), intent(in) :: T(:)
        !! Temperature in °C.
    character(len=*), intent(in) :: gas
        !! Gas.
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    real(real64), intent(out) :: k(:)
        !! Vapor-liquid constant. Filled with NaNs if gas not found.

    ! variables
    integer(int32) :: i

    if(heavywater > 0)then
        i = findgas_efgh(gas, efgh_D2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k =  f_kd_D2O(T, efgh_D2O(i))
        endif
    else
        i = findgas_efgh(gas, efgh_H2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k = f_kd_H2O(T, efgh_H2O(i))
        endif
    endif

end subroutine

pure function iapws_g704_ngases(heavywater)result(n)
    !! Returns the number of gases.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    integer(int32) :: n
        !! Number of gases.

    if(heavywater > 0)then
        n = ngas_D2O
    else
        n = ngas_H2O
    endif
end function

function iapws_g704_gases(heavywater)result(gases)
    !! Returns the list of available gases.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(iapws_g704_gas_t), pointer :: gases(:)
```

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```
        !! Available gases.

    ! variables
    integer(int32) :: i, n

    if(allocated(f_gases))then
        deallocate(f_gases)
    endif

    if(heavywater > 0)then
        allocate(f_gases(ngas_D2O))
        do i=1, ngas_D2O
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_D2O(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_D2O(i)%gas)
        enddo
    else
        allocate(f_gases(ngas_H2O))
        do i=1, ngas_H2O
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_H2O(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_H2O(i)%gas)
        enddo
    endif
    gases => f_gases
end function

function iapws_g704_gases2(heavywater)result(gases)
    !! Returns the available gases as a string.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    character(len=:), pointer :: gases
        !! Available gases

    ! variables
    integer(int32) :: i, j, k, ngas
    type(iapws_g704_gas_t), pointer :: f_gases(:)

    f_gases => iapws_g704_gases(heavywater)
    ngas = size(f_gases)

    k = 0
    do i=1, ngas
        k = k + len(f_gases(i)%gas)
    enddo

    if(allocated(f_gases_str))then
```

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```
        deallocate(f_gases_str)
    endif
    allocate(character(len=k+ngas) :: f_gases_str)

    i = 1
    j = 1
    k = 1
    do i=1, ngas
        do j=1, len(f_gases(i)%gas)
            f_gases_str(k:k) = f_gases(i)%gas(j:j)
            k = k + 1
        enddo
        f_gases_str(k:k) = ","
        k = k + 1
    enddo
    f_gases_str(len(f_gases_str):len(f_gases_str)) = ""
    gases => f_gases_str

end function

end module
```

IAPWS G704: Gas solubilities

- *iapws_g704.f90*: Module for IAPWS G7-04

```
module iapws_g704
    !! Module for IAPWS G7-04
    use iso_fortran_env
    use ieee_arithmetic
    implicit none
    private

integer(int32), parameter :: lengas = 5
integer(int32), parameter :: ngas_H2O = 14
integer(int32), parameter :: ngas_D2O = 7

type :: iapws_g704_gas_t
    !! Derived type containing a allocatable string for representing a gas.
    character(len=:), allocatable :: gas !! Gas
end type
type(iapws_g704_gas_t), allocatable, target :: f_gases(:)
character(len=:), allocatable, target :: f_gases_str

!> Absolute temperature in KELVIN
real(real64), parameter ::  T_KELVIN = 273.15d0

!! Parameters from IAPWS G7-04
!> critical temperature of water in K
real(real64), parameter ::  Tc1_H2O = 647.096d0
!> critical pressure of the water in K
real(real64), parameter ::  pc1_H2O = 22.064d0
!> critical temperature of heavy water MPa
real(real64), parameter ::  Tc1_D2O = 643.847d0
!> critical pressure of heavywater MPa
```

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```
real(real64), parameter ::  pc1_D2O = 21.671d0

!> solvent coefficient for kd in water
real(real64), parameter :: q_H2O = -0.023767d0
!> solvent coefficient for kd in heavywater
real(real64), parameter :: q_D2O = -0.024552d0

!! ABC coefficients for gases in water.
type :: abc_t
    character(len=lengas) :: gas
    real(real64) :: A
    real(real64) :: B
    real(real64) :: C
end type

type :: efgh_t
    character(len=lengas) :: gas
    real(real64) :: E
    real(real64) :: F
    real(real64) :: G
    real(real64) :: H
end type

!> ai and bi coefficients for water
real(real64), dimension(6, 2), parameter :: aibi_H2O = 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 heavywater
real(real64), dimension(5, 2), parameter :: aibi_D2O = reshape([&
-7.8966570d0, 24.7330800d0, -27.8112800d0,  9.3559130d0, -9.2200830d0, &
1.00d0, 1.89d0, 2.00d0, 3.00d0, 3.60d0], [5, 2])

!> ABC constants water.
type(abc_t), dimension(ngas_H2O), parameter :: abc_H2O = &
    [abc_t("He", -3.52839d0, 7.12983d0, 4.47770d0),&
     abc_t("Ne", -3.18301d0, 5.31448d0, 5.43774d0),&
     abc_t("Ar", -8.40954d0, 4.29587d0, 10.52779d0),&
     abc_t("Kr", -8.97358d0, 3.61508d0, 11.29963d0),&
     abc_t("Xe", -14.21635d0, 4.00041d0, 15.60999d0),&
     abc_t("H2", -4.73284d0, 6.08954d0, 6.06066d0),&
     abc_t("N2", -9.67578d0, 4.72162d0, 11.70585d0),&
     abc_t("O2", -9.44833d0, 4.43822d0, 11.42005d0),&
     abc_t("CO", -10.52862d0, 5.13259d0, 12.01421d0),&
     abc_t("CO2", -8.55445d0, 4.01195d0, 9.52345d0),&
     abc_t("H2S", -4.51499d0, 5.23538d0, 4.42126d0),&
     abc_t("CH4", -10.44708d0, 4.66491d0, 12.12986d0),&
     abc_t("C2H6", -19.67563d0, 4.51222d0, 20.62567d0),&
     abc_t("SF6", -16.56118d0, 2.15289d0, 20.35440d0)]

!> ABC constants for heavywater
type(abc_t), dimension(ngas_D2O), parameter :: abc_D2O = &
    [abc_t("He", -0.72643d0, 7.02134d0, 2.04433d0),&
     abc_t("Ne", -0.91999d0, 5.65327d0, 3.17247d0),&
     abc_t("Ar", -7.17725d0, 4.48177d0, 9.31509d0),&
```

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```
     abc_t("Kr", -8.47059d0, 3.91580d0, 10.69433d0),&
     abc_t("Xe", -14.46485d0, 4.42330d0, 15.60919d0),&
     abc_t("D2", -5.33843d0, 6.15723d0, 6.53046d0),&
     abc_t("CH4", -10.01915d0, 4.73368d0, 11.75711d0)]

!> ci and di coefficients for water
real(real64), dimension(6, 2), parameter :: cidi_H2O = reshape([&
1.99274064d0, 1.09965342d0, -0.510839303d0, -1.75493479d0, -45.5170352d0, -6.
↪7469445d5,&
1.0d0/3.0d0, 2.0d0/3.0d0, 5.0d0/3.0d0, 16.0d0/3.0d0, 43.0d0/3.0d0, 110.0d0/3.0d0], [6,
↪2])

!> ci and di coefficients for heavywater
real(real64), dimension(4, 2), parameter :: cidi_D2O = reshape([&
2.7072d0, 0.58662d0, -1.3069d0, -45.663d0, &
0.374d0, 1.45d0, 2.6d0, 12.3d0], [4,2])

!> EFGH constants for water
type(efgh_t), dimension(ngas_H2O), parameter :: efgh_H2O = &
[efgh_t("He", 2267.4082d0, -2.9616d0, -3.2604d0, 7.8819d0),&
 efgh_t("Ne", 2507.3022d0, -38.6955d0, 110.3992d0, -71.9096d0),&
 efgh_t("Ar", 2310.5463d0, -46.7034d0, 160.4066d0, -118.3043d0),&
 efgh_t("Kr", 2276.9722d0, -61.1494d0, 214.0117d0, -159.0407d0),&
 efgh_t("Xe", 2022.8375d0, 16.7913d0, -61.2401d0, 41.9236d0),&
 efgh_t("H2", 2286.4159d0, 11.3397d0, -70.7279d0, 63.0631d0),&
 efgh_t("N2", 2388.8777d0, -14.9593d0, 42.0179d0, -29.4396d0),&
 efgh_t("O2", 2305.0674d0, -11.3240d0, 25.3224d0, -15.6449d0),&
 efgh_t("CO", 2346.2291d0, -57.6317d0, 204.5324d0, -152.6377d0),&
 efgh_t("CO2", 1672.9376d0, 28.1751d0, -112.4619d0, 85.3807d0),&
 efgh_t("H2S", 1319.1205d0, 14.1571d0, -46.8361d0, 33.2266d0),&
 efgh_t("CH4", 2215.6977d0, -0.1089d0, -6.6240d0, 4.6789d0),&
 efgh_t("C2H6", 2143.8121d0, 6.8859d0, -12.6084d0, 0.0d0),&
 efgh_t("SF6", 2871.7265d0, -66.7556d0, 229.7191d0, -172.7400d0)]

 !> EFGH constants for heavywater
type(efgh_t), dimension(ngas_D2O), parameter :: efgh_D2O = &
[efgh_t("He", 2293.2474d0, -54.7707d0, 194.2924d0, -142.1257), &
 efgh_t("Ne", 2439.6677d0, -93.4934d0, 330.7783d0, -243.0100d0),&
 efgh_t("Ar", 2269.2352d0, -53.6321d0, 191.8421d0, -143.7659d0),&
 efgh_t("Kr", 2250.3857d0, -42.0835d0, 140.7656d0, -102.7592d0),&
 efgh_t("Xe", 2038.3656d0, 68.1228d0, -271.3390d0, 207.7984d0),&
 efgh_t("D2", 2141.3214d0, -1.9696d0, 1.6136d0, 0.0d0),&
 efgh_t("CH4", 2216.0181d0, -40.7666d0, 152.5778d0, -117.7430d0)]

public :: iapws_g704_gas_t
public :: iapws_g704_kh, iapws_g704_kd
public :: iapws_g704_ngases
public :: iapws_g704_gases, iapws_g704_gases2

contains

!> @brief Find the index of the gas in the ABC table.
!! @param[in] gas Gas.
!! @param[in] abc ABC table.
pure function findgas_abc(gas, abc)result(value)
    implicit none
```

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```
    !! arguments
    character(len=*), intent(in) :: gas
    type(abc_t), dimension(:), intent(in) :: abc
    !! returns
    integer(int32) :: value
    !! local variables
    integer(int32) :: i

    value = 0

    do i=1, size(abc)
        if(trim(gas) .eq. abc(i)%gas)then
            value = i
            exit
        endif
    end do
end function

!> @brief Find the index of the gas in the ABC table.
!! @param[in] gas Gas.
!! @param[in] efgh ABC table.
pure function findgas_efgh(gas, efgh)result(value)
    implicit none
    !! arguments
    character(len=*), intent(in) :: gas
    type(efgh_t), dimension(:), intent(in) :: efgh
    !! returns
    integer(int32) :: value
    !! local variables
    integer(int32) :: i

    value = 0

    do i=1, size(efgh)
        if(trim(gas) .eq. efgh(i)%gas)then
            value = i
            exit
        endif
    end do
end function

pure elemental function f_p1star_H2O(T)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau = 1 - Tr
    value = exp(1/(Tr) * sum(aibi_H2O(:,1)*tau**(aibi_H2O(:,2)))) * pc1_H2O
end function
```

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```
pure elemental function f_p1star_D2O(T)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau = 1 - Tr
    value = exp(1/(Tr) * sum(aibi_D2O(:,1)*tau**(aibi_D2O(:,2)))) * pc1_D2O
end function

pure elemental function f_kh_p1star_H2O(T, abc)result(value)
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau = 1 - Tr
    value = exp(abc%A/Tr + abc%B*(tau**0.355d0)/Tr + abc%C*exp(tau)*Tr**(-0.41d0))
end function

pure elemental function f_kh_p1star_D2O(T, abc)result(value)
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! return
    real(real64) :: value
    !! variables
    real(real64) :: Tr
    real(real64) :: tau

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau = 1 - Tr
    value = exp(abc%A/Tr + abc%B*(tau**0.355d0)/Tr + abc%C*exp(tau)*Tr**(-0.41d0))
end function

pure elemental function ft_H2O(tau)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: tau
    !! return
    real(real64) :: value
    value = sum(cidi_H2O(:,1) * tau**(cidi_H2O(:,2)))
end function

pure elemental function ft_D2O(tau)result(value)
    implicit none
```

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```
    !! arguments
    real(real64), intent(in) :: tau
    !! return
    real(real64) :: value
    value = sum(cidi_D2O(:,1) * tau**(cidi_D2O(:,2)))
end function

pure elemental function f_kh_H2O(T, abc)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! returns
    real(real64) :: value
    value = f_kh_p1star_H2O(T, abc) * f_p1star_H2O(T)
end function

pure elemental function f_kh_D2O(T, abc)result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(abc_t), intent(in) :: abc
    !! returns
    real(real64) :: value
    value = f_kh_p1star_D2O(T, abc) * f_p1star_D2O(T)
end function

pure elemental function f_kd_H2O(T, efgh) result(value)
    implicit none
    !! arguments
    real(real64), intent(in) :: T
    type(efgh_t), intent(in) :: efgh
    !! returns
    real(real64) :: value
    !! local variables
    real(real64) :: Tr
    real(real64) :: tau
    real(real64) :: p1
    real(real64) :: p2
    real(real64) :: p3
    real(real64) :: p4

    Tr = (T+T_KELVIN)/Tc1_H2O
    tau  = 1-Tr

    p1 = q_H2O*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_H2O(tau)
    p3 = (efgh%F + efgh%G*tau**(2.0d0/3.0d0) + efgh%H*tau)
    p4 = exp(-T/100.0d0)

    value = exp(p1 + p2 + p3 * p4)

end function

pure elemental function f_kd_D2O(T, efgh) result(value)
    implicit none
```

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```
    !! arguments
    real(real64), intent(in) :: T
    type(efgh_t), intent(in) :: efgh
    !! returns
    real(real64) :: value
    !! local variables
    real(real64) :: Tr
    real(real64) :: tau
    real(real64) :: p1
    real(real64) :: p2
    real(real64) :: p3
    real(real64) :: p4

    Tr = (T+T_KELVIN)/Tc1_D2O
    tau  = 1-Tr

    p1 = q_D2O*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_D2O(tau)
    p3 = (efgh%F + efgh%G*tau**(2.0d0/3.0d0) + efgh%H*tau)
    p4 = exp(-T/100.0d0)

    value = exp(p1 + p2 + p3 * p4)

end function

pure subroutine iapws_g704_kh(T, gas, heavywater, k)
    !! Compute the henry constant for a given temperature.
    implicit none

    ! arguments
    real(real64), intent(in) :: T(:)
        !! Temperature in °C.
    character(len=*), intent(in) :: gas
        !! Gas.
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    real(real64), intent(out) :: k(:)
        !! Henry constant. Filled with NaNs if gas not found.

    ! variables
    integer(int32) :: i

    if(heavywater > 0)then
        i = findgas_abc(gas, abc_D2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k =  f_kh_D2O(T, abc_D2O(i))
        endif
    else
        i = findgas_abc(gas, abc_H2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k = f_kh_H2O(T, abc_H2O(i))
        endif
```

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```
    endif

end subroutine

pure subroutine iapws_g704_kd(T, gas, heavywater, k)
    !! Compute the vapor-liquid constant for a given temperature.
    implicit none

    ! arguments
    real(real64), intent(in) :: T(:)
        !! Temperature in °C.
    character(len=*), intent(in) :: gas
        !! Gas.
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    real(real64), intent(out) :: k(:)
        !! Vapor-liquid constant. Filled with NaNs if gas not found.

    ! variables
    integer(int32) :: i

    if(heavywater > 0)then
        i = findgas_efgh(gas, efgh_D2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k =  f_kd_D2O(T, efgh_D2O(i))
        endif
    else
        i = findgas_efgh(gas, efgh_H2O)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k = f_kd_H2O(T, efgh_H2O(i))
        endif
    endif

end subroutine

pure function iapws_g704_ngases(heavywater)result(n)
    !! Returns the number of gases.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    integer(int32) :: n
        !! Number of gases.

    if(heavywater > 0)then
        n = ngas_D2O
    else
        n = ngas_H2O
    endif
end function
```

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```
function iapws_g704_gases(heavywater)result(gases)
    !! Returns the list of available gases.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(iapws_g704_gas_t), pointer :: gases(:)
        !! Available gases.

    ! variables
    integer(int32) :: i, n

    if(allocated(f_gases))then
        deallocate(f_gases)
    endif

    if(heavywater > 0)then
        allocate(f_gases(ngas_D2O))
        do i=1, ngas_D2O
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_D2O(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_D2O(i)%gas)
        enddo
    else
        allocate(f_gases(ngas_H2O))
        do i=1, ngas_H2O
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_H2O(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_H2O(i)%gas)
        enddo
    endif
    gases => f_gases
end function

function iapws_g704_gases2(heavywater)result(gases)
    !! Returns the available gases as a string.
    implicit none

    ! arguments
    integer(int32), intent(in) :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    character(len=:), pointer :: gases
        !! Available gases

    ! variables
    integer(int32) :: i, j, k, ngas
    type(iapws_g704_gas_t), pointer :: f_gases(:)

    f_gases => iapws_g704_gases(heavywater)
```

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```
    ngas = size(f_gases)

    k = 0
    do i=1, ngas
        k = k + len(f_gases(i)%gas)
    enddo

    if(allocated(f_gases_str))then
        deallocate(f_gases_str)
    endif
    allocate(character(len=k+ngas) :: f_gases_str)

    i = 1
    j = 1
    k = 1
    do i=1, ngas
        do j=1, len(f_gases(i)%gas)
            f_gases_str(k:k) = f_gases(i)%gas(j:j)
            k = k + 1
        enddo
        f_gases_str(k:k) = ","
        k = k + 1
    enddo
    f_gases_str(len(f_gases_str):len(f_gases_str)) = ""
    gases => f_gases_str

end function

end module
```

- *iapws_g704.f90*: C API for the IAPWS module.

```
module iapws_g704_capi
    !! C API for the IAPWS module.
    use iso_fortran_env
    use iso_c_binding
    use iapws_g704
    implicit none
    private

    type, bind(C) :: c_char_p
        type(c_ptr) :: p
    end type
    type :: capi_gas_t
        character(kind=c_char, len=1), allocatable :: gas(:)
    end type
    type(capi_gas_t), allocatable, target :: c_gases(:)
    type(c_char_p), allocatable, target :: char_pp(:)
    character(len=:), allocatable, target :: c_gases_str

    public :: iapws_g704_capi_kh, iapws_g704_capi_kd
    public :: iapws_g704_capi_ngases
    public :: iapws_g704_capi_gases

contains
```

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```
subroutine iapws_g704_capi_kh(T, gas, heavywater, k, size_gas, size_T)bind(C)
    !! Compute the henry constant for a given temperature.
    implicit none

    ! arguments
    type(c_ptr), value :: T
        !! Temperature in °C.
    type(c_ptr), intent(in), value :: gas
        !! Gas.
    integer(c_int), intent(in), value :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(c_ptr), intent(in), value :: k
        !! Henry constant. Filled with NaNs if gas not found.
    integer(c_int), intent(in), value :: size_gas
        !! Size of the gas string.
    integer(c_size_t), intent(in), value :: size_T
        !! Size of T and k.

    ! variables
    character, pointer, dimension(:) :: c2f_gas
    real(real64), pointer :: f_T(:)
    character(len=size_gas) :: f_gas
    real(real64), pointer :: f_k(:)
    integer(int32) :: i

    call c_f_pointer(gas, c2f_gas, shape=[size_gas])
    call c_f_pointer(T, f_T, shape=[size_T])
    call c_f_pointer(k, f_k, shape=[size_T])

    do i=1, size_gas
        f_gas(i:i) = c2f_gas(i)
    enddo
    call iapws_g704_kh(f_T, f_gas, heavywater, f_k)
end subroutine

subroutine iapws_g704_capi_kd(T, gas, heavywater, k, size_gas, size_T)bind(C)
    !! Compute the vapor-liquid constant for a given temperature.
    implicit none

    ! arguments
    type(c_ptr), value :: T
        !! Temperature in °C.
    type(c_ptr), intent(in), value :: gas
        !! Gas.
    integer(c_int), intent(in), value :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(c_ptr), intent(in), value :: k
        !! Vapor-liquid constant. Filled with NaNs if gas not found.
    integer(c_int), intent(in), value :: size_gas
        !! Size of the gas string.
    integer(c_size_t), intent(in), value :: size_T
        !! Size of T and k.

    ! variables
    character, pointer, dimension(:) :: c2f_gas
    real(real64), pointer :: f_T(:)
```

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```
    character(len=size_gas) :: f_gas
    real(real64), pointer :: f_k(:)
    integer(int32) :: i

    call c_f_pointer(gas, c2f_gas, shape=[size_gas])
    call c_f_pointer(T, f_T, shape=[size_T])
    call c_f_pointer(k, f_k, shape=[size_T])

    do i=1, size_gas
        f_gas(i:i) = c2f_gas(i)
    enddo
    call iapws_g704_kd(f_T, f_gas, heavywater, f_k)
end subroutine

pure function iapws_g704_capi_ngases(heavywater)bind(C)result(n)
    !! Returns the number of gases.
    implicit none

    ! arguments
    integer(c_int), intent(in), value :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    integer(c_int) :: n
        !! Number of gases.

    n = iapws_g704_ngases(heavywater)
end function

function iapws_g704_capi_gases(heavywater)bind(C)result(gases)
    !! Returns the list of available gases.
    implicit none

    ! arguments
    integer(c_int), intent(in), value :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(c_ptr) :: gases
        !! Available gases.

    ! variables
    integer(int32) :: i, j, ngas, n

    type(iapws_g704_gas_t), pointer :: f_gases(:) => null()
    f_gases => iapws_g704_gases(heavywater)
    ngas = size(f_gases)

    if(allocated(c_gases))then
        deallocate(c_gases)
    endif
    allocate(c_gases(ngas))

    if(allocated(char_pp))then
        deallocate(char_pp)
    endif
    allocate(char_pp(ngas))

    do i=1, ngas
        if(allocated(c_gases(i)%gas))then
```

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```
            deallocate(c_gases(i)%gas)
        endif
        n = len(f_gases(i)%gas)
        allocate(c_gases(i)%gas(n+1))
        do j=1, n
            c_gases(i)%gas(j) = f_gases(i)%gas(j:j)
        enddo
        c_gases(i)%gas(n+1) = c_null_char
        char_pp(i)%p = c_loc(c_gases(i)%gas)
    enddo
    gases = c_loc(char_pp)
end function

function iapws_g704_capi_gases2(heavywater)bind(C)result(gases)
    !! Returns the available gases as a string.
    implicit none

    ! arguments
    integer(c_int), intent(in), value :: heavywater
        !! Flag if D2O (1) is used or H2O(0).
    type(c_ptr) :: gases
        !! Available gases.

    ! variables
    character(len=:), pointer :: f_gases_str => null()
    f_gases_str => iapws_g704_gases2(heavywater)

    if(allocated(c_gases_str))then
        deallocate(c_gases_str)
    endif
    allocate(character(len=len(f_gases_str)) :: c_gases_str)

    c_gases_str = f_gases_str
    c_gases_str(len(f_gases_str):len(f_gases_str)) = c_null_char

    gases = c_loc(c_gases_str)

end function

end module
```

4.1.2 C

- *iapws.h*: Main C header for the whole library.

```
/**
 * @file iapws.h
 * @brief Main C header for the IAPWS library.
 */
#ifndef IAPWS_H
#define IAPWS_H
#include "iapws_g704.h"
#endif
```

IAPWS G704: Gas solubilities

- *iapws_g704.h*: C header.

```
/**
 * @file iapws_g704.h
 * @brief C header for the module iapws_g704.
 */

#ifndef IAPWS_G704_H
#define IAPWS_G704_H

extern void iapws_g704_capi_kh(double *T, char *gas, int heavywater, double *k, int␣
↪size_gas, size_t size_T);
extern void iapws_g704_capi_kd(double *T, char *gas, int heavywater, double *k, int␣
↪size_gas, size_t size_T);
extern int iapws_g704_capi_ngases(int heavywater);
extern char **iapws_g704_capi_gases(int heavywater);
extern char *iapws_g704_capi_gases2(int heavywater);

#endif
```

4.2 pyipaws

4.2.1 IAPWS G704: Gas solubilities

C extension wrapping the iapws_g704 module of the Fortran iapws library.

pyiapws.g704.**gases**()

gases(heavywater: bool) –> tuple

Get the available gases.

pyiapws.g704.**gases2**()

gases(heavywater: bool) –> str

Get the available gases as a string.

pyiapws.g704.**kd**()

kd(T: array, gas, heavywater: bool) –> mview

Get the vapor-liquid constant for gas in H2O or D2O for T. If gas not found returns NaNs

pyiapws.g704.**kh**()

kh(T: array, gas: str, heavywater :bool) –> mview

Get the Henry constant for gas in H2O or D2O for T. If gas not found returns NaNs

pyiapws.g704.**ngases**()

gases(heavywater: bool) –> int

Get the number of available gases.

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