
iapws Documentation

Release 0.2.0

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Jun 20, 2023

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GETTING STARTED

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

1.1 iapw

Modern Fortran IAPWS

iapws 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.

On windows, `msys2` needs to be installed.

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>=10.0
gfortran>=10.0
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

  ! 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,
```

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```

→ "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*/
    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);
}

```

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```

/* 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}")
print(gases_str)
for gas in gases_list:
    print(gas)

heavywater = True
gases_list = pyiapws.g704.gases(heavywater)
gases_str = pyiapws.g704.gases2(heavywater)

```

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```
ngas = pyiapws.g704.ngases(heavywater)
print(f"Gases in D20: {ngas}")
print(gases_str)
for gas in gases_list:
    print(gas)
```


IAPWS - THEORETICAL BACKGROUND

2.1 IAPWS G7-04

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

2.1.1 Henry Contant: k_H

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

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

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

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

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

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

Both equations have the form:

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

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

2.1.2 Vapor-Liquid Distribution Constant: k_D

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

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

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

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

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

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

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

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

- n is 6 for H_2O and 4 for D_2O

2.1.3 Molar fractions

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.

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

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 .

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

The molar fractions can be converted to solubilities 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 .

$$\begin{aligned} S_X[mg.kg^{-1}.bar^{-1}] &= x_2[bar^{-1}] \cdot \frac{M_X[g.mol^{-1}]}{M_{solvent}[g.mol^{-1}]} \cdot 10^6 \\ S_X[cm^3.kg^{-1}.bar^{-1}] &= \frac{S_X[mg.kg^{-1}.bar^{-1}]}{M_X[g.mol^{-1}]} \cdot V_m[mol.L^{-1}] \end{aligned} \quad (2.1.9)$$

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.

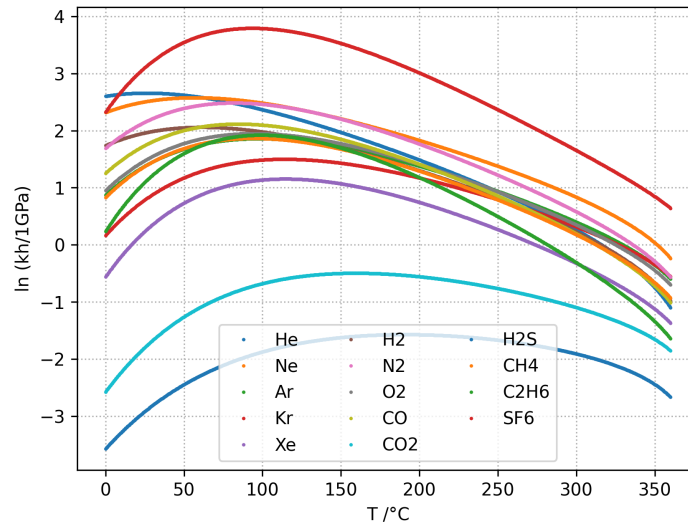


Fig. 2.1.1: kh in H_2O

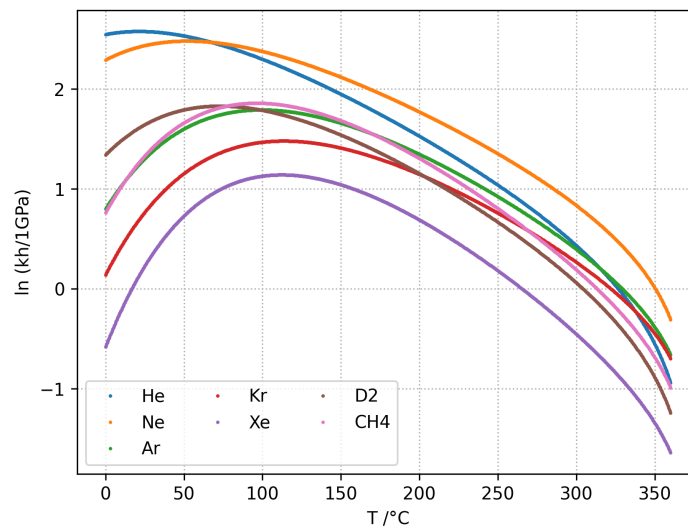
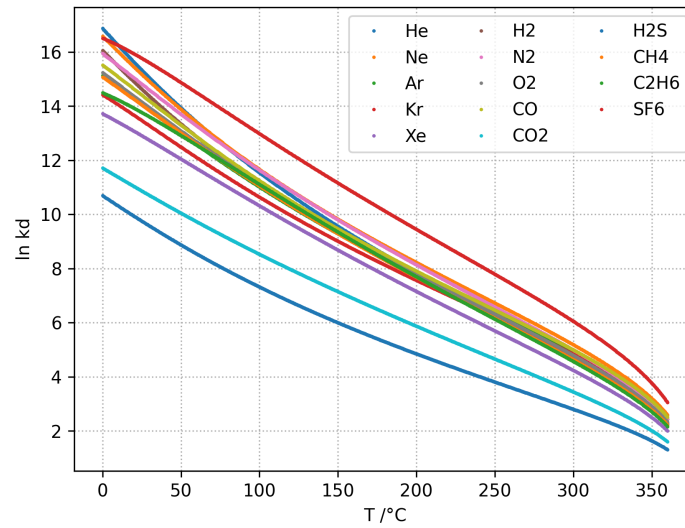
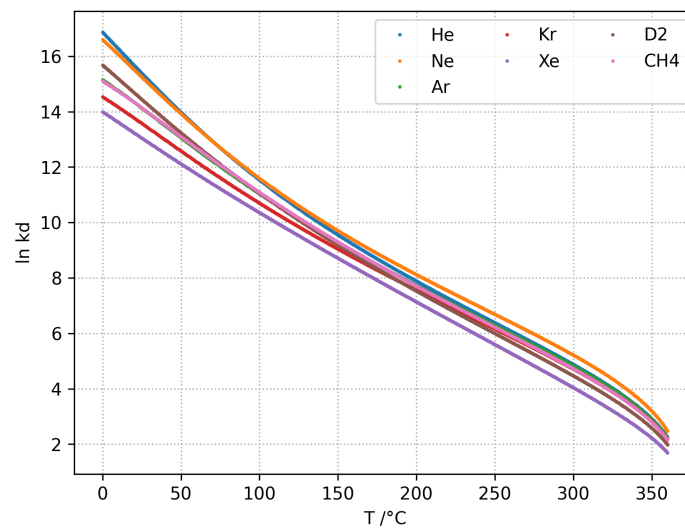


Fig. 2.1.2: kh in D_2O

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: k_h in H_2O Fig. 2.1.4: k_d in D_2O

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/iapws/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

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pyiapws

3.3.3 Contributors

Milan Skocic

3.3.4 Commits

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

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_D20 = 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_D20
tau = 1 - Tr
value = exp(1/(Tr) * sum(aibi_D20(:,1)*tau**(aibi_D20(:,2)))) * pc1_D20
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_D20
  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_D20(:,1) * tau**(cidi_D20(:,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_H20(T, abc) * f_p1star_H20(T)
end function

pure elemental function f_kh_D20(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_D20(T, abc) * f_p1star_D20(T)
end function

pure elemental function f_kd_H20(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_H20*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_H20(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_D20(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_D20
tau = 1-Tr

p1 = q_D20*efgh%F
p2 = efgh%E/(T+T_KELVIN)*ft_D20(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_D20)
    if(i==0)then
      k = ieee_value(1.0d0, ieee_quiet_nan)
    else
      k = f_kh_D20(T, abc_D20(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_D20)
    if(i==0)then
        k = ieee_value(1.0d0, ieee_quiet_nan)
    else
        k = f_kd_D20(T, efgh_D20(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_D20
    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_D20))
        do i=1, ngas_D20
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_D20(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_D20(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_D20 = 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_D20(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_D20
  tau = 1 - Tr
  value = exp(1/(Tr) * sum(aibi_D20(:,1)*tau**(aibi_D20(:,2)))) * pc1_D20
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_D20(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_D20
  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_H20(tau)result(value)
  implicit none
  !! arguments
  real(real64), intent(in) :: tau
  !! return
  real(real64) :: value
  value = sum(cidi_H20(:,1) * tau**(cidi_H20(:,2)))
end function

pure elemental function ft_D20(tau)result(value)
  implicit none

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```

    !! arguments
    real(real64), intent(in) :: tau
    !! return
    real(real64) :: value
    value = sum(cidi_D20(:,1) * tau**(cidi_D20(:,2)))
end function

pure elemental function f_kh_H20(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_H20(T, abc) * f_p1star_H20(T)
end function

pure elemental function f_kh_D20(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_D20(T, abc) * f_p1star_D20(T)
end function

pure elemental function f_kd_H20(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_H20*efgh%F
    p2 = efgh%E/(T+T_KELVIN)*ft_H20(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_D20(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_D20
tau = 1-Tr

p1 = q_D20*efgh%F
p2 = efgh%E/(T+T_KELVIN)*ft_D20(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_D20)
  if(i==0)then
    k = ieee_value(1.0d0, ieee_quiet_nan)
  else
    k = f_kh_D20(T, abc_D20(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

```

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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_D20)
        if(i==0)then
            k = ieee_value(1.0d0, ieee_quiet_nan)
        else
            k = f_kd_D20(T, efgh_D20(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
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_D20
    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_D20))
        do i=1, ngas_D20
            if(allocated(f_gases(i)%gas))then
                deallocate(f_gases(i)%gas)
            endif
            n = len(trim(abc_D20(i)%gas))
            allocate(character(len=n) :: f_gases(i)%gas)
            f_gases(i)%gas = trim(abc_D20(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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