# NFP user manual

Universitat Politècnica de Catalunya

Manel Soria, Caleb Fuster, Arnau Miró

NFP 2.0 - Manual version 1.0 - November 2021

# Contents

# 1   Introduction

NFP[1], standing for Non-ideal Fluid Properties is an open source Thermodynamics calculator for pure fluids (not mixtures), intended to be used in the context of rocket engines, cryogenics fluids, hydrogen storage, refrigeration and other applications. NFP is a library, designed for applications where real fluid properties have to be used as a part of more complex calculation such as algebraic or differential equation solvers.

This is a user manual of NFP and only an overview of the Thermodynamics behind the calculations is given. For a more detailed information, please check [1][2][3].

NFP is encoded in Matlab and the reader of this manual is assumed to be familiar with Matlab.

## 1.1   NFP versus HGS

If the reader is using NFP and HGS together, for instance in the context of rocket engines, it is important to keep in mind the following points:

- NFP covers the liquid, liquid+vapour, vapour and supercritical regions of the fluids. In all cases, the fluids are treated as real. For instance, **in NFP the enthalpy is a function of temperature and pressure, not only temperature**. This means that, when using data of both codes, the user will find differences in all the properties, such as density or enthalpy.

- Unlike HGS, NFP is based on the interpolation of real properties obtained from the National Institute of Standards [4] and not on the evaluation of analytical expressions.

- **The references for entropy and enthalpy are different in both codes, so they should not be compared or used together without corrections**.

- The enthalpy of two different fluids, calculated with NFP, should not be used together without corrections. A notorious example are the para and ortho forms of H2 5.7.

- NFP returns specific properties such as $kJ/kg$, while HGS is designed to work with molar properties such as $kJ/mol$.

---

[1]Formerly known as INIST.

## 1.2 States of a fluid

In order to use and understand NFP, it important to keep in mind the different regions in the Thermodynamic diagram of a fluid. Using as an example $H_2$, in Figure 1 we can see five different regions.

Beginning with the subcritical isobar (in blue) at the left, we have:

- Subcooled liquid (or just liquid), in blue, at a temperature below the saturation temperature for the fluid pressure. Please see the zoomed area in Figure 2, where the difference between the isobar and the saturated liquid line is can be appreciated.

- Saturated liquid, in green, at the saturation temperature for the given pressure.

- Saturated vapor, in black, at the saturation temperature for the given pressure.

- Overheated vapor, in magenta, at a temperature above the saturation temperature for the fluid pressure.

For a supercritical isobar (at a pressure above the pressure of the critical point), we have a supercritical point (in red).

Note that, for the points on the saturation bell, the properties are only a function of the temperature or the pressure, but not both.

The source code to plot this diagram can be found in Section 5.4 as an example.
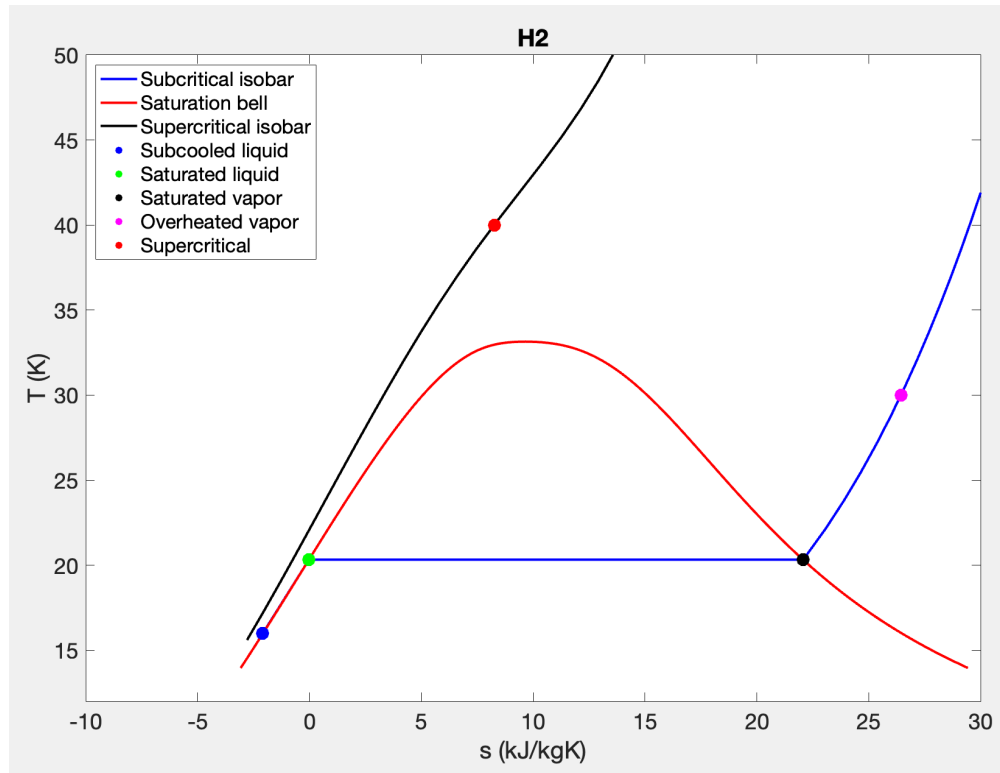


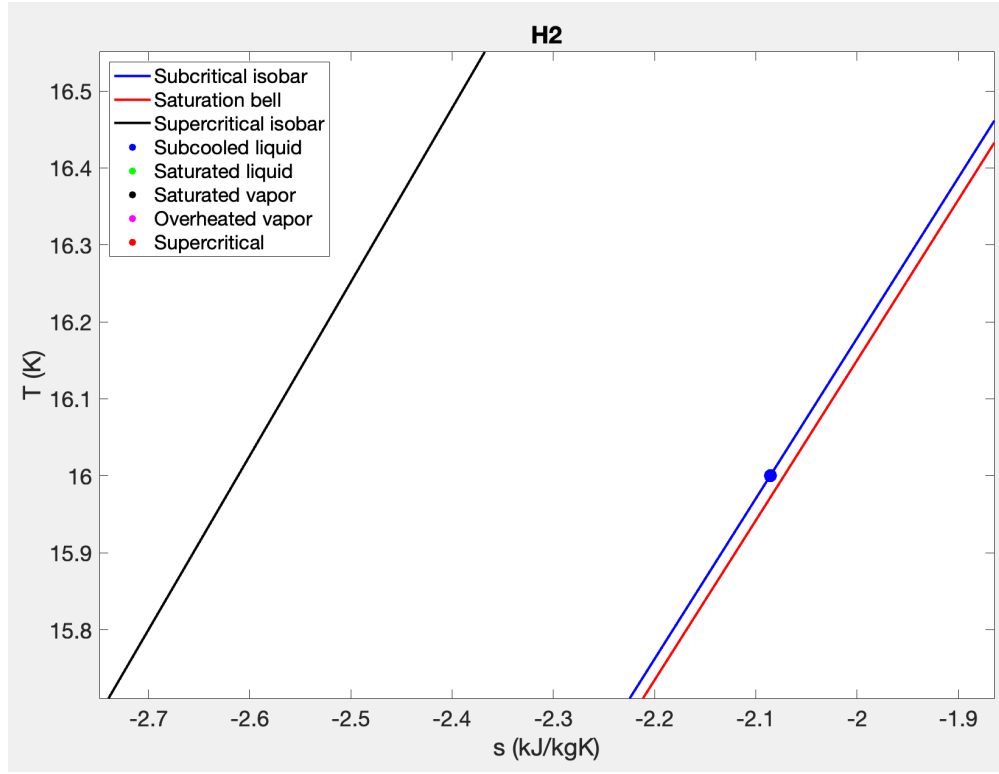Figure 1: Example: Regions in the $Ts$ diagram of $H_2$.

Figure 2: Example: Zoom of the $Ts$ diagram of $H_2$.

## 2 Using `NFP`

`NFP` is based on only two function calls: `NFP` and `NFP_plotisobar`. `NFP` is used for most of the operations so we begin with it.

### 2.1 Magnitudes available in `NFP`, symbols and units.

The magnitudes that can be obtained from `NFP`, followed by their symbol in `NFP` and their units are:

- $T$: Absolute temperature , `T`, $K$.

- $p$: Pressure , `p`, $bar$.

- $h$: Specific enthalpy , `h`, $kJ/kg$.

- $u$: Specific internal energy, `u`, $kJ/kg$.

- $s$ Specific entropy , `s`, $kJ/(kgK)$.

- $v$: Specific volume , `v`, $m^3/kg$.

- $\rho$: Density , `r`, $kg/m^3$.

- $a$: Sound velocity , `a`, $m/s$.

- $\mu$: Dynamic viscosity , `mu`,$Pa.s$.

- $k$: Thermal conductivity , `k` ,$W/(mK)$.

- $M$: Molecular mass , `MM`,$kg/mol$.

- $\mu_{JT}$: Joule-Thomson coefficient, `JT`, $bar/K$.

- $x$: Steam quality (for liquid-vapour equilibrium, $x = m_v/(m_l + m_v)$, `x`, []. Here $m_l$ and $m_v$ are the mass of the saturated liquid and the mass of the saturated vapour, respectively.

4

## 2.2  Obtaining the list of species available `NFP`

The command

```
NFP('Database')
```

returns a list with all the species currently available.

```
>> NFP('Database')
ans =
  1x6 cell array
    {'CH4'}    {'H2'}    {'He'}    {'O2'}    {'R134a'}    {'pH2'}
```

`pH2` stands for para-Hydrogen (see REFMANEL)

## 2.3  Calling `NFP`

`NFP` has a large number of possible queries, but most of them are arranged in a systematic pattern to ease its use.

- The **first argument** is the substance, such as `O2`.

- The **second argument** is a string that describes the property that has to be calculated, and the input parameters. The characters `l` and `v` and the end of the name of the property queried indicate saturated liquid and saturated vapour. For instance, `hl` and `hv` are the specific enthalpy of the saturated liquid and saturated vapour.

   In some cases, the property to be calculated is independent of the conditions, such as `tcrit` (the critical temperature). But usually, it is a function of one or more parameters. In the later case, the parameters are appended to the name of the property being calculated. For instance:

   - `'tsat_p'` stands for the saturation temperature as a function of the pressure.
   - `'r_pt'` stands for the density as a function of the pressure (assuming that the fluid is not in liquid-vapour equilibrium.
   - `'h_px'` stands for the specific enthalpy of a wet steam as a function of the saturation pressure and the quality.

- The **rest of the arguments** are the parameters specified by the second argument string. For instance, in the previous examples (assuming that the species of interest is $O_2$, the total call would be:

   - `NFS('O2',tsat_p',10)`: Query of the saturation temperature of $O_2$ at 10 bar.
   - `NFS('O2',r_pt',10,400)'`: Query of the density of $O_2$ at 10 bar, 400K.
   - `NFS('O2','h_px',10,0.5)`: Query of the $O_2$ as wet steam at 10 bar with a quality of 0.5.

   In all the cases, the arguments have to be given in alphabetical order, for instance `pt` rather than `tp`. The input and output units are as listed in Section 2.1.

**Example 2.**  Find the density, specific enthalpy and specific entropy of texttttH2 at 20K and 2bar.

```
>> NFP('H2','r_pt',2,20)
ans =
    71.3889
>> NFP('H2','h_pt',2,20)
ans =
    -2.4706
>> NFP('H2','s_pt',2,20)
ans =
    -0.1981
```

**Example 3.** Find the density, specific enthalpy and specific entropy of texttttH2 at 20K and 2bar.

```
>> NFP('H2','r_pt',2,20)
ans =
    71.3889
>> NFP('H2','h_pt',2,20)
ans =
    −2.4706
>> NFP('H2','s_pt',2,20)
ans =
    −0.1981
```

**Example 4.** Find the saturation temperature of textttttH2 at 2bar, and the density of the saturated liquid and vapour at the same pressure.

```
>> NFP('H2','rl_p',2)
ans =
    67.7138
>> NFP('H2','tsat_p',2)
ans =
    22.9104
>> NFP('H2','rl_p',2)
ans =
    67.7138
>> NFP('H2','rv_p',2)
ans =
     2.4827
```

## 2.4 Complete list of `NFP` queries

- Zero parameters queries.

  - Critical temperature `tcrit`. Example: NFP('H2','tcrit'). Query 1.
  - Critical pressure `pcrit`. Example: NFP('H2','pcrit'). Query 2.
  - Critical volume `vcrit`. Example: NFP('H2','vcrit'). Query 3.
  - Molecular mass `MM`. Example: NFP('H2','MM'). Query 4.

- One parameter queries

  - Saturation pressure and temperature queries:
    * Saturation temperature as a function of the pressure `tsat_p`. Example: NFP('H2','tsat_p',1). Query 5.
    * Saturation pressure as a function of the temperature `psat_t`. Example: NFP('H2','psat_t',20). Query 6.
  - Saturated liquid properties as a function of pressure:
    * Specific volume `vl_p`. Example: NFP('H2','vl_p',1). Query 7.
    * Specific density `rl_p`. Example: NFP('H2','rl_p',1). Query 8.
    * Specific energy `ul_p`. Example: NFP('H2','ul_p',1). Query 9.
    * Specific enthalpy `hl_p`. Example: NFP('H2','hl_p',1). Query 10.
    * Specific entropy `sl_p`. Example: NFP('H2','sl_p',1). Query 11.
    * Specific heat constant volume heat `cvl_p`. Example: NFP('H2','cvl_p',1). Query 12.
    * Specific heat constant pressure heat `cpl_p`. Example: NFP('H2','cpl_p',1). Query 13.

* Viscosity `mul_p`. Example: NFP('H2','mul_p',1). Query 14.
* Thermal conductivity `kl_p`. Example: NFP('H2','kl_p',1). Query 15.

– Saturated vapour properties as a function of pressure:
* Specific volume `vv_p`. Example: NFP('H2','vv_p',1). Query 16.
* Specific density `rv_p`. Example: NFP('H2','rv_p',1). Query 17.
* Specific energy `uv_p`. Example: NFP('H2','uv_p',1). Query 18.
* Specific enthalpy `hv_p`. Example: NFP('H2','hv_p',1). Query 19.
* Specific entropy `sv_p`. Example: NFP('H2','sv_p',1). Query 20.
* Specific heat constant volume heat `cvv_p`. Example: NFP('H2','cvv_p',1). Query 21.
* Specific heat constant pressure heat `cpv_p`. Example: NFP('H2','cpv_p',1). Query 22.
* Viscosity `muv_p`. Example: NFP('H2','muv_p',1). Query 23.
* Thermal conductivity `kv_p`. Example: NFP('H2','kv_p',1). Query 24.

– Saturated liquid properties as a function of temperature:
* Specific volume `vl_t`. Example: NFP('H2','vl_t',15). Query 25.
* Specific density `rl_t`. Example: NFP('H2','rl_t',15). Query 26.
* Specific energy `ul_t`. Example: NFP('H2','ul_t',15). Query 27.
* Specific enthalpy `hl_t`. Example: NFP('H2','hl_t',15). Query 28.
* Specific entropy `sl_t`. Example: NFP('H2','sl_t',15). Query 29.
* Specific heat constant volume heat `cvl_t`. Example: NFP('H2','cvl_t',15). Query 30.
* Specific heat constant pressure heat `cpl_p`. Example: NFP('H2','cpl_t',15). Query 31.
* Viscosity `mul_t`. Example: NFP('H2','mul_t',15). Query 32.
* Thermal conductivity `kl_t`. Example: NFP('H2','kl_t',15). Query 33.

– Saturated vapour properties as a function of temperature:
* Specific volume `vv_t`. Example: NFP('H2','vv_t',15). Query 34.
* Specific density `rv_t`. Example: NFP('H2','rv_t',15). Query 35.
* Specific energy `uv_t`. Example: NFP('H2','uv_t',15). Query 36.
* Specific enthalpy `hv_t`. Example: NFP('H2','hv_t',15). Query 37.
* Specific entropy `sv_t`. Example: NFP('H2','sv_t',15). Query 38.
* Specific heat constant volume heat `cvv_t`. Example: NFP('H2','cvv_t',15). Query 39.
* Specific heat constant pressure heat `cpv_t`. Example: NFP('H2','cpv_t',15). Query 40.
* Viscosity `muv_t`. Example: NFP('H2','muv_t',15). Query 41.
* Thermal conductivity `kv_t`. Example: NFP('H2','kv_t',15). Query 42.

– Wet vapour properties as a function of temperature and quality:
* Specific volume `v_tx`. Example: NFP('H2','v_tx',15,0.5). Query 43.
* Specific density `r_tx`. Example: NFP('H2','r_tx',15,0.5). Query 44.
* Specific energy `u_tx`. Example: NFP('H2','u_tx',15,0.5). Query 45.
* Specific enthalpy `h_tx`. Example: NFP('H2','h_tx',15,0.5). Query 46.
* Specific entropy `s_tx`. Example: NFP('H2','s_tx',15,0.5). Query 47.
* Specific heat constant volume heat `cv_tx`. Example: NFP('H2','cv_tx',15,0.5). Query 48.
* Specific heat constant pressure heat `cp_tx`. Example: NFP('H2','cp_tx',15,0.5). Query 49.
* Viscosity `mu_tx`. Example: NFP('H2','mu_tx',15,0.5). Query 50.

* Thermal conductivity k_tx. Example: NFP('H2','k_tx',15,0.5). Query 51.
    - Wet vapour properties as a function of pressure and quality:
        * Specific volume v_px. Example: NFP('H2','v_px',2,0.5). Query 52.
        * Specific density r_px. Example: NFP('H2','r_px',2,0.5). Query 53.
        * Specific energy u_px. Example: NFP('H2','u_px',2,0.5). Query 54.
        * Specific enthalpy h_px. Example: NFP('H2','h_px',2,0.5). Query 55.
        * Specific entropy s_px. Example: NFP('H2','s_px',2,0.5). Query 56.
        * Specific heat constant volume heat cv_px. Example: NFP('H2','cv_px',2,0.5). Query 57.
        * Specific heat constant pressure heat cp_px. Example: NFP('H2','cp_px',2,0.5). Query 58.
        * Viscosity mu_px. Example: NFP('H2','mu_px',2,0.5). Query 59.
        * Thermal conductivity k_px. Example: NFP('H2','k_px',2,0.5). Query 60.
    - Non-saturated properties as a function of pressure and temperature:
        * Specific volume v_pt. Example: NFP('H2','v_pt',2,300). Query 61.
        * Specific density r_pt. Example: NFP('H2','r_pt',2,300). Query 62.
        * Specific energy u_pt. Example: NFP('H2','u_pt',2,300). Query 63.
        * Specific enthalpy h_pt. Example: NFP('H2','h_pt',2,300). Query 64.
        * Specific entropy s_pt. Example: NFP('H2','s_pt',2,300). Query 65.
        * Specific heat constant volume heat cv_pt. Example: NFP('H2','cv_pt',2,300). Query 66.
        * Specific heat constant pressure heat cp_pt. Example: NFP('H2','cp_pt',2,300). Query 67.
        * Viscosity mu_pt. Example: NFP('H2','mu_pt',2,300). Query 68.
        * Thermal conductivity k_pt. Example: NFP('H2','k_pt',2,300). Query 69.
    - Temperature as a function of:
        * Pressure and entropy t_ps. Example: NFP('H2','t_ps',10,44). Query 70.
        * Pressure and enthalpy t_hp. Example: NFP('H2','t_hp',3962,300). Query 71.
- Special queries:
    - List of species available: Database. Example: NFP('Database'). Query 72.
    - Minimum isobar available for a species: minp. Example: NFP('H2','minp'). Query 73.
    - Maximum isobar available for a species: maxp. Example: NFP('H2','maxp'). Query 74.
    - Minimum temperature available for the lower isobar of a species: mint. Example: NFP('H2','mint'). Query 75.
    - Maximum temperature available for the lower isobar of a species: maxt. Example: NFP('H2','maxt'). Query 76.
    - Isobars available: isobars. Example: NFP('H2','isobars'). Query 77.

**Exercise 1**

For the case of $O_2$, select an arbitrary subcooled liquid state and a supercritical state. Find all the properties that NFP can obtain and check them in the [4].

# 3  NFP database

In the code, it is provided a small database but it can be increase using the function Download_NFPdatabase. By default the species provided are:

- $H_2$
- para-$H_2$
- $O_2$
- $H_2O$

- $CH_4$
- $CO_2$
- He
- R-134a

If there is more information in how the database is structured see [3].

# 4 NFP_plotisobar

This function create the T-s plot (as Fig.1) of any number of isobars and the saturation bell. It has some additional inputs to modify the colors of the isobars (Saturation bell always in red) and their linewidth.

```
NFP_plotisobar(dat,p,color,thickness)
    NFP_plotisobar:  plot isobar vector
    dat: species
    p: isobar vector
    color (optional): isobar colors
    thickness (optional): line thickness
```

```
NFP_plotisobar('O2',[10,20],'k',2)
```

Note that a wide range of temperatures is plotted. Later, the user can change the limits of the plot.

# 5 NFP additional examples

## 5.1 Determination of altitude from boiling point of water

A plane crashes in Los Andes mountain range and the survivors want to determine their altitude. They only have a thermometer and a recipient to boil water. They observe that the boiling point is 81ºC. Write a function that, using NFP and atmosisa allows to obtain the altitude from the boiling temperature.

```
function h=ex14_elevation(Tc)
p=NFP('H2O','psat_t',Tc+273.15);
options=optimset('display','none');
h=fsolve(@hastobezero,1000,options);
function r=hastobezero(h)
    [~,~,P,~]=atmosisa(h);
    P=P/1e5;
    r=P-p;
end
end
```

```
>> ex14_elevation(81)
ans =
     5.154127282540127e+03
```

## 5.2 Vaporization enthalpy

For $CH_4$, plot the vaporization enthalpy as a function of the saturation pressure.

```
% latent vaporisation heat vs. sat pressure
pv=linspace(1,NFP(sp,'pcrit'),50); % 50 values
for i=1:length(pv)
 dhv(i)= NFP(sp,'hv_p',pv(i))-NFP(sp,'hl_p',pv(i));
end
figure

plot(pv,dhv,'LineWidth',2);
title('C3H8 vaporisation heat vs. saturation pressure');
xlabel('Psat (bar)');
ylabel('\Delta h (kJ/khK)');
grid
set(gca,'FontSize',18)
```
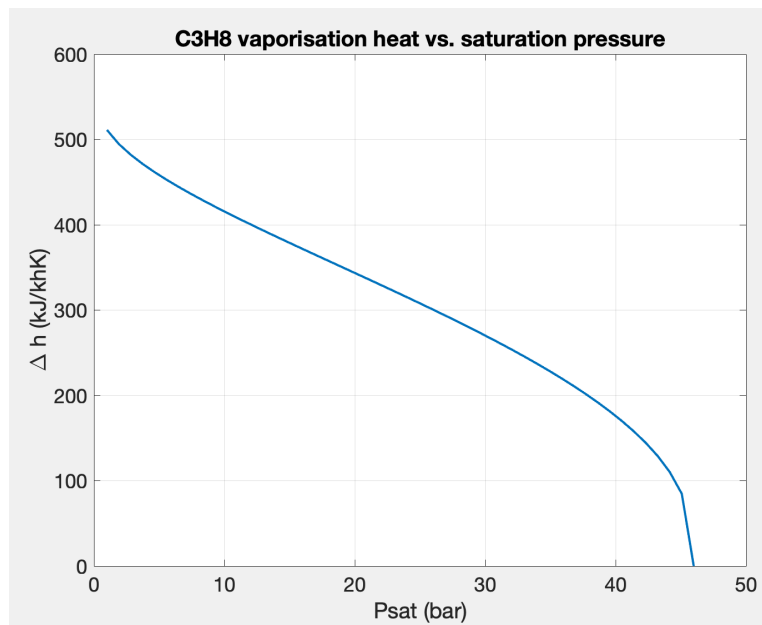


Figure 3: Example: Vaporization enthalpy of CH4 as a function of the saturation pressure.

## 5.3 Diagram of a process

NFP can be used to represent Thermodynamic process and cycles. As an example, consider the isentropic expansion of $CH_4$ from 100 bar, 200K to 5 bar. Determine final state and plot the expansion in a Ts diagram. In this example, we will assume that the final state is inside the saturation bell.

```matlab
clear
close all
sp='CH4';
NFP_plotisobar(sp,[1, 100],'k',2)
set(gca,'FontSize',18)


p1=100; % bar
T1=200; % K
p2=1; % bar
s1=NFP(sp,'s_pt',p1,T1) % kJ/kgK
s2=s1
sl=NFP(sp,'sl_p',p2)
sv=NFP(sp,'sv_p',p2)
x2=(s2-sl)/(sv-sl) % check that it is below 1 !
if x2>1
    error('huuu?? Not saturation conditions');
end
T2=NFP(sp,'Tsat_p',p2)
hold on
plot([s1 s2],[T1 T2],'-b','LineWidth',2);
SZ=120;
scatter(s1,T1,SZ,'og','filled')
scatter(s2,T2,SZ,'or','filled')

xlim([-1,5])
ylim([100,250])
```

### 5.4 Ts diagram of $H_2$

Plot the Ts diagram of $H_2$ to scale, drawing a point of each region.[2]

```
P1=1; T1=16;                        s1=NFP('H2','s_pt',P1,T1);
P2=1; T2=NFP('H2','tsat_p',P2);     s2=NFP('H2','sl_p',P2);
P3=1; T3=NFP('H2','tsat_p',P2);     s3=NFP('H2','sv_p',P3);
P4=1; T4=30;                        s4=NFP('H2','s_pt',P4,T4);

P5=40; T5=40;                       s5=NFP('H2','s_pt',P5,T5);
NFP_plotisobar('H2',P1,'b',2)
NFP_plotisobar('H2',P5,'k',2)

SZ=120;

hold on

scatter(s1,T1,SZ,'ob','filled')
scatter(s2,T2,SZ,'og','filled')
scatter(s3,T3,SZ,'ok','filled')
scatter(s4,T4,SZ,'om','filled')
scatter(s5,T5,SZ,'or','filled')
legend({'Subcritical isobar','Saturation bell','','Supercritical
    isobar','','','Subcooled liquid','Saturated liquid','Saturated
    vapor','Overheated vapor','Supercritical'},'Location','NW')
xlim([-10 30])
ylim([12 50])
set(gca,'FontSize',18)
```

**Exercise 2**

Plot a similar diagram for $pH_2$ . Find the appropriated limits for the pressure.

### 5.5 Isoenthalpic expansion - Pv diagram

A valve is connected to the bottom of a O2 tank. In the tank, we have saturated liquid at a pressure equal to 10 bar. At the valve outlet, the pressure has decreased to 7 bar. We are asked to obtain the O2 state after the valve, assuming that it is isoenthalpic and to plot the process in a pv diagram. Also, check that the entropy has increased.

clearvars close all

```
%Find initial state properties
p1=10;%bar
h1=NFP('O2','hl_p',p1);%kJ/kg
s1=NFP('O2','sl_p',p1);%kJ/kgK

p2=7;% bar
h2=h1;
hl2=NFP('O2','hl_p',p2);
hv2=NFP('O2','hv_p',p2);
x2=(h2-hl2)/(hv2-hl2);
if x2>1 || x2<0
    Error('ugg. This quality is not valid');
end
```

---

[2]This call of the legend command works on Matlab R2021a or greater

```matlab
% Check that entropy increases
T2=NFP('O2','tsat_p',p2);
sl2=NFP('O2','sl_p',p2);
sv2=NFP('O2','sv_p',p2);
s2=sl2+x2*(sv2-sl2);
Inc_s=s2-s1;
if Inc_s<0
    Error('ugg. Increment of entropy negative');
end
fprintf('Saturated vapour at T2=%f K \n',T2);
fprintf('Outlet quality is %8.4f\n',x2);
fprintf('Delta s = %8.4f kJ/kgK \n',s2-s1);

% Diagram
pv = linspace(1,NFP('O2','pcrit'),40); %bar

vl_p = NFP('O2','vl_p',pv);
vv_p = NFP('O2','vv_p',pv);

v1 = NFP('O2','vl_p',p1);

% v2 value (inside the saturation bell !)
v2 = NFP('O2','vl_p',p2) + x2*(NFP('O2','vv_p',p2)-NFP('O2','vl_p',p2));

fprintf('Specific volume at the exit = %8.4f m^3/kg \n',v2);

figure;
semilogx(vl_p,pv,'r','Linewidth',2);
hold on;
text(v1*1.05,p1+2,'1','Fontsize',14);
text(v2*1.05,p2+2,'2','Fontsize',14);
semilogx(vv_p,pv,'r','Linewidth',2);
semilogx(v1,p1,'ob','Linewidth',2);
semilogx(v2,p2,'ob','Linewidth',2);
semilogx([v1 v2],[p1 p2],'k','Linewidth',2);
xlabel('v','Fontsize',14);
ylabel('p','Fontsize',14);
title('O2 isoenthalpic expansion')
set(gca,'Fontsize',18)
```
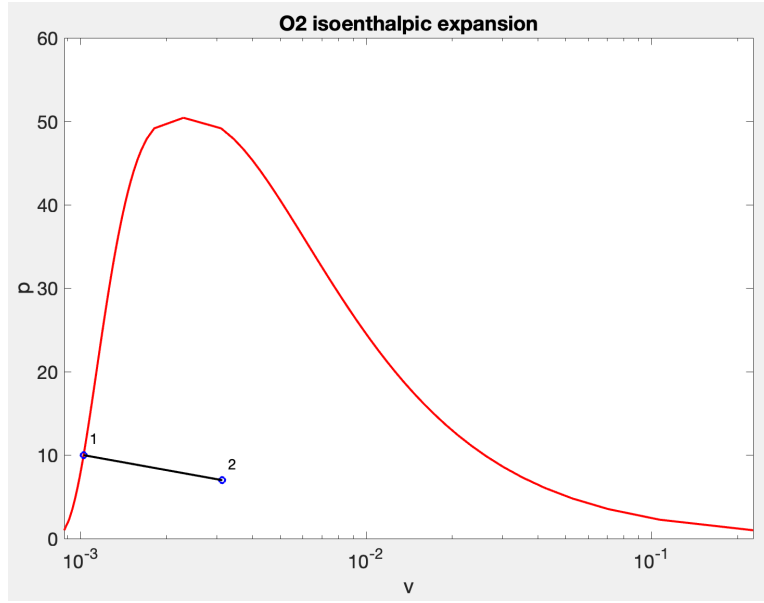
Figure 4: Example: isoenthalpic expansion of O2 in a Pv diagram

## 5.6 Estimation of Mars atmospheric conditions at ground level

The paper [5] gives a list of properties for mars atmospheric (Fig. 5). Use `NFP` to estimate them, assuming that the atmosphere is composed of $CO_2$ only.

**Table 1.** Operating conditions for Mars Condition 1-3

| Variable | Earth SLS | MC 1 | MC 2 | MC 3 |
|---|---|---|---|---|
| Density, $\rho$ [kg/m³] | 1.225 | 0.015 | 0.017 | 0.020 |
| Temperature, $T$ [K] | 288.20 | 248.20 | 223.20 | 193.20 |
| Gas Constant, $R$ [m²/s²/K] | 287.10 | 188.90 | 188.90 | 188.90 |
| Specific Heat Ratio, $\gamma$ [~] | 1.400 | 1.289 | 1.289 | 1.289 |
| Dynamic Viscosity, $\mu$ [Ns/m²] | $1.750 \cdot 10^{-5}$ | $1.130 \cdot 10^{-5}$ | $1.130 \cdot 10^{-5}$ | $1.130 \cdot 10^{-5}$ |
| Static Pressure, $p$ [Pa] | 101,300 | 703.10 | 716.60 | 729.70 |

Figure 5: Mars atmospheric conditions from [5]

```
clearvars
% From the paper
T=248.20; % K
p=703.10/1e5; % bar
rho=NFP('CO2','r_pt',p,T) % Density kg/m^3
gamma=NFP('CO2','cp_pt',p,T)/NFP('CO2','cv_pt',p,T) % gamma
mu=NFP('CO2','mu_pt',p,T) % dynamic viscosity
Ru=0.0083144621; % kJ/(kgK)
Rg=1000*Ru/NFP('CO2','MM') % kJ/(KgK)
```

```
rho =
    0.014995451861842
gamma =
    1.314601287981477
mu =
        1.246605979704258e−05
Rg =
        1.889242572626365e+02
```

As we can see, assuming a $CO_2$ atmosphere we obtain values quite close.

## 5.7   Ortho-Para hydrogen

The book "Ignition!: An Informal History of Liquid Rocket Propellants" by J.D.Clark says: "Each mole of hydrogen (2 grams) which changed from the ortho to the para state gave off 337 calories of heat in the process. And since it takes only 219 calories to vaporize one mole of hydrogen, you were in real trouble. For if you liquefied a mass of hydrogen, getting a liquid that was still almost three quarters ortho- hydrogen, the heat of the subsequent transition of that to para-hydro-gen was enough to change the whole lot right back to the gaseous state. All without the help of any heat leaking in from the outside"

Verify these claims using NFP and the comment in the book Thermodynamic properties of cryogenic fluids by Jacobsen, Richard T. Leachman, Jacob W. Lemmon, Eric W. Penoncello, Steven G

"For all comparisons and mixing with parahydrogen, the reference enthalpy and entropy of saturated liquid orthohydrogen at the normal boiling point should be changed to 702.98 kJ/kg and 0.018269 kJ/kg-K, respectively."

First we find the saturation temperatures at 1atm

```
P=1.013; % bar
T1p=NFP('pH2','tsat_p',P)
T1p =
    20.2765
T1o=NFP('H2','tsat_p',P)
T1o =
    20.3680
```

Now, we check the enthalpy values for both substances as sat liquid, 1atm

```
H1p=NFP('pH2','hl_p',P) % kJ/kg
H1p =
    −0.0090
H1o=NFP('H2','hl_p',P) % kJ/kg
H1o =
    −0.0092
```

We see that both are close to zero, while according to J.D.Clark the difference should be significant. The answer of course is that for each substance the reference enthalpy is different.

So, we impose H1o and the transition isobaric heat is:

```
H1o=702.98;

DeltaHop=H1p−H1o
DeltaHop =
    −702.9890
```

The heat is released in the transition from ortho (obtained from the gas state at 300K) to para, the stable form at 20K. 75% of the gas is ortho.

So, for 1mol, (about 2g), the heat released (in absolute value) is

```
Qop=abs(2e−3*(H1p−H1o)*0.239*1000) % cal
Qop =
  336.0288
```

Very close to the J.D.Clark value

Considering that only 3/4 of the gas is ortho, the transition heat is:

```
Qop=0.75*Qop
Qop =
  252.0216
```

Next check is the vaporization heat of 2 g for the para form:

```
Qvap=2e−3*(NFP('pH2','hv_p',P)−NFP('pH2','hl_p',P) )*0.239*1000
Qvap =
  212.9232
```

also very close

Meaning that ALL the $H_2$ just liquefied would evaporate even if the liquid could be stored in a perfectly adiabatic container.

## 5.8 Combustion of liquid $C_3H_8$ and $O_2$

1 mol/s of C3H8 and 5 mol/s of O2 enter a combustion chamber as as saturated liquid at 20bar. Find the products temperature, considering dissociation. Use `HGS` where needed, but remember to convert the `NFP` enthalpies to the `HGS` reference.

```
species={'C3H8',...
    'CO2',...
    'CO',...
    'O2',...
    'O',...
    'H2',...
    'H',...
    'OH',...
    'H2O'};

% Propellants enters at the combustion chamber  as saturated liquid at
% chamber pressure
P0=20; % bar

TO2=NFP('O2','tsat_P',P0)

TC3H8=NFP('C3H8','tsat_P',P0)

% 1 mol C3H8, 5 mol O2

np=[1;0;0;5;0;0;0;0;0];

% neq=hgseq(species,np,2000,P0)


deltah_O2=(NFP('O2','h_pT',P0,400)-NFP('O2','hl_P',P0))*NFP('O2','MM');
    % kJ/mol
%deltah_O2=0 % uncomment for gas phase propellants
hO2 = HGSsingle('O2','h',400)-deltah_O2 % enthalpy at inlet, in hgs
    reference


deltah_C3H8=(NFP('C3H8','h_pT',P0,400)-NFP('C3H8','hl_P',P0))*NFP('C3H8','MM');
    % kJ/mol
%deltah_C3H8=0  % uncomment for gas phase propellants
hC3H8 = HGSsingle('C3H8','h',400)-deltah_C3H8

Hin=np(1)*hO2+np(4)*hC3H8

[Tp,~,~,~] = HGStp(species,np,'H',Hin,P0)
```

**Exercise 3**

> Solve a similar problem for $CH_4$. The reaction products are expanded in a nozzle up to a pressure of 0.01 bar. Find the thrust in vacuum.

**Exercise 4**

Specific impulse of LOX LH2. Find the specific impulse in vacuum of mixtures of liquid H2 and O2, for a nozzle that expands the reaction product up to 0.01 bar. Assume that the chamber pressure is 100 bar. Plot the specific impulse as a function of the OF ratio (in mass).

**Exercise 5**

Repeat the previous exercise for different chamber pressures and plot the results.

**Exercise 6**

The difficult problem of liquid $H_2$ storage. A closed tank that contains 7kg of para-hydrogen as saturated liquid at 1 bar. Find:

1. The temperature of the $H_2$.

2. The density of the fluid, and the volume of the tank. Would it be larger or smaller to contain liquid water?. How many times?.

3. Assume that the tank, despite being well insulated, has a heat flow of $10W/m^2$ entering it. Calculate the pressure of the tank after $100s$. Assume it is perfectly rigid.

Warning: never try to keep a cryogenic fluid in liquid state inside a closed recipient.

# References

[1]  Yunus A. Çengel et al. *Thermodynamics: an engineering approach.* New York [etc.] : McGraw-Hill, 2006. ISBN: 9701056116.

[2]  Manel Soria. *Extension of Rocket Engines class notes.* Class Notes. 2021.

[3]  Caleb Fuster. *Study: Algorithms for Rocket Engine Thermochemistry.* Master Thesis. 2021. URL: https://upcommons.upc.edu/handle/2117/353102.

[4]  NIST. *NIST Chemistry WebBook - SRD 69.* 2017. DOI: https://doi.org/10.18434/T4D303. URL: https://webbook.nist.gov/chemistry/ (visited on 11/14/2021).

[5]  Witold J.F. Koning, Wayne Johnson, and Håvard F. Grip. "Improved mars helicopter aerodynamic rotor model for comprehensive analyses". In: *AIAA Journal* 57.9 (2019), pp. 3969–3979. ISSN: 00011452. DOI: 10.2514/1.J058045.