

Namelist "Species_Properties"

This data setup is only used in the full version of sunfluidh for the simulation of multi-species gas flows under low-Mach number hypothesis. Otherwise it can be omitted.

It is used to define every thermo-chemical properties of species to estimate physical properties of gas mixture such as heat capacity, thermal conductivity, transport coefficients of diffusion,

Data could be used or not, this depends on the context.

Not for the release SUNFLUIDH_EDU .

Full data set of the namelist

An example on a Helium/Air mixture is given here for helping the user about this data set.

```
&Species_Properties
  Species_Name           = "He" ,
  Species_molecular_Mass= 4.0D-03 ,
Reference_Molecular_Heat_Capacity = 5.193D+03 , Schmidt_Number           = 1.0
,
  Electric_Charge        = 0 ,      Lennard_Jones_Diameter
= 2.576D-10 , Lennard_Jones_Potential= 10.20 ,
  Thermochemical_Properties_Coefficients(1:7,1) = 2.50000000E+00
0.00000000E-00 0.00000000E-00 0.00000000E-00 0.00000000E-00
2.85315086E+05 1.62166556E+00 ,
  Thermochemical_Properties_Coefficients(1:7,2) = 2.50000000E+00
0.00000000E-00 0.00000000E-00 0.00000000E-00 0.00000000E-00
2.85315086E+05 1.62166556E+00 /
&Species_Properties
  Species_Name           = "Air" ,
  Species_molecular_Mass= 2.9D-02 ,
Reference_Molecular_Heat_Capacity = 1.048D+03 , Schmidt_Number           = 1.0
,
  Electric_Charge        = 0 ,      Lennard_Jones_Diameter
= 3.711D-10 , Lennard_Jones_Potential= 97.60 ,
  Thermochemical_Properties_Coefficients(1:7,1) = 0.03298677E+02
0.14082404E-02 -0.03963222E-04 0.05641515E-07 -0.02444854E-10
-0.10208999E+04 0.03950372E+02 ,
  Thermochemical_Properties_Coefficients(1:7,2) = 0.02926640E+02
0.14879768E-02 -0.05684760E-05 0.10097038E-09 -0.06753351E-13
-0.09227977E+04 0.05980528E+02 ,
  End_of_Data_Block= .true./
```



The Thermochemical_Properties_Coefficients are provided by the Chemkin data base. Don't forget to set the variable End_Of_Data_Block to .true. in the last namelist.

Definition of the data set

Species_Name

- type : character string with a maximum size of 6
- Name of the species present in the gas mixture
- Default name given by the user.

Species_molecular_Mass

- type : real value
- Molecular mass (mol/kg)
- Default value given by the user

Reference_Molecular_Heat_Capacity

- type : real value
- Species heat capacity (J/K/kg)
- Default value given by the user

Schmidt_Number

- type : real value
- The Schmidt number Sch is used to define the diffusion coefficient of the species from the kinematic viscosity as $D_i = \nu / Sch$.
This definition is enabled only when the data
"Multi_Species_Mixture_Law_for_Mass_Diffusion_Enabled = .false." (coming from the namelist "Fluid_Properties").
- Default value given by the user

Electric_Charge

- type : real value
- Electric charge of the ionized species in electronic unit
- Used only if chemical reactions are implied.
- Default value given by the user

Lennard_Jones_Diameter

- type : real value
- Diameter of Lennard-Jones (m)
- Default value given by the user

Lennard_Jones_Potential

- type : real value
- Potential of Lennard-Jones (dimensionless)
- Default value given by the user

Thermochemical_Properties_Coefficients

- type : real array - size array (7,2)
- These coefficients are used to define some physical quantities such as enthalpy, entropy, heat capacity, free enthalpy of species in respect with the temperature.
- This data setup is an array of size (7,2) , The first dimension corresponds to the number of coefficients considered (here 7) and the second to the number of temperature ranges considered (here 2).
 - The 1st range of T is 300K → 1000K
 - The 2nd range of T is 1000K → 5000K
- The coefficients come from the Chemkin data base.
- If we note a_i the 7 coefficients that belong to a specific temperature range, we read (with R the universal gas constant):
 - The species heat capacity : $\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$
 - The species enthalpy : $\frac{H}{R} = a_1 T + \frac{a_2 T^2}{2} + \frac{a_3 T^3}{3} + \frac{a_4 T^4}{4} + \frac{a_5 T^5}{5} + a_6$
 - The species entropy : $\frac{S}{R} = a_1 \log(T) + \frac{a_2 T^2}{2} + \frac{a_3 T^3}{3} + \frac{a_4 T^4}{4} + a_7$

End_of_Data_Block

- type : boolean value
- Specify the end of the data set constituted by one or several namelist "Species_Properties".

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<https://sunfluidh.lisn.upsaclay.fr/> - Documentation du code de simulation numérique SUNFLUIDH

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