

## Namelist "Chemical\_Reactions\_Features"

### **Not for the release SUNFLUIDH\_EDU .**

This data setup is recommended for expert users only. It can be omitted for non-reactive flows. It is only used in the full version of sunfluidh for the simulation of reactive gas flows under low-Mach number hypothesis.

It provides some information on the nature of the chemical reactions. The kinetic mechanisms must be described in specific files planned to be directly compiled with the code :

- ***polyn\_coef\_for\_rev\_reactions.inc*** : Polynomials coefficients for calculating the reversed kinetic rate constant.
- ***kinetics.inc*** : Calculation of the kinetic rate constants.
- ***reaction\_rates.inc*** : Calculation of the reaction rates.

An explanation note is included in each file.

Examples of chemical mechanisms are given in the sunfluidh directory :

/TRUNK/DATA/REACTIVE\_FLOW\_DATA

All new data set on chemical mechanisms must be defined in a specific directory which must be stated in the make file in order to download the files \*.inc in the SOURCES directory during the compilation procedure.

## Full data set of the namelist

The values are arbitrary chosen.

```
&Chemical_Reactions_Features  Chemical_Reactions_Enabled= .false. ,  
                               Number_of_Reactions = 1 ,  
                               Start_Time= 0.0 ,  
                               Reaction_Rate_Damping_Time= 0.0,  
                               Density_Dependency_Enabled      = .true.,  
                               Temperature_Dependency_Enabled = .true.,  
                               Heat_Capacity_Dependency_Enabled= .true.,  
                               Homogeneous_Reactor_Enabled     = .false. /
```

## Definition of the data set

### **Chemical\_Reactions\_Enabled**

- Type : boolean value
- This data allows the code to access (or not) to any specific procedures used for calculating the the chemical part of the reactive flow simulations.
- Default value= .false.

## Number\_of\_Reactions

- Type : integer value
- Number of chemical reactions
- Default value = 1

## Start\_Time

- Type : real value
- Time from which chemical reaction are activated
- Default value = 0.0

## Reaction\_Rate\_Damping\_Time

- type : real value
- Time range for which the reaction rates are damped (in order to reduce the stiffness of equations)
- Default value= 0.0

## Density\_Dependency\_Enabled

- Type : Boolean value
- Specify whether the reaction rates depend on the density
- Default value= .true.

## Temperature\_Dependency\_Enabled

- Type : Boolean value
- Specify whether the reaction rates depend on the temperature
- Default value= .true.

## Heat\_Capacity\_Dependency\_Enabled

- Type : Boolean value
- Specify whether the time-variation rate of the energy depends on the heat capacity of the species.
- Default value= .true.

## Homogeneous\_Reactor\_Enabled

- Type : Boolean value
- This option allows the user to test the kinetic mechanism in the case of a homogeneous reactor (without flow consideration)
- In this case, the Navier-stokes equations are not considered.
- Default value= .true.

From:

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

Permanent link:

[https://sunfluidh.limsi.fr/sunfluidh:chemical\\_reactions\\_features\\_namelist](https://sunfluidh.limsi.fr/sunfluidh:chemical_reactions_features_namelist)

Last update: **2016/11/28 17:40**

