

Brookesia



Basics for starting with Brookesia

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1 Installation

Brookesia is developed under the informatic language Python 3. It can be used on Linux, macOS, and Windows.

The necessary computations for the reduction procedure are done with the open-source Cantera software toolkit. The first step is thus to install it.

1.1 Cantera

Every necessary information for the installation of Cantera are provided on Cantera website :

<https://www.cantera.org/install/conda-install.html>

1.2 Brookesia

At the moment, Brookesia do not need installation. The only thing you need to do is to download the source files and use it properly !

1.2.1 Through command line on Linux and Mac

On a terminal, go to your future reduction working folder then type:

```
git clone https://github.com/Brookesia-py/Brookesia
```

1.2.2 By downloading the software on Github

1. Go to the following webpage
<https://github.com/Brookesia-py/Brookesia>
2. click on **Clone or download** button then **Download zip**
3. unzip the downloaded file on your future working folder

After that, all source files shall be on your working folder and you can directly start to work !

2 Basic usage

Before using Brookesia, make sure your Cantera environment is activated. On linux, type on a terminal:

```
source activate <path_to_cantera_environment>
```

2.1 Input file creation through the Graphic User Interface

On **Spyder** (normally installed with the Anaconda suite), load the file GUI_red_mech.py and run it. On command line, on Brookesia folder, just type:

```
python GUI_red_mech.py
```

Then, proceed to the following steps to operate a mechanism reduction (see the screen shots in Table 1):

On the **Main parameters** tab:

1. Load the kinetic mechanism
Example: C1_GRI30.cti
*Note: It is possible to load a previous input file by clicking on **load file** button*
2. Select the target species
Example: CH₄/CO/CO₂
3. Select the reduction methods you want to apply
Example: DRGEP_sp + SA_r
→ then new tabs must appear
4. Select the errors options (pts/QoI ; max/mean)
5. On the **Conditions** tab:
Define the canonical configurations you want to run
Example: Reactor (H,p) CH₄/air $\Phi = 0,5/1/1,5$ $p = 10^5$ Pa; $T = 1600$ K
6. On the **reduction** tab:
define all the options you want to specify (see 2.4 for details)
7. On the **GA** tab (if so):
define all the options you want to specify (see 2.4 for details)
8. On the **Main parameters** tab:
If necessary:
 - change the condition name and save it by clicking on the button Save current conditions
Example: First_example.inp → then saved in the _condition_input folder
 - change the folder name
Example: First_example_folder *Note: to this will be added the date and the hour of reduction (i.e. here 20191225_1200_First_example_folder)*
 - change the amount of outputs during the reduction process (verbose /show plot during reductions)

Run the reduction by clicking on **RUN** button

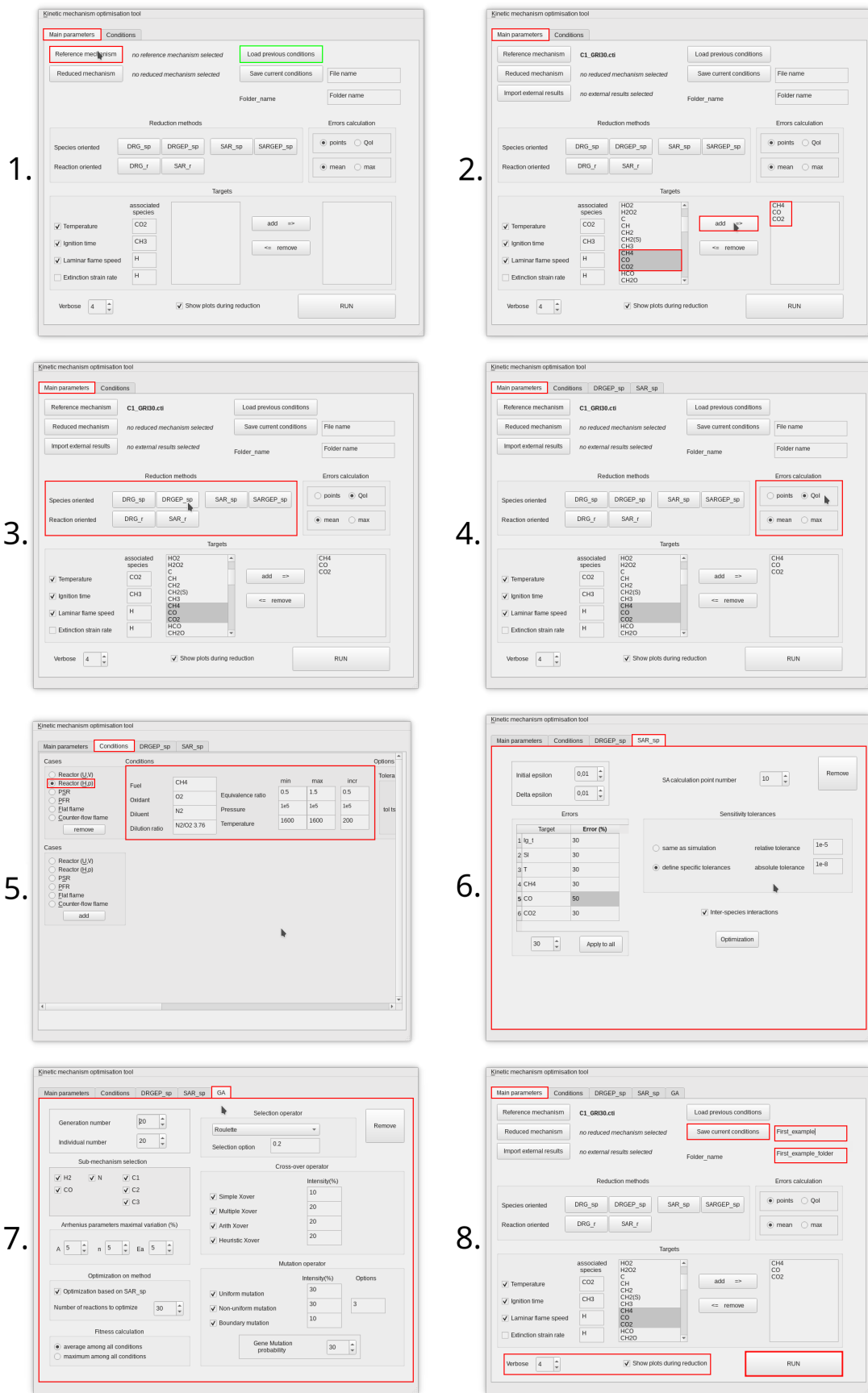


Table 1: Successive usual steps for the reduction and optimization of a kinetic mechanism

2.2 Input file modification on a text editor and tips

Input files (presented in appendices) are usually stored in the `_condition_input` folder. They are composed in three steps :

- ```
#=====
Main parameters
#=====
```

Corresponds to the informations displayed in "*Main parameters*" tab in GUI. Note: several species can be associated to the global data *T*, *igt*, *Sl*, and *K*. To do that just separate the associated species by a coma, i.e.

```
sp_T = CO2, CO
```

- ```
#=====
#           Simulation cases
#=====
```

Note: instead of entering fuel, oxidant, diluent, options, you can enter the mixture in the cantera format using "mixt" option (and "mixt2" for counterflow burner configurations), i.e.

```
mixt           = CH4:0.1 , O2:0.1 , N2:0.8
```

- ```
#=====
Operators
#=====
```

Corresponds to the informations displayed in "*Reduction operator*" and "*GA*" tabs in GUI. Note: if the number of values provided for the tolerance limit of target species is lower than the number of target species, only the first value will be retranscribed and applied to target species. Thus, if you want to define a tolerance threshold of 30% for all target species, you only need to enter the value 30 after the `max_error_sp` keyword, i.e.:

```
max_error_sp = 30
```

An example of input file and the corresponding keyword dictionary are presented in appendices

## 2.3 Running Brookesia from command line

From the head of the working folder, type:

```
python main_reduction.py _conditions_input/<name_of_the_input_file>
```

The argument "`_conditions_input/<name_of_the_input_file>`" is the path toward the reduction condition input file.

## 2.4 Focus on reduction and optimization options

### • Reduction options :

For all reduction methods, you can specify:

- The starting epsilon,
- The starting delta epsilon that will be applied between each iteration (subject to change during the reduction process)
- The number of calculation points distributed in each simulation
- The target tolerances
- The Inter Species Interactions loop
- The optimization after the reduction, if so, a new tab will appear

To facilitate the sensitivity analyses, it is possible to modify the tolerances (in the present example, relative/absolute tolerances are fixed at  $10^{-5}/10^{-8}$ , respectively)

### • Optimization options:

On the genetic algorithm tab, you can specify:

- the number of generation, of individuals,
- the sub-mechanism to optimize
- the variation range of reaction rate coefficients  $B, n$  and  $C$
- to constrain the reduction method to the important reactions identified during the reduction
- to define the fitness computation depending on the average error or the maximal error (among all targets and conditions)
- the selection method
- the cross-over method and corresponding intensity
- the mutation method and corresponding intensity. The gene mutation probability define the reaction probability to get its reaction rate coefficients modified

(a) Reduction tab, example of SAR

(b) Genetic algorithm tab

Figure 1: Results file main sections composition

### 3 Output files

The reduction shall now take place. If the calculations are operated on spyder and the option *Show plots during reduction* has been selected, you can follow the accuracy of the reduced models on the graphs displayed on the spyder console (see figure 2. a).

Once the reduction is finished, you can check the results on the new folder [date\_time\_name\_of\_the\_folder], (here: 191225\_1200\_First\_example\_folder). It contains the following elements:

- **File.** Conditions\_redopt.inp: the input file of the reduction
- **File.** \*.cti: the reference mechanism (here: C1\_GRI30.cti)
- **File.** red\_info.txt: contains informations of the reduction process
- **File.** X\_reduction\_results.csv: contains the simulation results of the *X* reduction step (here, 0\_reduction\_result.csv for the DRGEP\_sp step and 1\_reduction\_result.csv for the SA\_r step). See details, hereafter.
- **Folder.** Flame\_ref\_results (if so): store the \*.xml reference flame results used for *restore* cantera option to accelerate the new mechanism simulations
- **Folder.** Red\_mech: contains the reduced and optimized step named as follows: X(opt)\_B.cti where *X* represent the step number, (opt) is a character string added for the optimized kinetic mechanism, *B* is the reference mechanism name.

In the present example, the kinetic mechanism created are:

- 1\_C1\_GRI30.cti: reduced mechanism after DRGEP\_sp step
- 2\_C1\_GRI30.cti: reduced mechanism after SAR\_sp step
- 2opt\_C1\_GRI30.cti: optimized mechanism after genetic algorithm step

Simulation results are organized on a \*.csv file as presented in Figures 2. The first part of the file (a) indicate information concerning the reference mechanism, the reduction method and, if so, the genetic algorithm. The main information concerning the conditions of the simulation cases (canonical configuration, mixture composition, pressure, temperature, simulation tolerances, etc.) are reminded and the results of the reference simulation are provided. As indicated, in the Figure 2 b), after the reference results, the simulation results obtained with the reduced mechanism and, if so, the optimized mechanism are given. Error information are also provided.



| Kinetic mechanism information    |                                             |                   |                  |                      |                      |                      |                   |                      |                |
|----------------------------------|---------------------------------------------|-------------------|------------------|----------------------|----------------------|----------------------|-------------------|----------------------|----------------|
| Reduction method information     |                                             |                   |                  |                      |                      |                      |                   |                      |                |
| Genetic algorithm information    |                                             |                   |                  |                      |                      |                      |                   |                      |                |
| Simulation condition information |                                             |                   |                  |                      |                      |                      |                   |                      |                |
| 1                                | Reference mechanism                         | C1_CRI30.cti      |                  |                      |                      |                      |                   |                      |                |
| 2                                | Number of species:                          | 53                |                  |                      |                      |                      |                   |                      |                |
| 3                                | Number of reactions:                        | 323               |                  |                      |                      |                      |                   |                      |                |
| 4                                | DRGEP_sp_opt                                |                   |                  |                      |                      |                      |                   |                      |                |
| 5                                | DRGEP_sp computation time: 0 h 2 min 40 sec |                   |                  |                      |                      |                      |                   |                      |                |
| 6                                | GA computation time: 0 h 3 min 6 sec        |                   |                  |                      |                      |                      |                   |                      |                |
| 7                                | Fitness : 17.89                             |                   |                  |                      |                      |                      |                   |                      |                |
| 8                                |                                             | points mean mean  |                  |                      |                      |                      |                   |                      |                |
| 9                                |                                             |                   |                  |                      |                      |                      |                   |                      |                |
| 10                               | Case nb: 1                                  |                   |                  |                      |                      |                      |                   |                      |                |
| 11                               | config                                      |                   |                  |                      |                      |                      |                   |                      |                |
| 12                               | reactor UV                                  | fuel              | oxidant          | diluent              | phi                  |                      | diluent ratio     | mixt                 | P(Pa)          |
| 13                               | Step: Reference                             |                   |                  |                      |                      |                      |                   |                      |                |
| 14                               | Ignition delay time(s)                      | 0.000391788934086 |                  |                      |                      |                      |                   |                      |                |
| 15                               | Time(s)                                     |                   |                  |                      |                      |                      |                   |                      |                |
| 16                               |                                             |                   |                  |                      |                      |                      |                   |                      |                |
| 17                               |                                             | 6.96898287454E-06 | 1599.98436108629 | 3.13901515943511E-07 | 3.96561085459202E-08 | 3.72917461374255E-08 | 0.19959937832826  | 7.06690984655529E-08 | 6.520804780248 |
| 18                               |                                             | 7.66588116199E-05 | 1599.9157705015  | 7.30530349859615E-06 | 1.36345743091012E-07 | 2.25989161258767E-07 | 0.199561789238167 | 5.61482864939225E-07 | 3.699170559167 |
| 19                               |                                             | 0.000146348640365 | 1600.3375370618  | 3.19248049111343E-05 | 4.629005699837E-07   | 7.01117853950509E-07 | 0.199429013452512 | 1.79801613851135E-06 | 0.000181985    |
| 20                               |                                             | 0.00021038469111  | 1602.46736386875 | 0.000120451988454    | 1.61869969331524E-06 | 1.86447939503082E-06 | 0.199040586219956 | 5.03911554523351E-06 | 0.000612803    |
| 21                               |                                             | 0.000221061816796 | 1602.76466946078 | 0.000132508650667    | 1.77634274982721E-06 | 1.99983657764341E-06 | 0.19898327570414  | 5.43436615186445E-06 | 0.000665496    |
| 22                               |                                             | 0.000226095164481 | 1603.09230462217 | 0.0001458020889      |                      |                      | 6.2053470292      | 5.86400709803468E-06 | 0.000722565    |
| 23                               |                                             | 0.000231108512167 | 1603.45340239398 | 0.0001604705023      |                      |                      | 6.5432039427      | 6.3318964473999E-06  | 0.000784428    |
| 24                               |                                             | 0.000236131859852 | 1603.85148400041 | 0.0001766701921      |                      |                      | 6.8320993333      | 6.84244050496438E-06 | 0.000851548    |
| 25                               |                                             | 0.000241155207537 | 1604.2905224507  | 0.000194578573913    | 2.5932541849868E-06  | 2.65879882920028E-06 | 0.198760907382137 | 7.40082195152081E-06 | 0.000924447    |
| 26                               |                                             | 0.000246178555223 | 1604.77501967164 | 0.000214397839654    | 2.85663040581599E-06 | 2.85980093725249E-06 | 0.19868975780596  | 8.01298393004693E-06 | 0.010037228    |
| 27                               |                                             | 0.000251201902908 | 1605.3101007355  | 0.000236359420884    | 3.15022793143121E-06 | 3.07886966445343E-06 | 0.198612250914261 | 8.6859307878707E-06  | 0.01090062     |

(a) Reference result part

| Step name          |                                 |                   |                  |                   |                   |                   |                |                   |             |
|--------------------|---------------------------------|-------------------|------------------|-------------------|-------------------|-------------------|----------------|-------------------|-------------|
| Error information  |                                 |                   |                  |                   |                   |                   |                |                   |             |
| Simulation results |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 278                |                                 | 0.00160395913716  | 2645.49070935    |                   |                   |                   |                |                   |             |
| 279                |                                 | 0.0016736489659   | 2645.0356834017  |                   |                   |                   |                |                   |             |
| 280                |                                 | 0.00174333879465  | 2644.59075392    |                   |                   |                   |                |                   |             |
| 281                |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 282                | Step: Reduction                 |                   |                  |                   |                   |                   |                |                   |             |
| 283                | Temperature error: 0.0%         |                   |                  |                   |                   |                   |                |                   |             |
| 284                | Ignition delay time error: 0.0% |                   |                  |                   |                   |                   |                |                   |             |
| 285                | Target species errors:          |                   |                  |                   |                   |                   |                |                   |             |
| 286                | Ignition delay time(s)          | 0.000391788934086 |                  |                   |                   |                   |                |                   |             |
| 287                | Time(s)                         |                   |                  |                   |                   |                   |                |                   |             |
| 288                |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 289                |                                 | 6.96898287454E-06 | 1599.98436108629 | 3.13901516125E-07 | 3.96561085688E-08 | 3.72917461589E-08 | 0.199599378443 | 7.06690985063E-08 | 6.520804784 |
| 290                |                                 | 7.66588116199E-05 | 1599.9157705015  | 7.30531050344E-06 | 1.36345873829E-07 | 2.25989377954E-07 | 0.199561960593 | 5.6148340333E-07  | 3.69917410  |
| 291                |                                 | 0.000146348640365 | 1600.3375370618  | 3.19252398984E-05 | 4.62906874045E-07 | 7.0112740628E-07  | 0.199431730684 | 1.7986261199E-06  | 0.000181987 |
| 550                |                                 | 0.00160395913716  | 2645.49070935    |                   |                   |                   |                |                   |             |
| 551                |                                 | 0.0016736489659   | 2645.0356834017  |                   |                   |                   |                |                   |             |
| 552                |                                 | 0.00174333879465  | 2644.59075392    |                   |                   |                   |                |                   |             |
| 553                |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 554                | Step: Optimisation              |                   |                  |                   |                   |                   |                |                   |             |
| 555                | Temperature error: 0.0%         |                   |                  |                   |                   |                   |                |                   |             |
| 556                | Ignition delay time error: 2.7% |                   |                  |                   |                   |                   |                |                   |             |
| 557                | Target species errors:          |                   |                  |                   |                   |                   |                |                   |             |
| 558                | Ignition delay time(s)          | 0.000381335459774 |                  |                   |                   |                   |                |                   |             |
| 559                | Time(s)                         |                   |                  |                   |                   |                   |                |                   |             |
| 560                |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 561                |                                 | 6.96898287454E-06 | 1599.98243261138 | 4.46579238965E-07 | 3.9653371031E-08  | 5.14467813391E-08 | 0.199599356112 | 5.8113349674E-08  | 6.482192755 |
| 562                |                                 | 7.66588116199E-05 | 1599.86156229194 | 1.11918112835E-05 | 1.50452497861E-07 | 3.47913498386E-07 | 0.199562909092 | 4.62351424175E-07 | 3.634248743 |
| 563                |                                 | 0.000146348640365 | 1600.02962278649 | 4.6746238152E-05  | 4.43204212793E-07 | 1.02617822466E-06 | 0.199436629066 | 1.3650202658E-06  | 0.000172485 |

(b) Reduction/optimization results part

Figure 2: Results file main sections composition

## 4 First examples

Five input files are provided for a gentle start with Brookesia software. Input conditions are summarized in Table 2.

| Input file name          | 1_reactor.inp                                       | 2_JSR.inp                                                   | 3_Free_Flame.inp                                     | 4_diff.inp                   | 5_pp.inp                                                |
|--------------------------|-----------------------------------------------------|-------------------------------------------------------------|------------------------------------------------------|------------------------------|---------------------------------------------------------|
| kinetic mechanism        | C1_GRI30                                            | C1_GRI30                                                    | C1_GRI30                                             | C0_H2_Law                    | C1_GRI30                                                |
| Species (reaction)       | 53 (325)                                            | 53 (325)                                                    | 53 (325)                                             | 11 (32)                      | 53 (325)                                                |
|                          | Reactor (U,V)                                       | JSR                                                         | Free flame                                           | Diffusion flame              | Partially-premixed flame                                |
| conditions               | $\Phi=0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 1600$ K | $\Phi = 0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 600 - 1200$ K | $\Phi = 0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 300$ K | $p = 10^5$ Pa<br>$T = 300$ K | $\Phi = 1/0.5, 1.5/0.5$<br>$p = 10^5$ Pa<br>$T = 300$ K |
| Target(error)            | CH <sub>4</sub> (30)                                | CH <sub>4</sub> (30)                                        | CH <sub>4</sub> (30)                                 | H <sub>2</sub> (30)          | CH <sub>4</sub> (30)                                    |
|                          | CO(30)                                              | OH(30)                                                      | CO(30)                                               | H <sub>2</sub> O(30)         | CO(30)                                                  |
|                          | CO <sub>4</sub> (30)                                | CO <sub>2</sub> (30)                                        | CO <sub>2</sub> (30)                                 | H(30)                        | CO <sub>2</sub> (30)                                    |
|                          | $T(30)$                                             | $T(30)$                                                     | $T(30)$                                              | $T(30)$                      | $T(30)$                                                 |
|                          | Igt(30)                                             |                                                             | Sl(30)                                               | K(30)                        |                                                         |
| Error method             | points                                              | points                                                      | QoI                                                  | QoI                          | points                                                  |
| Reduction method         | DRGEP_sp + GA<br>SAR_sp + GA                        | DRGEP_sp<br>DRG_r + GA                                      | DRGEP_sp<br>SARGEPP_sp + GA                          | DRGEP_sp<br>DRG_r + GA       | DRG_sp<br>SAR_r + GA                                    |
| Final Species (reaction) | 15 (57)                                             | 22 (114)                                                    | 25 (133)                                             | 8 (12)                       | 24 (86)                                                 |
| Computation time         | 7 min                                               | 5 min                                                       | 2 h 08 min                                           | 35 min                       | 40 min                                                  |

Table 2: Summary presentation of the five input files provided as examples  
targets symbols:  $T$ : temperature,  $igt$ : ignition delay time,  $Sl$ : laminar flame speed,  $K$ : Extinction stretch rate

As an example, the results obtained with the successive kinetic mechanisms simulation of the reduction procedure given in 1\_reactor.inp are presented in Figure 3.

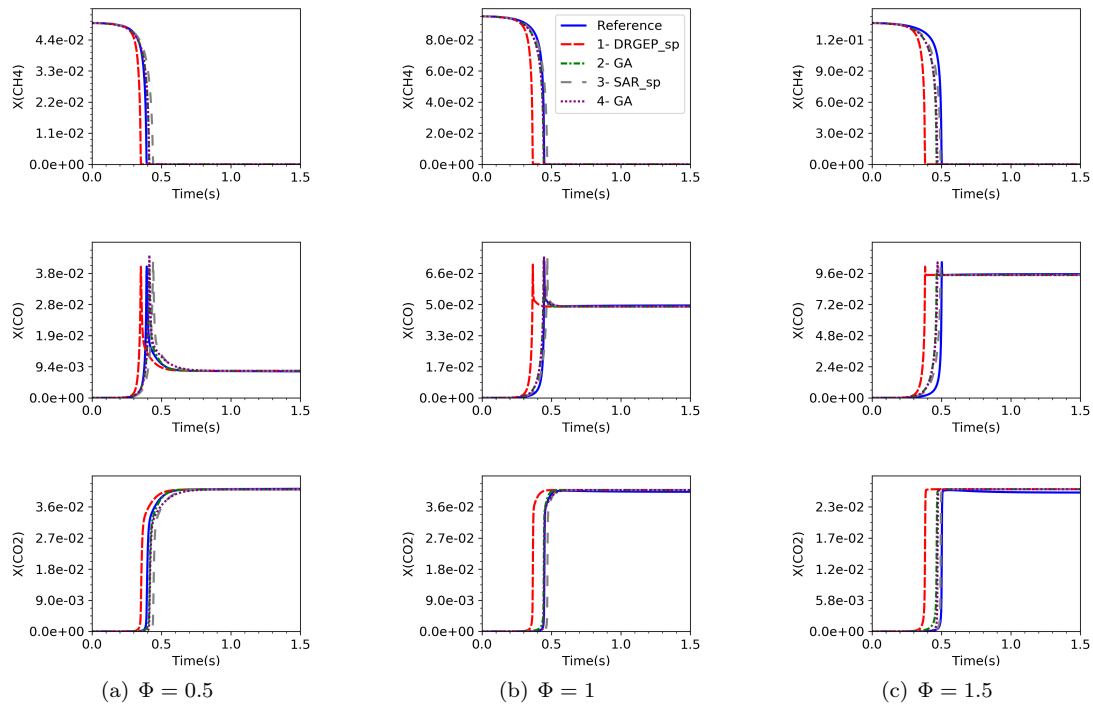


Figure 3: Simulation results obtained during the reduction process defined in the example 1\_reactor.inp

## 5 Appendices

### Input file example

```
#=====
Main parameters
#=====
main_path = TEST_1_reactor
mech = C1_GRI30.cti
verbose = 4
show_plots = True
tspc = CH4, CO, CO2
T_check = True
sp_T = CO2
Sl_check = False
sp_Sl = H
ig_check = True
sp_ig = CH3
K_check = False
sp_K = H
error_calculation = points
error_coupling = mean

#=====
Simulation cases
#=====

#=====> Case 1
config = reactor_UV
Ps = 100000.0
fuel = CH4
oxidant = O2
diluent = N2
diluent_ratio = N2/O2 3.76
Ts = 1600.0
Ps = 100000.0
phis = 0.5, 1.0, 1.5
n_pts = 250.0
delta_npts = 20.0
t_max_coeff = 5.0
Scal_ref = H2O
grad_curv_ratio = 0.5
tign_nPoints = 130.0
tign_dt = 1e-09
tol_ts = 1e-06, 1e-12

#=====
Operators
#=====

#=====> Op: DRGEP_sp
operator = DRGEP_sp
eps = 0.02
delta_eps = 0.01
n_points = 10.0
max_error_sp = 30, 30, 30
max_error_T = 30
max_error_ig = 30
inter_sp_inter = True
optim = True
#=====> Optimization
n_gen = 5
n_indiv = 5
```

```

error_fitness = mean
Arrh_max_variation = 5, 5, 5
optim_on_meth = False
nb_r2opt = 30
selection_operator = Roulette
selection_options = 0.2
Xover_operator = simple_Xover, multiple_Xover, arith_Xover, heuristic_Xover
Xover_pct = 10, 20, 20, 20
Xover_opt = , , ,
mut_operator = uniform_mutation, non_uniform_mutation, boundary_mutation
mut_pct = 30, 30, 10
mut_opt = , 3,
mut_intensity = 20
sub_mech_sel = H2, CO, C1, C2, C3, N

```

```

=====> Op: SAR_sp
operator = SAR_sp
eps = 0.02
delta_eps = 0.01
n_points = 10.0
max_error_sp = 30.0, 30.0, 30.0
max_error_T = 30.0
max_error_ig = 30.0
inter_sp_inter = True
optim = True
ttol_sensi = [1e-05, 1e-08]
=====> Optimization
n_gen = 5
n_indiv = 5
error_fitness = mean
Arrh_max_variation = 8, 3, 3
optim_on_meth = False
nb_r2opt = 30
selection_operator = Roulette
selection_options = 0.2
Xover_operator = simple_Xover, multiple_Xover, arith_Xover, heuristic_Xover
Xover_pct = 10, 20, 30, 20
Xover_opt = , , ,
mut_operator = uniform_mutation, non_uniform_mutation, boundary_mutation
mut_pct = 10, 70, 40
mut_opt = , 3,
mut_intensity = 30
sub_mech_sel = H2, CO

```

## Input file keyword dictionary

### Main parameters keywords

|                   |                                                                                                      |
|-------------------|------------------------------------------------------------------------------------------------------|
| main_path         | name of the folder containing all results (to this will be added the date and the hour of reduction) |
| mech              | reference mechanism name                                                                             |
| verbose           | rules the amount of information displayed during the reduction process (range between 0 and 10)      |
| show_plots        | for spyder essentially, select to display or not the simulation results during the reduction process |
| tspc              | name of target species                                                                               |
| T_check           | add (True) or not (False) the temperature as target                                                  |
| sp_T              | temperature associated species to manage reduction with DRG methods                                  |
| Sl_check          | add (True) or not (False) the flame speed as target                                                  |
| sp_Sl             | flame speed associated species to manage reduction with DRG methods                                  |
| ig_check          | add (True) or not (False) the ignition delay time as target                                          |
| sp_ig             | ignition delay time associated species to manage reduction with reduction methods                    |
| K_check           | add (True) or not (False) the extinction stretch rate as target                                      |
| sp_K              | extinction stretch rate associated species to manage reduction with reductions methods               |
| error_calculation | error method (point / QoI)                                                                           |
| error_coupling    | error interpretation (max / mean)                                                                    |

### Configuration keywords

|                 |                                                                                      |
|-----------------|--------------------------------------------------------------------------------------|
| config          | configuration (reactor_UV, reactor_HP, free_flame, diff_flame, pp_flame, tp_flame)   |
| reactor_UV      | adiabatic, constant volume reactor                                                   |
| JSR             | Jet-stirred reactor                                                                  |
| PFR             | Plug-flow reactor (!) <i>beta version</i>                                            |
| reactor_HP      | adiabatic, constant pressure reactor                                                 |
| free_flame      | freely propagative adiabatic flame                                                   |
| diff_flame      | counterflow diffusion flame                                                          |
| pp_flame        | partially-premixed flame                                                             |
| tp_flame        | twin-premixed flames                                                                 |
| mixt            | initial mixture composition (e.g. mixt = CH4:0.1, O2:0.1, N2:0.8)                    |
| fuel            | fuel species                                                                         |
| oxidant         | oxidant species                                                                      |
| diluent         | diluent species                                                                      |
| diluent_ratio   | dilution ratio (%)                                                                   |
| Ts              | initial temperature(s) (K)                                                           |
| Ps              | initial pressure(s) (Pa)                                                             |
| phis            | equivalent ratio(s)                                                                  |
| tol_ts          | simulation transient tolerances                                                      |
| n_pts           | <i>for reactors:</i> simulation point number (for reactors)                          |
| delta_npts      | <i>for reactors:</i> tolerance in simulation point number                            |
| t_max_coeff     | <i>for reactors:</i> final time of the simulations (multiple of ignition delay time) |
| Scal_ref        | <i>for reactors:</i> reference scalar for grad and curve interpretation              |
| grad_curv_ratio | <i>for reactors:</i> grad/curv options for time discretization                       |
| t_max           | <i>for JSR:</i> residence time on the reactor (s)                                    |
| xmax            | <i>for free_flames:</i> dimension of the computational domain (m)                    |

### Configuration keywords

|                 |                                                                                                                                          |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------|
| tol_ss          | <i>for flames:</i> simulation steady-state tolerances                                                                                    |
| transport_model | <i>for flames:</i> transport model (Mix/Mult)                                                                                            |
| pts_scatter     | <i>for flames:</i> initial grid                                                                                                          |
| slope           | <i>for flames:</i> Cantera refining criteria<br>normalized maximum difference in value between two adjacent points                       |
| curve           | <i>for flames:</i> Cantera refining criteria<br>normalized maximum difference in slope between two adjacent intervals                    |
| ratio           | <i>for flames:</i> Cantera refining criteria<br>add points if the ratio of the spacing on either side of a grid point exceeds this value |
| prune           | <i>for flames:</i> Cantera refining criteria<br>remove point if the slope or curve criteria are satisfied to the level of "prune"        |
| xmax            | <i>for free_flames:</i> dimension of the computational domain (m)                                                                        |
| fuel_1          | <i>for counterflow flames:</i> bottom burner fuel species                                                                                |
| oxidant_1       | <i>for counterflow flames:</i> bottom burner oxidant species                                                                             |
| diluent_1       | <i>for counterflow flames:</i> bottom burner diluent species                                                                             |
| diluent_ratio_1 | <i>for counterflow flames:</i> bottom burner diluent species                                                                             |
| Ts_1            | <i>for counterflow flames:</i> bottom burner initial temperature(s) (K)                                                                  |
| phis_1          | <i>for counterflow flames:</i> bottom burner equivalent ratio(s)                                                                         |
| mdots_1         | <i>for counterflow flames:</i> bottom burner mass flux (kg/m <sup>2</sup> /s)                                                            |
| fuel_2          | <i>for counterflow flames:</i> top burner fuel species                                                                                   |
| oxidant_2       | <i>for counterflow flames:</i> top burner oxidant species                                                                                |
| diluent_2       | <i>for counterflow flames:</i> top burner diluent species                                                                                |
| diluent_ratio_2 | <i>for counterflow flames:</i> top burner diluent ratio                                                                                  |
| Ts_2            | <i>for counterflow flames:</i> top burner temperature(s) (K)                                                                             |
| phis_1          | <i>for counterflow flames:</i> top burner equivalent ratio(s)                                                                            |
| mdots_2         | <i>for counterflow flames:</i> top burner mass flux (kg/m <sup>2</sup> /s)                                                               |
| width           | <i>for counterflow flames:</i> interval between the bottom and the top burner (m)                                                        |

### Reduction method keywords

|                |                                                                                                                                                                                                                          |
|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| operator       | reduction operator (DRG_sp, DRGEP_sp, DRG_r, SAR_sp, SAR_r, SARGE_sp)                                                                                                                                                    |
| eps            | starting cut-off threshold $\epsilon$                                                                                                                                                                                    |
| delta_eps      | starting delta epsilon (subject to change during the reduction process)                                                                                                                                                  |
| n_points       | number of calculation points distributed in each simulation                                                                                                                                                              |
| max_error_sp   | target tolerances<br>Note: if the number of values provided for the tolerance limit of target species is lower to the number of target species, only the first value will be retranscribed and applied to target species |
| max_error_T    | temperature tolerances                                                                                                                                                                                                   |
| max_error_ig   | ignition delay time tolerances                                                                                                                                                                                           |
| max_error_Sl   | flame speed tolerances                                                                                                                                                                                                   |
| max_error_K    | extinction stretch rate tolerances                                                                                                                                                                                       |
| inter_sp_inter | application of the Target Species Interaction loop (True/False)                                                                                                                                                          |
| ttoi_sensi     | sensitivity analyses relative/absolute tolerances                                                                                                                                                                        |

### Genetic Algorithm keywords

|                    |                                                                                                                                                                       |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| optim              | genetic algorithm optimization (True/False)                                                                                                                           |
| n_gen              | generation number                                                                                                                                                     |
| n_indiv            | individual number                                                                                                                                                     |
| error_fitness      | fitness computation option<br>mean: computation based on the average error / max: computation based on the maximal error among all targets and conditions on all /max |
| Arrh_max_variation | variation range of reaction rate coefficients B,n and C                                                                                                               |
| optim_on_meth      | optimization method constrained to the important reactions identified by reduction methods (True/False/DRG/SA)                                                        |
| nb_r2opt           | number of reaction to optimize                                                                                                                                        |
| selection_operator | selection operator                                                                                                                                                    |
| selection_options  | selection operator option                                                                                                                                             |
| Xover_operator     | cross-over operator                                                                                                                                                   |
| Xover_pct          | cross-over operator use rate (% of the number of individuals)                                                                                                         |
| mut_operator       | mutation operator                                                                                                                                                     |
| mut_pct            | mutation operator use rate (% of the number of individuals)                                                                                                           |
| mut_opt            | mutation options 'leave empty if not necessary                                                                                                                        |
| mut_intensity      | probability of a reaction to get its reaction rate coefficients modified by mutation operator                                                                         |
| sub_mech_sel       | sub-mechanism to optimize                                                                                                                                             |