

# Brookesia



## Tutorial for starting with Brookesia

*version, 11/05/2020*

# Contents

<b>1</b>	<b>Installation</b>	<b>2</b>
1.1	Cantera . . . . .	2
1.2	Brookesia . . . . .	2
1.2.1	Necessary python modules for proper use of Brookesia . . . . .	2
1.2.2	Through command line on Linux and Mac . . . . .	2
1.2.3	By downloading the software on Github . . . . .	2
<b>2</b>	<b>Basic for reduction and subsequent optimization of detailed mechanisms</b>	<b>3</b>
2.1	Input file creation through the Graphic User Interface . . . . .	3
2.2	Input file modification on a text editor . . . . .	4
2.3	Running Brookesia from command line . . . . .	6
2.4	Reduction and optimization options . . . . .	6
2.5	Output files . . . . .	7
<b>3</b>	<b>Data importation</b>	<b>8</b>
3.1	Start from a previously reduced kinetic mechanism . . . . .	8
3.2	Import results file . . . . .	8
<b>4</b>	<b>First examples</b>	<b>10</b>
<b>5</b>	<b>Appendices</b>	<b>12</b>

# 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, install the required modules and use it properly!

### 1.2.1 Necessary python modules for proper use of Brookesia

To use Brookesia, the modules Pandas (<https://pandas.pydata.org/>) and Scipy (<https://www.scipy.org/>) must be installed. On a terminal <sup>1</sup>, go to your future reduction working folder then type:

```
conda activate <name_of_your_environment>
conda install pandas
conda install scipy
conda install matplotlib
conda install numpy
```

### 1.2.2 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
```

### 1.2.3 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!

---

<sup>1</sup>On Windows, start Anaconda then click on:  
Environment → Name\_of\_your\_environment → ► → Open Terminal

## 2 Basic for reduction and subsequent optimization of detailed mechanisms

Before using Brookesia, make sure your Cantera environment is activated.

On Anaconda: click on Environments tab then on your environment name.

On a terminal, type:

```
conda 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.

By 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  
Table 1 example: C1\_GRI30.cti  
*Note: It is possible to skip all the following steps by loading a previous input file by clicking on **load file** button*
2. Select the target species  
Table 1 example: CH<sub>4</sub>/CO/CO<sub>2</sub>
3. Select the reduction methods you want to apply  
Table 1 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  
Table 1 example: Reactor (H,p) CH<sub>4</sub>/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 section 2.4 for details)
7. On the **GA** tab (if so):  
define all the options you want to specify (see section 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  
Table 1 example: First\_example.inp → then saved in the \_condition\_input folder
  - change the folder name  
Table 1 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

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.

## 2.2 Input file modification on a text editor

Saved input files (presented in appendices) are stored in an ASCII file, in the `_condition_input` folder. It may sometimes be more convenient to modify this text file directly than resorting to the GUI. Those input files can be then run by command line from a terminal (see next section).

They are composed in three parts:

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

Corresponds to the information 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 information 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 transcribed and applied to target species. Thus, if you want to define a tolerance limit 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

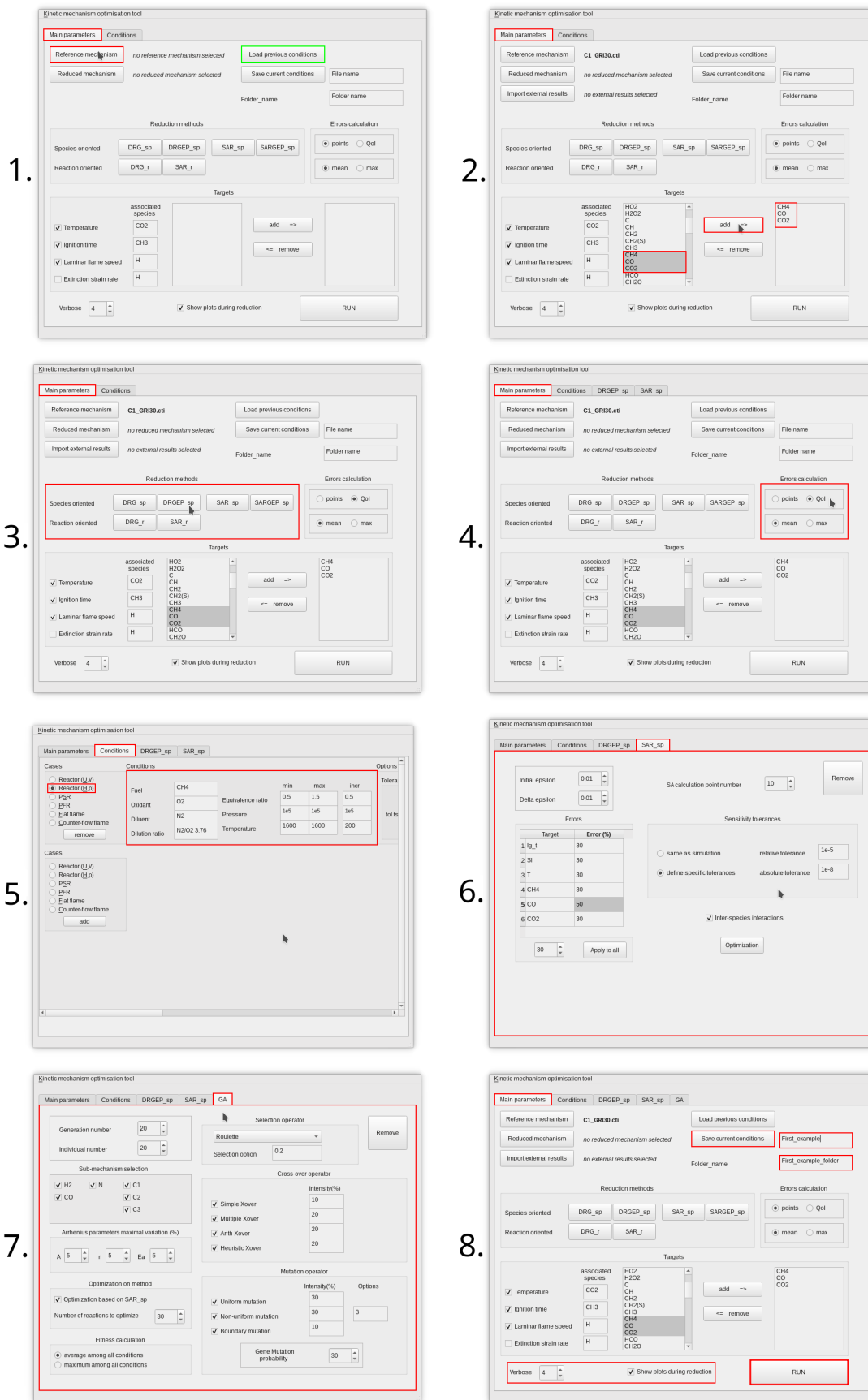


Table 1: Successive usual steps for the reduction and optimization of a kinetic mechanism

## 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 Reduction and optimization options

### • Reduction options :

Seven reduction methods are implemented in Brookesia :

- DRG - oriented species (DRG\_sp)
- DRGEP - oriented species (DRGEP\_sp)
- Sensitivity analysis - oriented species (SAR\_sp)
- Sensitivity analysis with graph search - oriented species (SARGEP\_sp)
- DRG - oriented reactions (DRG\_r)
- Sensitivity analysis - oriented reactions (SAR\_r)
- Computational Singular Perturbation - QSSA candidate identification and oriented reactions reduction (CSP)

For all reduction methods, you can specify (Figure 1 a.):

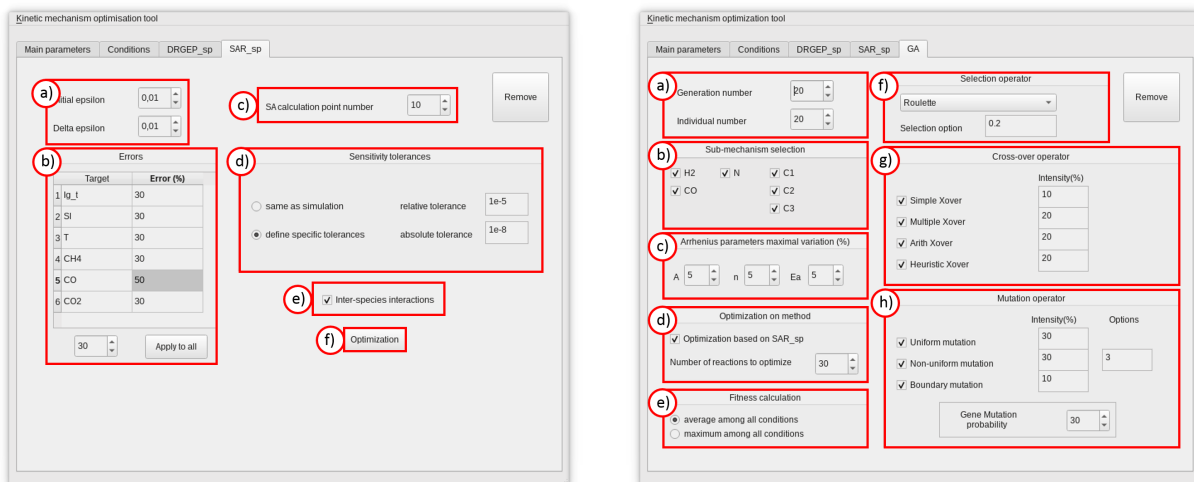
- a) The starting epsilon,
- b) The starting delta epsilon that will be applied between each iteration (subject to change during the reduction process)
- c) The number of calculation points distributed in each simulation
- d) The target tolerances
- e) The Inter Species Interactions loop
- f) The optimization 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 (Figure 1 b.):

- a) the number of generation, of individuals,
- b) the sub-mechanism to optimize
- c) the variation range of reaction rate coefficients  $B$ ,  $n$  and  $C$
- d) to constrain the reduction method to the important reactions identified during the reduction
- e) to define the fitness computation depending on the average error or the maximal error (among all targets and conditions)
- f) the selection method
- g) the cross-over method and corresponding intensity
- h) 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 Sensitivity Analysis based Reduction

(b) Genetic algorithm tab

Figure 1: Composition of the operator tabs (description in section 2.4)

## 2.5 Output files

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: input file of the reduction
- **File.** \*.cti: reference mechanism (here: C1\_GRI30.cti)
- **File.** red\_info.txt: contains information 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 follow:  
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 written in 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.



| Reference mechanism |                                             |                   |                  |                      |                      |                      |                        |                      |                |
|---------------------|---------------------------------------------|-------------------|------------------|----------------------|----------------------|----------------------|------------------------|----------------------|----------------|
| 1                   | Reference mechanism                         | C-1 GR130.cti     |                  |                      |                      |                      |                        |                      |                |
| 2                   | Number of species:                          | 53                |                  |                      |                      |                      |                        |                      |                |
| 3                   | Number of reactions:                        | 325               |                  |                      |                      |                      |                        |                      |                |
| 4                   | ORSEP_sp_opt                                |                   |                  |                      |                      |                      |                        |                      |                |
| 5                   | ORSEP_sp computation time: 0 h 2 min 40 sec |                   |                  |                      |                      |                      |                        |                      |                |
| 6                   | GA computation time: 0 h 3 min 6 sec        |                   |                  |                      |                      |                      |                        |                      |                |
| 7                   | Fitness : 17.89                             |                   |                  |                      |                      |                      |                        |                      |                |
| 8                   |                                             |                   |                  |                      |                      |                      |                        |                      |                |
| 9                   |                                             |                   |                  |                      |                      |                      |                        |                      |                |
| 10                  | Case nb: 1                                  |                   |                  |                      |                      |                      |                        |                      |                |
| 11                  | config                                      | fuel              | oxidant          | diluent              | phi                  | diluent_ratio        | mixt                   |                      | P(Pa)          |
| 12                  | reactor UV                                  | CH4               | O2               |                      |                      | 3.761                | CH4:0.5,O2:2.0,N2:7.52 |                      |                |
| 13                  | Step Reference                              |                   |                  |                      |                      |                      |                        |                      |                |
| 14                  | Ignition delay time(s):                     | 0.000391788934086 |                  |                      |                      |                      |                        |                      |                |
| 15                  | Time(s)                                     |                   |                  |                      |                      |                      |                        |                      |                |
| 16                  |                                             |                   |                  |                      |                      |                      |                        |                      |                |
| 17                  |                                             | 6.9689828745E-06  | 1599.98436198629 | 3.13901515943511E-07 | 3.96561085459202E-08 | 3.72917461374255E-08 | 0.19959937832826       | 7.06690984655529E-08 | 6.520804780245 |
| 18                  |                                             | 7.66588116199E-05 | 1599.9157705015  | 7.30530349858615E-06 | 1.36345743091012E-07 | 2.25899161258767E-07 | 0.199561769238167      | 5.61482864939225E-07 | 3.699170559167 |
| 19                  |                                             | 0.000146348640365 | 1600.33755370618 | 3.19248049111343E-05 | 4.629005699837E-07   | 7.01117853509508E-07 | 0.199429013452512      | 1.79860161385135E-06 | 0.000181989    |
| 20                  |                                             | 0.000216038469111 | 1602.46736366975 | 0.000120451988454    | 1.61889689331524E-06 | 1.86447939503082E-06 | 0.19900586219956       | 5.03911554523351E-06 | 0.000612803    |
| 21                  |                                             | 0.000221061816796 | 1602.76466846078 | 0.000132508650667    | 1.77634274982721E-06 | 1.9983657764341E-06  | 0.19899327570414       | 5.43436615186445E-06 | 0.000665498    |
| 22                  |                                             | 0.000226085164481 | 1603.09230462217 | 0.000145802088       |                      |                      | 4.2053470292           | 5.8640070803468E-06  | 0.000722565    |
| 23                  |                                             | 0.000231108512167 | 1603.45340239398 | 0.000160470502       |                      |                      | 8.6543205927           | 6.33188964473999E-06 | 0.000784428    |
| 24                  |                                             | 0.00023611859852  | 1603.85148400041 | 0.00017670192        |                      |                      | 8.6320993333           | 6.84244950496438E-06 | 0.000851549    |
| 25                  |                                             | 0.000241155207537 | 1604.2905224507  | 0.000194578573913    | 2.5932541849898E-06  | 2.65879882920203E-06 | 0.198769073821137      | 7.40082195152081E-06 | 0.000924447    |
| 26                  |                                             | 0.000246178555223 | 1604.77501967164 | 0.000214397839654    | 2.85663040581599E-06 | 2.85800093725240E-06 | 0.19868975780596       | 8.01298303004693E-06 | 0.001003728    |
| 27                  |                                             | 0.000251201902908 | 1605.310107355   | 0.000236359420884    | 3.15022793143121E-06 | 3.07886966445343E-06 | 0.198612250914261      | 8.6859307878707E-06  | 0.001090062    |

(a) Reference result part

|     |                                 |                   |                  |                   |                   |                   |                |                   |             |
|-----|---------------------------------|-------------------|------------------|-------------------|-------------------|-------------------|----------------|-------------------|-------------|
| 278 | 0.00160395913716                | 2645.49070935     |                  |                   |                   |                   |                |                   |             |
| 279 | 0.0016736489659                 | 2645.03568340817  |                  |                   |                   |                   |                |                   |             |
| 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:          | CH4 error: 0.0%   | CO error: 0.0%   | CO2 error: 0.0%   |                   |                   |                |                   |             |
| 286 | Ignition delay time(s):         | 0.000391788934086 |                  |                   |                   |                   |                |                   |             |
| 287 | Time(s)                         |                   |                  |                   |                   |                   |                |                   |             |
| 288 |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 289 |                                 | 6.9689828745E-06  | 1599.98436198629 | 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 | 2.25899377954E-07 | 0.199561960593 | 5.6148340333E-07  | 3.69917410  |
| 291 |                                 | 0.000146348640365 | 1600.33755370618 | 3.19252398884E-05 | 4.62906874045E-07 | 7.0112740628E-07  | 0.199431730684 | 1.7986261199E-06  | 0.000181987 |
| 550 | 0.00160395913716                | 2645.49070935     |                  |                   |                   |                   |                |                   |             |
| 551 | 0.0016736489659                 | 2645.03568340817  |                  |                   |                   |                   |                |                   |             |
| 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:          | CH4 error: 1.9%   | CO error: 5.9%   | CO2 error: 1.0%   |                   |                   |                |                   |             |
| 558 | Ignition delay time(s):         | 0.00038135459774  |                  |                   |                   |                   |                |                   |             |
| 559 | Time(s)                         |                   |                  |                   |                   |                   |                |                   |             |
| 560 |                                 |                   |                  |                   |                   |                   |                |                   |             |
| 561 |                                 | 6.9689828745E-06  | 1599.98243246138 | 4.46579238965E-07 | 3.9653371031E-08  | 5.14467813391E-08 | 0.199599356112 | 5.8113349674E-08  | 6.482192753 |
| 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  | 0.000172483 |

(b) Reduction/optimization results part

Figure 2: Results file main sections composition

## 3 Data importation

### 3.1 Start from a previously reduced kinetic mechanism

It is possible to continue a reduction/optimization process previously started while keeping the initial data (i.e. i.e. simulation reference results and reaction rate constants) of the detailed baseline mechanism. To do this, you must import the reference mechanism and specify the reduced mechanism from which you wish to start.

Procedure for specifying the reduced mechanism:

- from the GUI: click on the **Reduced mechanism** button on **Main parameter** tab.
- in an input file: in the **Main parameters** section, use the keyword **mech\_prev\_red**, e.g.:  
`mech_prev_red = red_mech.cti`

### 3.2 Import results file

In section 2.1, the reference results are calculated at the beginning of the reduction process from the detailed mechanism. It is also possible to conduct the reduction/optimization process from imported reference

| column | reactor_HP        | reactor_UV | JSR      | free_flame      | burner_flame   | diff_flame         | pp_flame |
|--------|-------------------|------------|----------|-----------------|----------------|--------------------|----------|
| 1      | config            |            |          |                 |                |                    |          |
| 2      | fuel (*)          |            |          |                 |                |                    |          |
| 3      | oxidant (*)       |            |          |                 |                |                    |          |
| 4      | diluent (*)       |            |          |                 |                |                    |          |
| 5      | phi (*)           |            |          |                 |                |                    |          |
| 6      | diluent_ratio (*) |            |          |                 |                |                    |          |
| 7      | mixt (*)          |            |          |                 |                |                    |          |
| 8      | P (Pa)            |            |          |                 |                |                    |          |
| 9      | Ti (K)            |            | time (s) | Ti (K)          |                | fuel2 (*)          |          |
| 10     |                   |            | rtol_ts  |                 |                | oxidant2 (*)       |          |
| 11     |                   |            | atol_ts  |                 |                | diluent2 (*)       |          |
| 12     | ig_time (s)       |            |          | rtol_ss         |                | phi2 (*)           |          |
| 13     |                   |            |          | atol_ss         |                | diluent_ratio2 (*) |          |
| 14     |                   |            |          | transport_model |                | mixt2              |          |
| 15     |                   |            |          | Sl (m/s)        | mdot (kg/m2/s) | mdot2              |          |
| 16     |                   |            |          |                 |                | Ti (K)             |          |
| 17     |                   |            |          |                 |                | rtol_ts            |          |
| 18     |                   |            |          |                 |                | atol_ts            |          |
| 19     |                   |            |          |                 |                | rtol_ss            |          |
| 20     |                   |            |          |                 |                | atol_ss            |          |
| 21     |                   |            |          |                 |                | transport_model    |          |
| 22     |                   |            |          |                 |                | K_max(1/s)         |          |

Table 2: Simulation condition information layout in the imported result files

data. It allows, for instance, to use data simulated by another kinetic mechanisms than the one to be reduced/optimized as references, or also to define experimental data as references.

The input file for external results has to be filled in the same way than the output file provided by Brookesia (see figure 2). Thus, the easiest way to fill a new input result file is probably to start from a former output result file. If the value of a target for optimization or reduction is not provided in the input file, it is simply skipped for the evaluation of the simulation quality. For instance, it is possible to include in the experimental data panel experiments containing only ignition delay times while the optimization targets include ignition delay time as well as the evolution of CH<sub>4</sub>, CO, and NO species. In the same way, flame structure experimental measurements containing only the profile of NO can be included even if the targets are CH<sub>4</sub>, CH, and NO.

Results input files must be csv semicolon-separated file. Comments must be preceded by the hash symbol (#). The key-word "*Case*" is used to separate the different input conditions. This line is followed by the conditions specification, constituted, themselves in two lines. The first is a headline and the second contains the condition information. The column order must respect the arrangement presented in Table 2.

Important: when reference data are imported, the simulation conditions are only defined by those provided in the data file. In GUI, the **Conditions** tab is removed.

Procedure for importing a results file:

- from the GUI: after defining the reference kinetic mechanism, click on the button **import external results**. Then, a window will appear to specify the units of the data (molar concentrations / molar fractions).
- in an input file: in the **Main parameters** section, use the keyword `ext_results_file`, e.g.:  
`ext_results_file = red_mech.cti`  
then specify the nature of the imported data with the keywords `conc_units`, e.g.:

conc\_units = Molar\_fraction

## 4 First examples

Five input files are provided for a gentle start with Brookesia software. Input conditions are summarized in Table 3.

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.

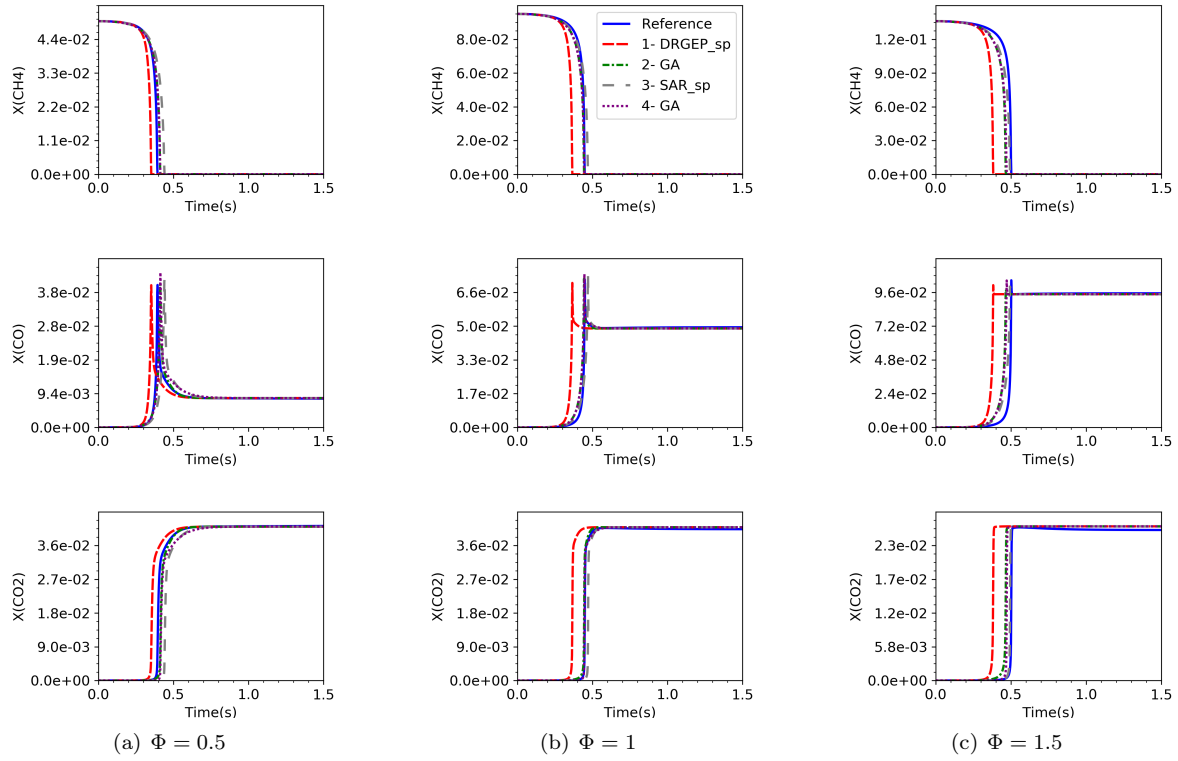


Figure 3: Simulation results obtained during the reduction process defined in the example `1_reactor.inp`

|                          |                                                                              |                                                                                     |                                                                             |                                                                          |                                                                                 |                                                                                          |
|--------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-----------------------------------------------------------------------------|--------------------------------------------------------------------------|---------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Input file name          | 1_reactor.inp                                                                | 2_JSR.inp                                                                           | 3_Free_Flame.inp                                                            | 4_diff.inp                                                               | 5_pp.inp                                                                        | 6_import_Sl                                                                              |
| kinetic mechanism        | C1_GRI30                                                                     | C1_GRI30                                                                            | C1_GRI30                                                                    | C0_H2_Law                                                                | C1_GRI30                                                                        | C3_Gong_red_a                                                                            |
| Species (reaction)       | 53 (325)                                                                     | 53 (325)                                                                            | 53 (325)                                                                    | 11 (32)                                                                  | 53 (325)                                                                        | 28 (118)                                                                                 |
|                          | Reactor (U,V)                                                                | JSR                                                                                 | Free flame                                                                  | Diffusion flame                                                          | Partially-premixed flame                                                        | Free flame                                                                               |
| conditions               | CH <sub>4</sub> /air<br>$\Phi=0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 1600$ K  | CH <sub>4</sub> /air<br>$\Phi = 0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 600 - 1200$ K | H <sub>2</sub> /air<br>$\Phi = 0.5, 1, 1.5$<br>$p = 10^5$ Pa<br>$T = 300$ K | CH <sub>4</sub> /air<br>$p = 10^5$ Pa<br>$T = 300$ K                     | CH <sub>4</sub> /air<br>$\Phi = 1/0.5, 1.5/0.5$<br>$p = 10^5$ Pa<br>$T = 300$ K | C <sub>2</sub> H <sub>6</sub> /air<br>$\Phi = 0.6 - 1.8$<br>$p = 10^5$ Pa<br>$T = 300$ K |
| Target(error)            | CH <sub>4</sub> (30)<br>CO(30)<br>CO <sub>4</sub> (30)<br>$T(30)$<br>Igt(30) | CH <sub>4</sub> (30)<br>OH(30)<br>CO <sub>2</sub> (30)<br>$T(30)$                   | CH <sub>4</sub> (30)<br>CO(30)<br>CO <sub>2</sub> (30)<br>$T(30)$<br>Sl(30) | H <sub>2</sub> (30)<br>H <sub>2</sub> O(30)<br>H(30)<br>$T(30)$<br>K(30) | CH <sub>4</sub> (30)<br>CO(30)<br>CO <sub>2</sub> (30)<br>$T(30)$               | Sl                                                                                       |
| Error method             | points                                                                       | points                                                                              | QoI                                                                         | QoI                                                                      | points                                                                          | points                                                                                   |
| Reduction method         | DRGEP_sp + GA<br>SAR_sp + GA                                                 | DRGEP_sp<br>DRG_r + GA                                                              | DRGEP_sp<br>SARGEP_sp + GA                                                  | DRGEP_sp<br>DRG_r + GA                                                   | DRG_sp<br>SAR_r + GA                                                            | GA                                                                                       |
| Final Species (reaction) | 15 (57)                                                                      | 23 (114)                                                                            | 20 (100)                                                                    | 8 (11)                                                                   | 26 (87)                                                                         | 28 (118)                                                                                 |
| Computation time         | 7 min                                                                        | 5 min                                                                               | 2 h 08 min                                                                  | 35 min                                                                   | 40 min                                                                          | 23 min                                                                                   |

Table 3: 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

## 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                                                                             |
| mech_prev_red     | starting reduced mechanism name                                                                      |
| ext_results_file  | name of the external file containing reference conditions and corresponding results                  |
| conc_units        | concentration unit of the imported external data (Molar_fraction/mol_m3)                             |
| show_plots        | for Spyder essentially, select to display or not the simulation results during the reduction process |
| verbose           | rules the amount of information displayed during the reduction process (range between 0 and 10)      |
| tspc              | name of target species                                                                               |
| ig_check          | add (True) or not (False) the ignition delay time as target                                          |
| K_check           | add (True) or not (False) the extinction stretch rate as target                                      |
| Sl_check          | add (True) or not (False) the flame speed as target                                                  |
| T_check           | add (True) or not (False) the temperature as target                                                  |
| sp_ig             | ignition delay time associated species to manage reduction with reduction methods                    |
| sp_K              | extinction stretch rate associated species to manage reduction with reductions methods               |
| sp_Sl             | flame speed associated species to manage reduction with DRG methods                                  |
| sp_T              | temperature associated species to manage reduction with DRG 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) |

### Configuration keywords

|                 |                                                                                                                                          |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------|
| 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)                                                                        |
| 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, SARGEP_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 transcribed 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)                                                                                                                                                        |
| ttol_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                                                                                                                                             |