CERFACS

Procedure to register developed mechanisms at CERFACS.

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Abstract

The aim of this document is to give people an overview on the strategy in terms of mechanism development as well as the exact procedure to make them usable for other people.

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1 CERFACS strategy

If a mechanism is referred to in an official document (a project report, a paper, a PhD thesis, internship report), it must be registered :

- if a mechanism has been used in Cantera and in AVBP, it must be registered on the chemistry website and in AVBP code at the same time. A mail should be sent both to wirtz@cerfacs.fr (for Cantera) and to vermorel@cerfacs.fr (for AVBP).
- for some particular cases, if a mechanism is only used in Cantera, it is sufficient to register it on the chemistry website. A mail should be sent to wirtz@cerfacs.fr only.

2 Mechanism naming

Your mechanisms should be named in a proper manner before being integrated in Cantera and in AVBP. It is specified in the following page : https://chemistry.cerfacs.fr/en/avbp/arc-in-avbp/.

3 Procedure to register mechanisms for Cantera

Before starting, you need to have the following files, depending on your mechanism :

Mechanism type	File needed
Detailed	.cti
Skeletal	.cti
ARC	.cti of the associated skeletal, .cti of the ARC and cantera .f90 of the ARC

You will also need a **small paragraph** describing the following for the chemistry website :

- **the person(s) who derived it. (@authors)**
- a **reference of a paper or a website** if there is any of it.
- if the mechanism should be **public** (everybody can access it) or **private** (it is protected by passwords)
- **reduction conditions** in terms of **cases** (auto-ignition, laminar flame speed, counterflow diffusion flame, etc ...), of **fuel** (hydrogen, methane, both, etc ...) , **oxidizer** (pure oxygen, air, etc ...) and **operating conditions** (high pressure, specific temperature, etc ...) (@configuration).
- from **which detailed mechanism** (and skeletal mechanism if necessary) it comes from (@detailed mechanism).
- an **example of validation** that is done from this scheme (*.zip* or *.png*).
- more if you have anything else to say.

  Here is an example :

```
This mechanism has been derived by Antoine Pestre at CERFACS.
This mechanism is for public use.
It is derived from the detailed Polimi scheme C1C3_NOx_180501 using ARCANE.
Skeletal mechanism associated can be found here.
This mechanism can be used for the CH4 and H2 combustion in air at
atmospheric conditions. High temperature auto-ignition mechanisms are also
included.
Validity has been evaluated for 1D premixed flames on the following range :
P = 0.3 bar - 5 bar, T = 233 K - 650 K, phi = 0.5 - 1.6.
Validity has been evaluated for 0D auto-ignition reactors on the following
range :
P = 0.3 bar - 1 bar, T = 2000K - 3000K, phi =1.
Validity has been evaluated for 1D flamelets the following range :
P = 1 bar, T = 300K, chist = 1e-3 s^-1 - 25 s^-1.
The ARC mechanism comprises  15 transported species, 9 QSS species, and
138 reactions.
```

For ARC mechanisms, do not forget to fill in the header as illustrated.

```
@details Generated by ARCANE custom kinetics routine to compute the chemical source
terms.
@authors Antoine Pestre
@date 15/12/2020
@cantera version 2.3
@detailed mechanism Polimi scheme C1C3_NOx_180501
@configuration CH4/air and H2/air
1D premixed flame : P = 0.3 bar - 5 bar, T = 233 K - 650 K, phi = 0.5 - 1.6.
0D auto-ignition : P = 0.3 bar - 1 bar, T = 2000K - 3000K, phi =1.
1D flamelets : P = 1 bar, T = 300K, chist = 1e-3 s^-1 - 25 s^-1.
```