INTRODUCTION

At CERFACS, with the help of the tool YARC from Prof. Pepiot (Pepiot, 2008), it is possible to develop Analytically Reduced Chemistries, or ARC. Such chemistries usually cannot be cast in a classical "reaction mechanism" format, due to the presence of Quasi-Steady State (QSS) species. Thus, such chemistries come with a specific subroutine for the computation of species source terms. The official chemistry tool Cantera was not designed to be able to deal with these chemistry descriptions. In order to test ARC ability on a variety of canonical test cases, the CERFACS version of Cantera has been adapted to overwrite the classical evaluation of species source terms. For more information about ARC and reduced chemistries, the reader is referred, e.g., to publications by Prof. P. Pepiot (Pepiot and Pitsch, 2008b,a) or Prof. T. Lu (Lu and Law, 2005, 2008a,b).

This short note will explain how to run a CERFACS-Cantera computation with an ARC **already implemented in the CERFACS-Cantera source code**, and provide a list of the various ARC currently implemented in the code. *The following discussion is only valid for the sources available on the CERFACS Gitlab NITROX !*

How can I perform a CERFACS-Cantera computation with a referenced ARC ?

It is believed that you are already a "confirmed" user, so you know at least how to launch simple 0D/1D simulations via a python script such as the one provided on the CERFACS-Cantera webpage. If it is not the case, maybe you should start with the basics: see the tutorials from the CERFACS-Cantera formation !

To perform a computation with an ARC mechanism **already implemented in the CERFACS-Cantera source code**, follow these few steps:

1. **The ARC mechanism file**: Start with the mechanism file in a Cantera format (.xml or .cti extensions). Since we are dealing with mechanisms already "hard-coded", the chemistry you seek should be referenced on the Cantera website. When this is the case, it will appear in bold in Table 1. However, as will be seen in the following section, some ARC already available in the CERFACS-Cantera code that are not referenced on the website as of yet ! This is not a problem: **all available mechanisms referenced in Table 1 are present in the database that comes along with the sources** (see `data/inputs` directory).

   Note that, in any case, ARC mechanism files are obtained from the associated skeletal/detailed mechanism: simply remove all reactions except a dummy one -for example: `reaction('2 O <=> O2', [0.000000e+00, 0.0, 0.0])`, and keep only the transported species in the list featured in the gas definition. Click to see an example. **The species should appear in the SAME order than that in your subroutine !!**

2. If it is not already present, add the proper (see Table 1) "kinetic" keyword in the gas definition of your mechanism file. You can add it in between the "reaction" and "transport" keyword, for instance. Click to see an example, of an .xml ARC mechanism file (the kinetic flag in this case is `ch4_nox_22_320_18_tj`).

3. Use your usual python script ! Note that you might also need simplified transport related files adapted to your ARC. If not available on the Cantera website, you might need to generate them ! The new CERFACS-Cantera code accepts "mixture_database.dat" AVBP format. See the associated short note.

List of available ARC in the CERFACS-Cantera

The discussion is summarized in Table 1.

Name	File name	"kinetic" keyword	Fuel/Air
LU13	LU13.cti	sankaran_13	CH_4/Air
CH4_NOX_22_320_18_TJ	CH4_NOX_22_320_18_TJ.xml	ch4_nox_22_320_18_tj	CH_4/Air
C2H4_18_320_11_AF	C2H4_18_320_11_AF.cti	c2h4_18_320_11_af	C_2H_4/Air
C3H8_22_173_12_FC	C3H8_22_173_12_FC.cti	c3h8_22_173_12_fc	C_3H_8/Air
C7H16_25_210_27_FC	C7H16_25_210_27_FC.cti	c7h16_25_210_27_fc	C_7H_{16}/Air
C12H26_NOX_27_452_20_TJ	C12H26_NOX_27_452_20_TJ.xml	c12h26_nox_27_452_20_tj	$C_{12}H_{26}$/Air
NC12H26_25_373_27_TJ	NC12H26_25_373_27_TJ.xml	c12h26_25_373_27_tj	$C_{12}H_{26}$/Air
HYCHEM_NOX_29_548_17_AF	HYCHEM_NOX_29_548_17_AF.cti	hychemnox_29_548_17_af	Jet A
HYCHEM_27_272_12_AF	HYCHEM_27_272_12_AF.cti	hychem_27_272_12_af	Jet A

Table 1: ARC available in the CERFACS-Cantera. Those in bold are available on the Cantera website.

REFERENCES

Lu, T., and C. K. Law, 2005, A directed relation graph method for mechanism reduction: Proceedings of the Combustion Institute, **30**, 1333–1341.

———, 2008a, A criterion based on computational singular perturbation for the identification of quasi steady state species: A reduced mechanism for methane oxidation with no chemistry: Combustion and Flame, **154**, 761–774.

———, 2008b, Strategies for mechanism reduction for large hydrocarbons: n-heptane: Combustion and flame, **154**, 153–163.

Pepiot, P., 2008, Automatic strategies to model transportation fuel surrogates: Phd thesis, Stanford University.

Pepiot, P., and H. Pitsch, 2008a, A chemical lumping method for the reduction of large chemical kinetic mechanisms: Combustion Theory and Modelling, **12:6**, 1089 – 1108.

———, 2008b, An efficient error propagation based reduction method for large chemical kinetic mechanisms: Combustion and Flame, **154**, 67–81.