INTRODUCTION

At CERFACS, kinetic mechanisms (ARC, global) are usually developed to be employed in the LES solver AVBP. In such an environment, the chemistry needs to be simplified for the simulations to be efficient. Detailed transport properties are very costly to obtain, and are therefore usually approximated. One common approximation consists in assuming constant (but non necessarily unity) Lewis and Prandtl numbers throughout the computation. The CERFACS version of Cantera has been adapted to do so. Interested readers are referred to the AVBP Handbook for further information regarding simplified transport properties.

This short note will explain how to run a CERFACS-Cantera computation with simplified transport properties. *The following discussion is only valid for the sources available on the CERFACS Gitlab NITROX !*

How can I perform a CERFACS-Cantera computation with "AVBP-like" transport properties ?

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 !

Follow these few steps:

1. **Get the mechanism file**: Start with a mechanism file in a Cantera format (.xml or .cti extensions). You can peruse the Cantera mechanism section to get one suited to your needs.

2. If it is not already done, **add the proper "transport" keyword** in the gas definition that you will employ:

   ```
   transport = 'AVBP'
   ```

   You should also verify that the transport is not directly set in your python script !

3. **Get the transport data file(s)**. In the new CERFACS-Cantera 2.3, it is now possible to directly use AVBP's mixture_database.dat file. This file is available via the AVBP source code. To use it in your Cantera simulation, simply place it in your working directory.

   Note: Although not recommended, "old" users familiar with the AVBP V6X input_thermo.dat *and* input_premix.dat *can still use them as in previous CERFACS-Cantera releases !*

4. Make sure that the species order you use in your Cantera mechanism file (.cti/.xml) is the same as that provided in the AVBP transport file(s).

5. **Make sure that the name of your gas instance in the Cantera mechanism (.cti/.xml) file matches that provided in the mixture_database.dat.** Usually,

the gas instance in cantera is labelled 'gas', but sometimes several instances are present so be careful.

For example, say you want to run a simulation with the classical 2 step BFER mechanism. Based on the species order, you would need to use the gas instance currently labeled "CH4_BFER_avbp7" in accordance with the mixture_database.dat entry "CH4-AIR-2S-BFER_FLAMMABLE": so you would need to change the gas instance name from "CH4_BFER_avbp7" to "CH4-AIR-2S-BFER_FLAMMABLE" in the 2S_CH4_BFER.cti.

6. Use your usual python script ! Note that you should also verify that the transport is not set directly in your python scripts...