User's Manual for Chemkin, Cantera, & Open-source Chemical Reaction Kinetics Solvers

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1 Introduction

A framework for an open-source chemical reaction kinetics solver is developed from the governing equations of thermodynamics. Later, the framework is translated into a computer code written in MATrix LABoratory. Furthermore, parser programs are written to call Chemkin and Cantera functions to solve reaction kinetics and provide a comparison with the open-source solver. This user's manual aims to provide basic information on the files included in the folders as well as sub-folders. The user is encouraged to tally the file list provided here with the files present in the folder, before running any MATLAB scripts. Besides, new users may find some of the terms used in this manual to be unfamiliar or confusing. We have tried to limit the use of such terms and concepts, but some are simply unavoidable. The user is, thus, encouraged to read the following paper (provide reference to the ASME IMECE paper) in order to develop a complete understanding of this effort.

2 Folders and File Description

The main folder consists of three sub-folders, one each for open-source, Chemkin, and Cantera based solvers. The user is advised to install the necessary software, i.e., MATLAB in order to view/execute/edit the files. While Chemkin functions can be called from a MATLAB script using the provided MEX (parser) file, Cantera[1] requires installation on the machine prior to function calls from MATLAB.

[1] More information on Cantera and installation instructions are provided here.

The following folders exist under the main directory:

- Cantera
- Chemkin
- Open-source

All folders consist of some common files or sub-folders in order to provide a standalone environment for execution in MATLAB. The common sub-folder, "Species", consists of text files containing thermo-fits for each species considered in the study. The files common to the three solvers are:

- *importonce.m*: Imports data from the reaction-input file and prepares the pre-requisites for the solver (driver + Ordinary Differential Equation function file).
- *stoichiometricmatrix.m*: Imports the species coefficients from the reaction data and prepares the corresponding matrices for later use.
- *thermdatextractor2.m*: Extracts data from the accompanying files consisting of the thermo-fit data for the species considered. See the "Species" folder to view the files.
- *thermofits3.m*: Calculates the thermodynamic data for each species using the NASA Polynomials.
- *troeform.m*: Calculates the TROE parameters for the high-pressure fall-off reactions.
- *reactions data new.xlsx*: An Microsoft® Office Excel file that consists of reaction kinetics data, customized for easy import using the in-house written *importonce.m* file.

In addition to the common files mentioned above, several other files are required for seamless execution in MATLAB.

2.1 Cantera

The Cantera sub-folder consists of the following files (other than the common files):

- *alldata.mat*: A .mat file that is prepared by the *importonce.m* and *stoichiometricmatrix.m* files and consists of the necessary inputs to the main driver file as well as the ODE function file.
- *allreaxcantera01molef.m*: This is the main driver file that consists of user input such as initial pressure, temperature, and mole fractions along with the Cantera function calls, ode solver and other relevant inputs.

- *allreaxcanode01.m*: This is the function file that consists of all the relevant ODEs.
- *h2o2_saud_all.cti*: This file consists of the relevant H_2-O_2 reaction kinetics data that is called by Cantera through the MATLAB script. It can be edited using an advanced text-file editor, such as, Notepad++.

2.2 Chemkin

The Chemkin subfolder consists of the following files (other than the common files):

- *alldata.mat*: Similar to Cantera. See 2.1.
- *allreax01cksimple.m*: This is the main driver file that consists of the necessary inputs and calls the ODE function file.
- *allreaxodev01cksimple.m*: The ODE function file. For more details, see 2.1.
- *chemkinmainfunction.m*: This function calls the Chemkin solver via the MEX file and returns the production/destruction rates of species, to be used later in the main MATLAB-based solver.
- MEX-related files:
  - *depkin.dll*
  - *depkin.lib*
  - *inputMueller.txt*
  - *mexdepkin.c*
  - *mexdepkin.h*
  - *mexdepkin.mexw64*
  - *Mueller1999.asc*
  - *Mueller1999.dat*
  - *Mueller1999.xlsx*
  - *Mueller1999_tran.asc*

2.3 Open-source

This sub-folder consists of the following files (other than the common files):

- *allreax01.m*: The main driver file similar to Cantera and Chemkin driver files.
- *allreaxodev01.m*: The ODE function file similar to Cantera and Chemkin ODE function files.