Numerical Implementation of Reaction Diffusion Manifolds - REDIM

F. C. Minuzzi

August 9, 2017

Abstract

This is an report for the basic aspects of how to develop a REDIM table based on flamelets as initial conditions, and does not intend to give a theoretical description of the method. The fuel to be considered is ethanol, and two parameters will be used for parametrizing the manifold. [1]

In order to obtain the slow manifold that will represent the state of the system, one has to integrate the REDIM equation given by

$$\begin{cases} \dfrac{\boldsymbol{\Psi}(\boldsymbol{\theta})}{\partial t} = \left(I - \boldsymbol{\Psi}_{\boldsymbol{\theta}}\boldsymbol{\Psi}_{\boldsymbol{\theta}}^{+}\right)\left[\mathbf{F}(\boldsymbol{\Psi}) - \dfrac{1}{\rho}\left(\mathbf{D}\boldsymbol{\Psi}_{\boldsymbol{\theta}\boldsymbol{\theta}}\mathbf{grad}(\boldsymbol{\theta}) \circ \mathbf{grad}(\boldsymbol{\theta})\right)\right] \\ \boldsymbol{\Psi}^{o} = \boldsymbol{\Psi}_{\text{in}}(\theta) \end{cases} \tag{1}$$

where θ is the vector which parametrizes the manifold.

The path to successfully develop a REDIM table for simulation starts with the generation of the initial guess $\boldsymbol{\Psi}_{\text{in}}(\theta)$ for the integration of the REDIM equation. For that, the free software INSFLA will be used, but there is no prohibition to use any other 1D code.

INSFLA can be used either by the GUI or compilation through the terminal in UNIX systems. As the initial guess used in this report is based on flamelets simulations, several counterflow solutions are performed with INSFLA. The inputs files for the program are 4: INP, which has the basics definitions for the simulations, such as boundary conditions and solver conditions: MEC, which has the kinetic mechanism in the INSFLA format; MOLNEW with the transport properties and THERMO with the thermodynamic data.

It is possible to convert the CHEMKIN basic format of kinetic mechanism to the INSFLA format, with the program MecConv. The code is very easy to handle and just need the input `inp.mech`. This file has the elements, species, thermodynamics data and the reaction mechanism, in this order. After running the code, the mechanism in INSFLA format, as the THERMO file will be displayed, and other files. The transport properties for the MOLNEW file is equal to CHEMKIN format.

With that files, one can write the INP file, which is the input file for INSFLA generate the files needed for integration. In the GUI, one can only change the input parameters, and for whom compile direct from the source, INP can be manipulated freely. Fig. 1 shows a INP example for counterflow flame of ethanol. In this file, the block options is reserved for the properties of the calculation. The meanings of each input can be found in the INSFLA guide.

[1] This report was developed by the author at KIT - Karlsruhe Institute of Technology, under the supervision of Prof. Ulrich Maas, in the Summer/2017.

```
OPTIONS
REGRID  2/PCON     /IMPULS -2/STORE   1/EXTRA   2/J_OUT   1/PROFIL
W_IN    1/W_OUT   1/T_IN    1/T_OUT   1/V_IN    1/FUSO    4/Tecplo
OUTPUT  3/TSO      /InnerB   /Plot    2/
END
GAS PHASE SPECIES
H2      ,H       ,CH4     ,CH3     ,CH2     ,CH      ,CH2O    *
HCO     ,CO2     *CO      ,O2      ,O       ,OH      ,HO2     *
H2O2    ,H2O     ,C2H     ,HCCO    ,C2H2    ,C2H3    ,C2H4    ,
C2H5    ,C2H6    ,CH2OH   ,CH3O    ,HCCOH   ,H2CCCH  ,C3H2    ,
CH2(S)  ,CH2CO   ,C2O     ,HCOH    ,CH3OH   ,CH2HCO  ,C3H6    ,
AC3H5   ,PC3H5   ,SC3H5   ,CH2CHCHO,PC3H4   ,AC3H4   ,CH3CO   ,
CH2CHCO ,CH3CHCO ,CH3HCO  ,CHOCHO  ,IC3H7   ,NC3H7   ,C2H5OH  ,
C2H4OH  ,CH3CHOH ,CH3CH2O ,Set_0001,HCOOH   ,C3H8    ,HOC2H4O2,
N2      ,        ,        ,        ,        ,        ,
END
Left boundary
P       :    1.0E00
T       :  298.0E00
v       :       1.9
C2H5OH  :      1.00
O2      :      0.00
N2      :      0.00
CO2     :       0.0
H2O     :       0.0
END
Right boundary
P       :    1.0E00
T       :  298.0E00
PHI     :  -4.8E+05
O2      :     21.00
N2      :     79.00
C2H5OH  :      0.00
CO2     :      0.00
H2O     :       0.0
END
Conditions
WFT =       1.0
WFP =       1.0
WFU =       1.0
WFR =       1.0
AMPL=    1700.0
RMAX=    0.5E-1
SIGM=   2.5E-02
TE  =  1.00E+02
NT  =   20.0E00
NMAX=    1.0E00
NG  =   70.0E00
RI  =    0.0E00
RO  =   0.05E00
GE  =     0.0E0
RTOL=   1.0E-03
ATOL=   1.0E-08
STEP=   1.0E-08
RS  =   1.0E-09
END
```

Figure 1: Example of INP file.

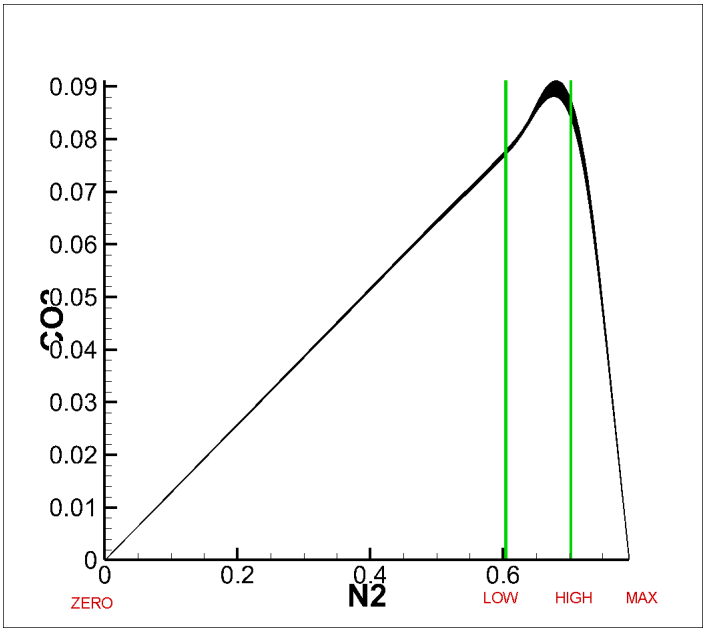

Figure 2: Example where the points in the PREPREDIM are used.

The ideia for generating the flamelets is to solve several counterflows flames until it reaches the extinction, either varying the PHI (i.e., the pressure gradient), keeping all other parameters the same, or varying both inlets velocities. In order to capture the ignition, one has to solve a counterflow flame for a very low time step in order to make the flame burn. This can be done either by setting a very high temperature in one stream and a very low temperature (usually 298K), and using this as initial profile for a new simulation with 298K on both sides. Other way of doing that, only for the ones who compile from the source, is manipulating the `fort.3` file obtained by a cold mixture simulation. After having the first ignited flame, one can easily change the parameters to generate the next ones, until reaches the extinction point.

After generating the flamelets solution, it is necessary to generate a mesh of the initial condition (this mesh is generated only for the parameters that will be used to parametrize the manifold). For this, the program PREPREDIM can be used.

The PREPREDIM uses as input the flamelets generated by the INSFLA calculations. All considered solutions (which generally are in the `file.29`) should be putted together in a file. The head of the `fort.3` should be in the head of this file also. The `Inp-PREPREDIM` file has the parameters for generating the mesh. The space of flamelets solutions are divided in three sections. The values **zero, low, high** and **max** defines the points in the $x-$direction where the mesh starts and finishes (zero and max, respectively) and the region where a refining of the mesh should be performed (between low and high). It should be pointed out that if zero is set to 0, an error will occur in the REDIM integration, so if one wants to starts the mesh in 0, a value such as 0.001 should be defined.

The values **nlow, nstoi** and **nhig** defines the number of points between each zone in the space of flamelets solutions. The **number of entries** defines how many variables will be used in the parameter (e.g. 1 if is only one species, or 2 if its a sum of species) and the **position and value** is the position where the parameter is in the species block of the `fort.3` file. Running PREPREDIM will give the Out-PREPREDIM file, which will be used as initial condition in the next step, the REDIM integration. Figure 3 shows the head of the input of

PREPREDIM.

```
-----------------------------------------------------------------------
- Range and number of points for first variable direction
- Domain can be decomposed in up to three subdomains (zones)
- lgeor = T : xnew as geometric row in first zone
- lgeol = T : xnew as geometric row in third zone
- distmr : max allowed distance in first zone
- distml : max allowed distance in third zone
-----------------------------------------------------------------------
0.001  23.5000  25.800  27.381     zero,low,high,max
40  20  10             nlow, nstoi,nhig
 T 2.5                        lgeor,distr
 T 0.2                        lgeol,distl
-----------------------------------------------------------------------
- Number of points for second variable direction
-----------------------------------------------------------------------
55                  nsecond
-----------------------------------------------------------------------
- Parameter vector for first variable direction N2
-----------------------------------------------------------------------
  1              number of entries
  59 1.0          position and value
-----------------------------------------------------------------------
- Parameter vector for second variable direction CO2
-----------------------------------------------------------------------
  1              number of entries
  11 1.0          position and value
-----------------------------------------------------------------------
```

Figure 3: Head of the input of PREPREDIM.

```
**************************************************************************
OPTIONS
InMan   1/          /ILDM    1/Plot    1/Trans   4/Resf    2/          /
State   3/Output  1/ManPar    /TSO      /Theta    2/          /          /
END
**************************************************************************
Species
H2        H         CH4       CH3       CH2
CH        CH2O      HCO       CO2       CO
O2        O         OH        HO2       H2O2
H2O       C2H       HCCO      C2H2      C2H3
C2H4      C2H5      C2H6      CH2OH     CH3O
HCCOH     H2CCCH    C3H2      CH2(S)    CH2CO
C2O       HCOH      CH3OH     CH2HCO    C3H6
AC3H5     PC3H5     SC3H5     CH2CHCHO  PC3H4
AC3H4     CH3CO     CH2CHCO   CH3CHCO   CH3HCO
CHOCHO    IC3H7     NC3H7     C2H5OH    C2H4OH
CH3CHOH   CH3CH2O   Set_0001  HCOOH     C3H8
HOC2H4O2  N2
End
**************************************************************************
****   BLOCK FOR LOW-DIMENSIONAL MANIFOLD                              ****
**************************************************************************
Parametrization first cell
    + 1.0  *N2                                      -2.00E-01:-2.00E-01
    + 1.0  *CO2                                     -2.00E-01:-2.00E-01
End
**************************************************************************
```

Figure 4: `Inp-xxx-init` file.

In the REDIM integration, the folder **0-input** has the all the input files. Inside, the **0-mech** has the files for mechanism, thermodynamics and transport properties. Two files are important here: the `Inp-xxx-init` and `Inp-extra-init` (where xxx is a name given by the user for identification). In the `Inp-xxx-init`, the first block is the options for the HOMREA integration, while the second is the species (just as in the INP file

Figure 5: `Inp-extra-init` file.

of INSFLA). Below, the user has to define the parametrization variables for the REDIM. Figure 4 shows an example of the `Inp-xxx-init` file.

The `Inp-extra-init` has the values for the time step and number of iterations. The same parameters should be defined in the `Inp-extra-restart` and `Inp-xxx-restart` files. `Inp-extra-restart`, only one iteration and a very small time step shuld be choosen (e.g. 10^{-10}). Then, the `go` executables can be run, first the `init` (which is run only to define the state for the simulation) and then the `restart`, which will generate the REDIM table in the `Out-REDIM` file. Figure 5 shows the `Inp-extra-init` file.

One command usually used in Linux system is the `ulimit -s unlimited`, so the output files can have unlimited size (this can happens for very long tables with mechanisms with thousand of species). The `conv.dat` file has the total, the mean and the maximum errors in the integration. Usually, values below 10^1 for the mean error indicates a good converged result. One can also identified the number of iterations needed for convergence, which can be done using the time-scale analysis based on the eigenvalues of the Jacobian.