OppDif

Modeling opposed-flow diffusion flames

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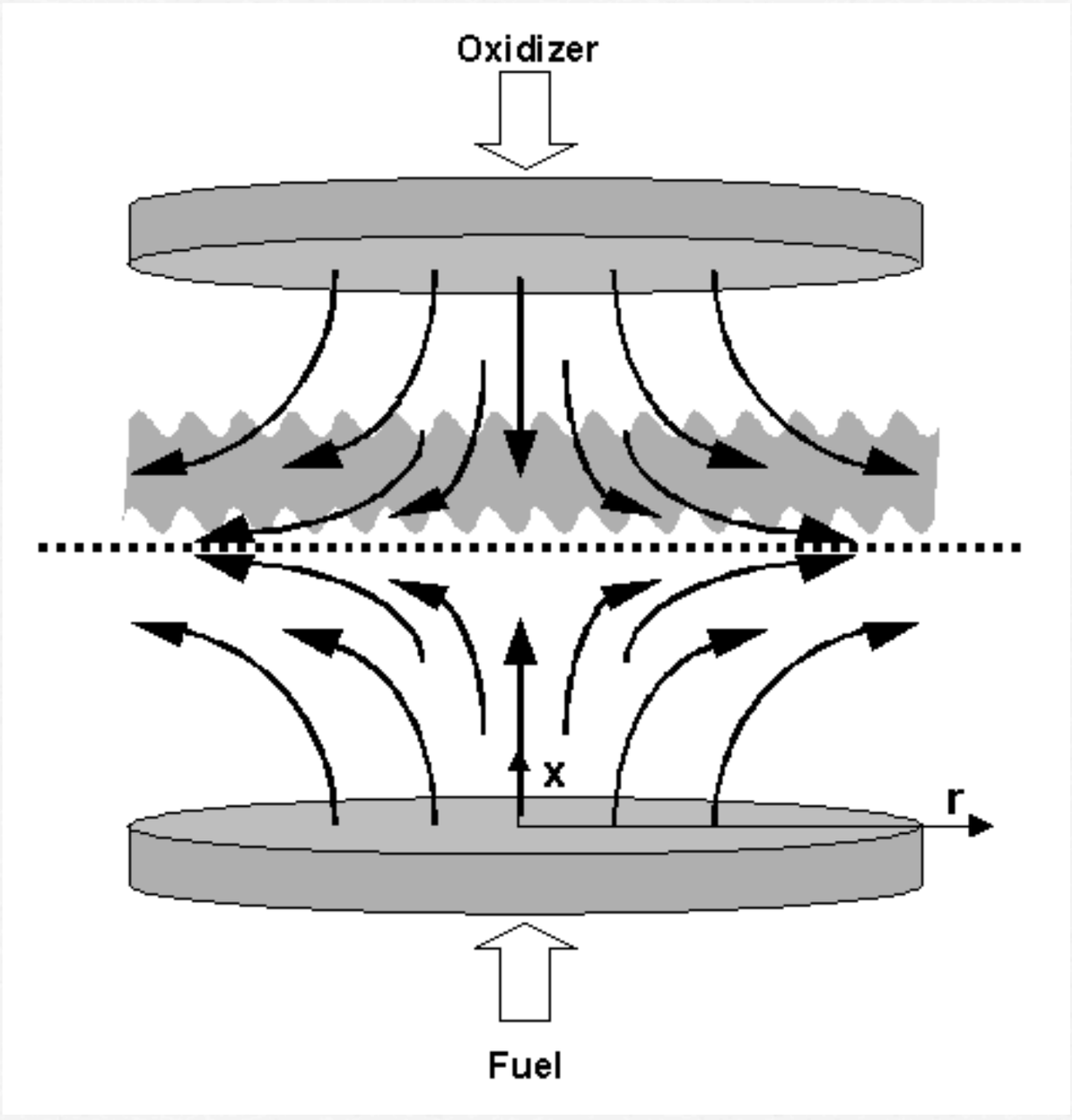
Introduction

OPPDIF computes the diffusion flame between two opposing nozzles. A similarity transformation reduces the flow field to a one-dimensional problem, either for an axisymmetric flow or for a 2-dimensional planar case. For the radially axisymmetric case, the similarity solution assumes that the radial component of velocity is linear in radius and the dependent variables become functions of the axial direction only. For the planar case, the velocity (perpendicular to the axis of the opposed flow) is linear with the distance in the direction, and again the dependent variables become functions of the axial direction only.

OPPDIF solves for the temperature, species mass fractions, axial and perpendicular velocity components, and perpendicular pressure gradient.

Introduction



The opposed-flow geometry makes an attractive experimental configuration, because the flames are flat, allowing for detailed study of the flame chemistry and structure. OPPDIF allows simulation of both premixed and non-premixed flames.

The axisymmetric geometry consists of two concentric, circular nozzles directed towards each other. This configuration produces an axisymmetric
flow field with a stagnation plane between the nozzles.

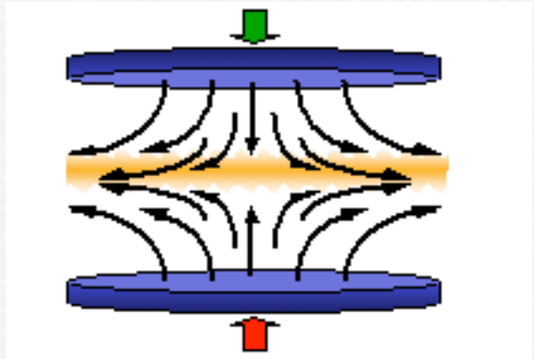
The location of the stagnation plane (line) on the momentum balance of the two streams. When the streams are premixed, two premixed flames exist, one on either side of the stagnation plane. When one stream contains fuel and the other oxidizer, a diffusion flame is established. Since most fuels require more air than fuel by mass, the diffusion flame usually sits on the oxidizer side of the stagnation plane; fuel diffuses through the stagnation plane to establish the flame in a stoichiometric mixture.

OppDif Application

Keyword Syntax and Rules

Rule	*Description*
1	The first character-string in the line must be a Keyword; the length of the character-string depends on Keyword descriptions.
2	Any further input associated with the Keyword can appear anywhere after the Keyword, through column 80. The specific starting column is not important, as long as there is at least one space after the Keyword.
3	When more than one piece of information is required, the order in which the information appears is important, and the pieces are delimited by one or more blank spaces.
4	Numbers may be stated in integer, floating-point, or "E" format. The application converts the numbers to the proper type, including conversion to double precision.
5	Species names must appear exactly as they are specified in the Gas-phase Kinetics Pre-processor input.
6	If more information is input than required, then the last read inputs are used. For example, if contradictory keywords are encountered, the last one read is taken.
7	A "comment" line is one that has either a period (.), slash (/), or exclamation mark (!) as the first non-blank character. In addition, on any Keyword line, any input that follows an exclamation mark is taken as a comment. All input lines, including comments, are printed to the output.
8	The keyword END must be the last line.

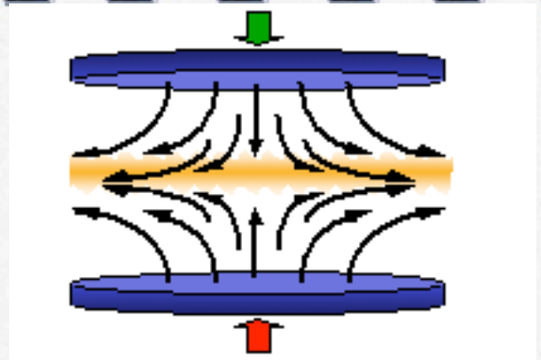
Input File: Keywords



Problem Type Keywords

Keyword	*Description*
AXIS	Radial axisymmetric coordinate system. **Default:** Coordinate system is radial axisymmetric.
PLAN	Planar coordinate system. **Default:** Coordinate system is radial axisymmetric.
TGIV	Energy equation is not included. User specifies a temperature profile using the `TEMP` keyword. **Default:** None. Either TGIV or ENRG is required.
ENRG	Energy equation is included. A temperature profile specified by the `TEMP` keyword will be used as an initial guess in this case. **Default:** None. Either TGIV or ENRG is required.
NOFT	Skip the fixed temperature problem and include the energy equation on the first attempt. **Default:** Fixed temperature solution is obtained before adding the energy equation.
LINE	Linear profile used to set up initial solution estimates. **Default:** PLAT
PLAT	Plateau profile used to set up initial solution estimates. **Default:** PLAT
QFUN	Enable the user-defined heat-loss function; a sample of `FUNCTION OPQFUN` can be found in the file *oppdif_user_functions.f* and described in *Equation 2.2*. **Units:** $cal/sec/cm^2$ **Default:** none, optional input.
TINF	Ambient temperature needed in user routine `FUNCTION OPQFUN`. The sample `OPQFUN` computes the gas radiation to/from the surroundings of temperature `TINF` based on the optically-thin limit model. The emissivity of the gas mixture is computed based on an empirical formula. **Units:** K **Default:** none, optional input.
END	This keyword must appear on the last line of the input data.

Input File: Keywords



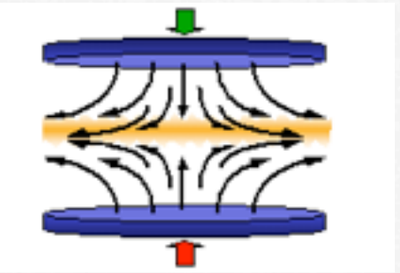
Grid Parameter Keywords

NPTS	The number of initial mesh points. The inclusion of NPTS will generate an equally spaced mesh of NPTS points between 0 and XEND. The user can also specify an initial nonuniform mesh using the keyword GRID, in which case the NPTS input is not needed. **Example:** NPTS 11 **Default:** 6; unless GRID keywords are included.
GRID	The use of this keyword allows the user to input an initial grid. Up to NMAX of these GRID inputs can be included. Each GRID line contains the coordinate of a mesh point. The GRID keywords are a grouped list and the grid coordinates must appear in ascending order. The use of this keyword is optional. If no GRID keywords are included, the grid will have equally spaced grid points based on NPTS. **Example:** GRID 0.0 **Units:** cm **Default:** none; NPTS=6 assumed if no GRID keywords are included.
GRAD	Parameter that controls the degree of mesh adaptation based on the maximum first derivative, or gradient in the solution. **Example:** GRAD 0.5 **Default:** 0.1
CURV	Parameter that controls the degree of mesh adaptation based on the second gradient, or curvature, in the solution. **Example:** CURV 0.7 **Default:** 0.5

NTOT	Maximum number of grid points allowed for this job. **Example:** NTOT 200 **Default:** NTOT= maximum grid dimension set by OPPDIF driver program **Restart:** cannot be changed on restart.
NADP	Number of mesh points that TWOPNT can add during each grid refinement. **Example:** NADP 2 **Restart:** cannot be changed on restart.
XEND	Physical length of the computational domain, or value of x at the end of the domain. Note that the fuel inlet is assumed to be located at $x = 0$. **Example:** XEND 10.0 **Units:** cm **Default:** none; XEND keyword is required.
XCEN	Center of the mixing region; used in defining the initial profile for the LINE or PLAT options. Note that the fuel inlet is assumed to be located at $x = 0$. **Example:** XCEN 3.0 **Units:** cm **Default:** XEND * 0.35
WMIX	Width of the mixing region; used in defining the initial profile for the LINE or PLAT options. **Example:** WMIX 2.0 **Units:** cm **Default:** XEND * 0.5

Input File: Keywords

Flame Definition Keywords

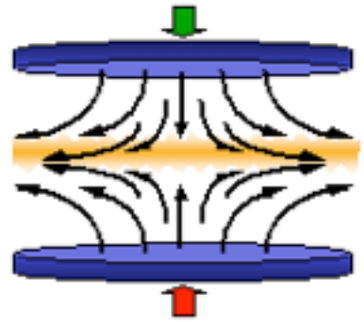


VFUE	Fuel inlet velocity (at $x = 0$). **Example:** VFUE 100. **Units:** cm/sec **Default:** none; VFUE must be specified.
VOXI	Oxidizer inlet velocity (at $x =$ XEND). **Example:** VOXI 100. **Units:** cm/sec **Default:** none; VOXI must be specified.
AFUE	Radial gradient in fuel inlet velocity (at $x = 0$). **Example:** AFUE 5.0 **Units:** 1/sec **Default:** 0.
AOXI	Radial gradient in oxidizer inlet velocity (at $x =$ XEND). **Example:** AOXI 5.0 **Units:** 1/sec **Default:** 0.
TFUE	Fuel inlet temperature (at $x = 0$). **Example:** TFUE 300. **Units:** K **Default:** none; TFUE must be specified.
TOXI	Oxidizer inlet temperature (at $x =$ XEND). **Example:** TOXI 300. **Units:** K **Default:** none; TOXI must be specified.
TMAX	Maximum temperature for use with profiles defined by the LINE or PLAT options. **Example:** TMAX 2500. **Units:** K **Default:** 2200.
PRES	The initial pressure of the gas mixture. **Example:** PRES 0.5 **Units:** atm **Default:** 1.

FUEL	Species name and the number of moles of that species in the fuel mixture. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all FUEL entries. Note that both FUEL and OXID can be specified as a premixed fuel/oxidizer mixture to run premixed flame calculations. **Example:** FUEL H2 0.2 **Units:** moles or mole fraction. **Default:** None, at least one FUEL entry.
OXID	Species name and number of moles of that species in the oxidizer mixture. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all OXID entries. Note that both FUEL and OXID can be specified as a premixed fuel/oxidizer mixture to run premixed flame calculations. **Example:** OXID O2 0.3 **Units:** moles or mole fraction. **Default:** None, at least one OXID entry.
PROD	Species name and number of moles of that species expected in the products of combustion of the fuel and oxidizer in stoichiometric proportions. The product mixture is used to define the initial profiles specified using the LINE or PLAT keywords. The mole fractions of the species will be normalized from the input mole quantities, so the absolute magnitudes of the input quantities are unimportant, as long as they are consistent for all PROD entries. **Example:** PROD H2O 0.2 **Units:** moles or mole fraction. **Default:** None, species input is required.
TEMP	Specifies an initial (for ENRG) or given (for TGIV) temperature profile in pairs of grid location and temperature, $(x;T)$. **Example:** TEMP 0.0 300. **Units:** cm; K **Default:** A linear temperature profile is assumed between the TOXI and TFUE values.

Input File: Keywords

Sensitivity Option Keywords



MULT	Use the multicomponent formula for diffusion velocities, *Equation 6-7*. **Default:** Use the mixture-averaged formula (MIX).
MIX	Use the mixture-averaged formula for diffusion velocities, *Equation 6-8*. **Default:** Use the mixture-averaged formula.
TDIF	Include thermal diffusion in the calculation of diffusion velocities. **Default:** Thermal diffusion is neglected.
ASEN	Inclusion of this Keyword causes all the first-order sensitivity coefficients with respect to the rate constants to be determined. **Default:** no sensitivities computed. **Restart:** can be changed.
HSEN	Inclusion of this Keyword causes all the first order sensitivity coefficients with respect to the species' heats of formation to be determined. **Default:** no sensitivities computed. **Restart:** can be changed.

Example

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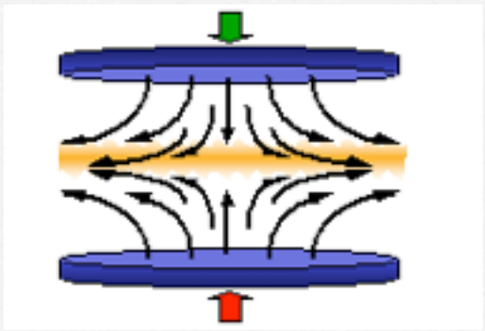


Conditions:

Vfuel=100 cm/s
Voxi=82,44 cm/s
Tfuel=300 K
Toxi=300 K
D= 2 cm
Pressure=1 Atm
Mole Frac CH4=0,5
Mole Frac N2= 0,5
Mole Frac O2= 0,21
Mole Frac N2= 0,79

Kinetic Mechanism: GRI-Mech 3.0 :
http://www.me.berkeley.edu/gri_mech/

Results :

1. Temperature profiles versus Mixture Fraction
2. Hdot Profiles versus Mixture Fraction
3. Species Profile

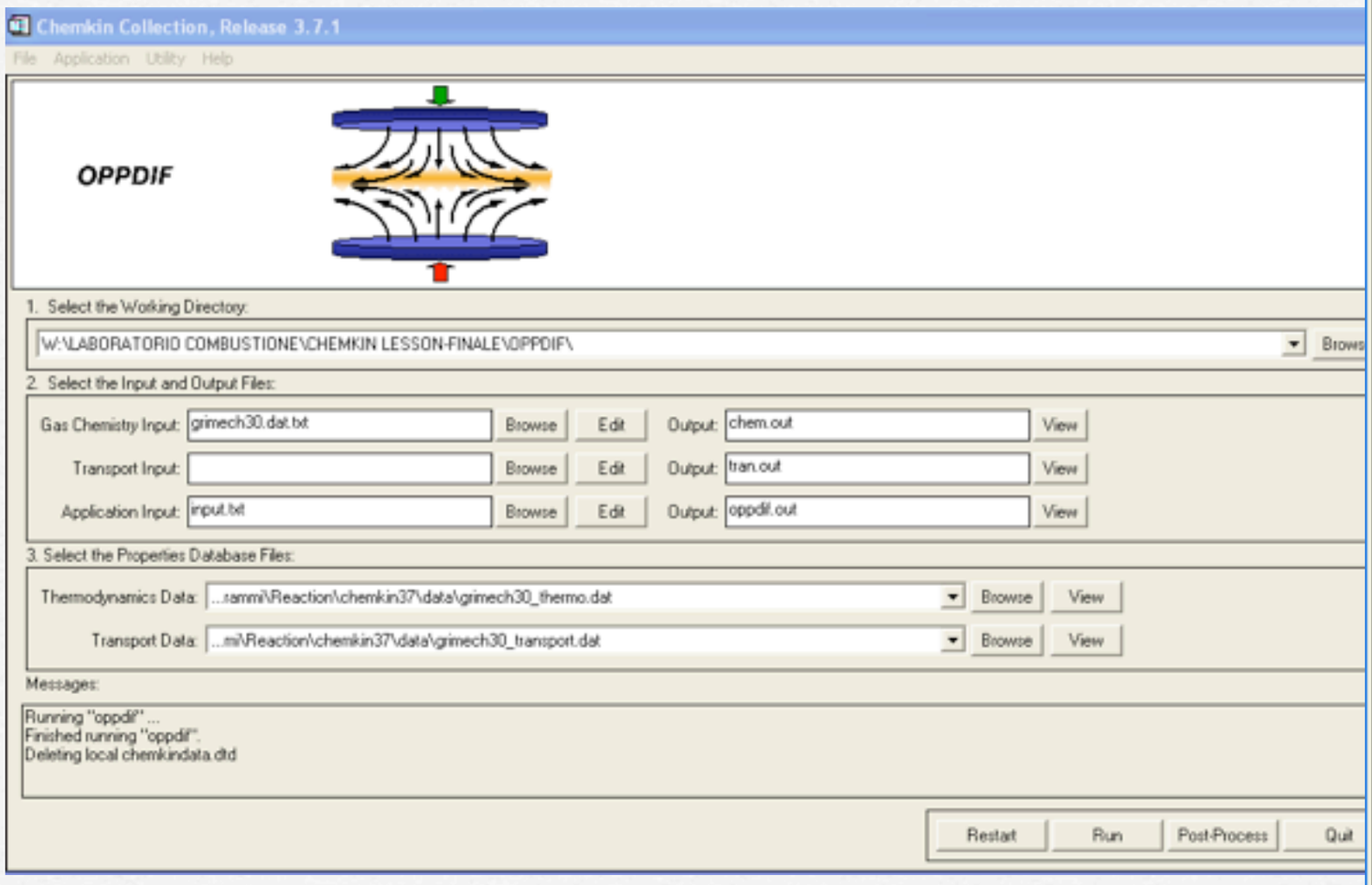
Input File

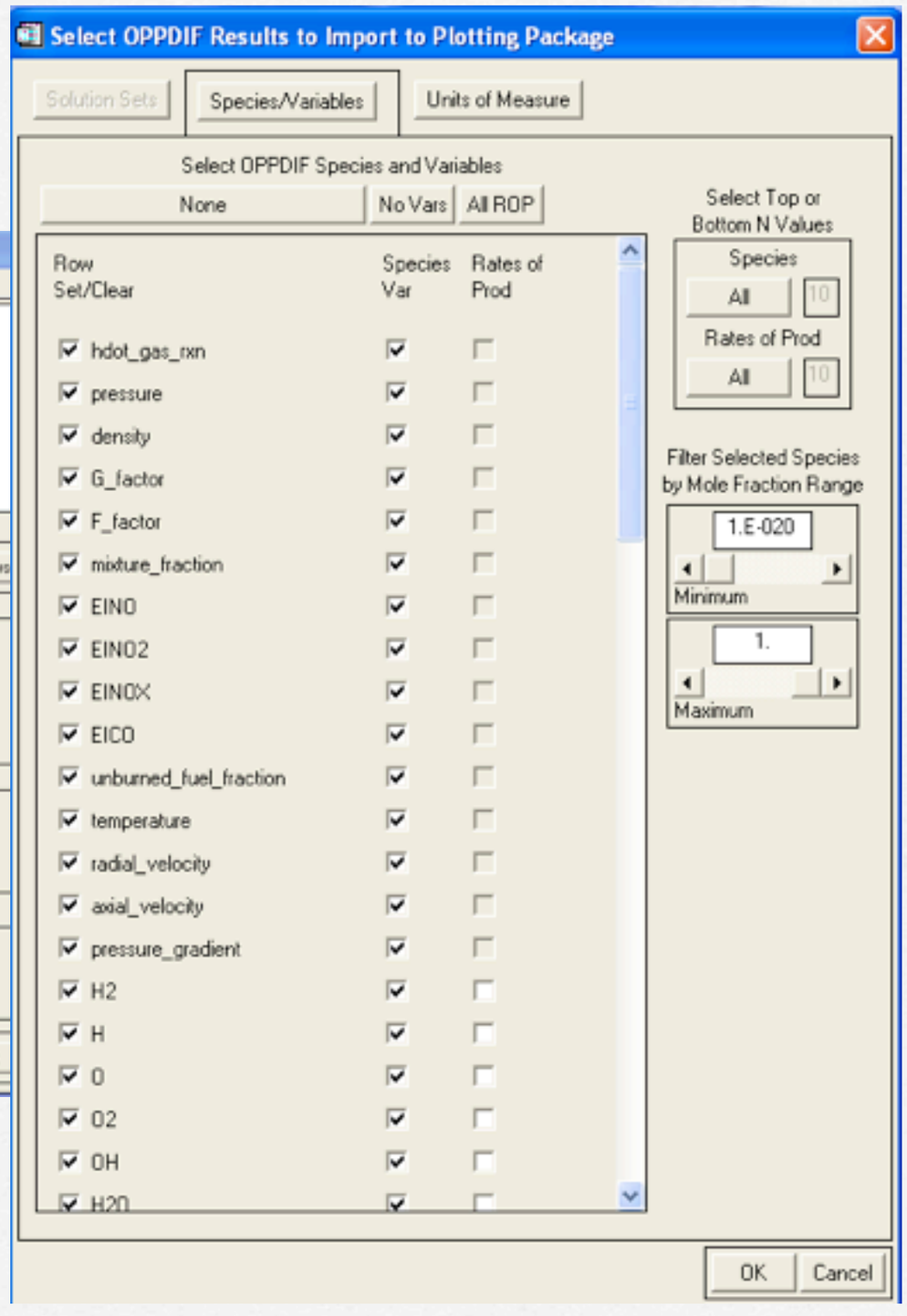
```
MIX
TDIF
PCAD 0.7
RGTC 1.0
ENRG
PLAT
AFUE    0
AOXI    0
VFUE   100
VOXI  82.44
TFUE   300
TOXI   300
TMAX  2000

GRID  0.
GRID  0.05
GRID  0.1
GRID  0.25
GRID  0.5
GRID  0.75
GRID  0.9
GRID  1.0
GRID  1.05
GRID  1.1
GRID  1.15
GRID  1.25
GRID  1.30
GRID  1.35
GRID  1.4
GRID  1.45
GRID  1.5
GRID  1.55
GRID  1.6
GRID  1.65
GRID  1.7
GRID  1.75
GRID  1.8
GRID  1.85
GRID  1.9
GRID  1.95
GRID  2.0
XEND  2.0
XCEN  1.0
WMIX  1.5

PRES  1.0
IRET  20
UFAC  2.
SFLR  -1.E-4
PRNT  11
TIME 200 1.E-6
TIM2 200 1.E-6
GRAD 0.5
CURV 0.5
FUEL CH4  0.5
FUEL N2   0.5
OXID N2 0.79
OXID O2 0.21
/
PROD H2O   0.3
PROD N2    0.7
/
RTOL  1.E-3
ATOL  1.E-6
ATIM  1.E-6
RTIM  1.E-3
/
END
```

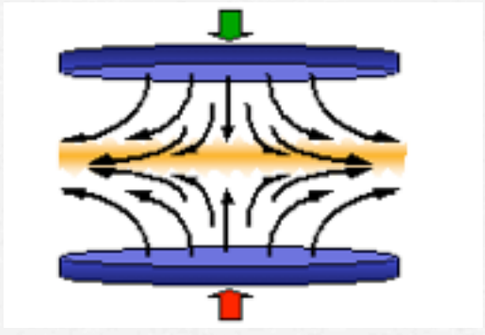
Graphical Post-process



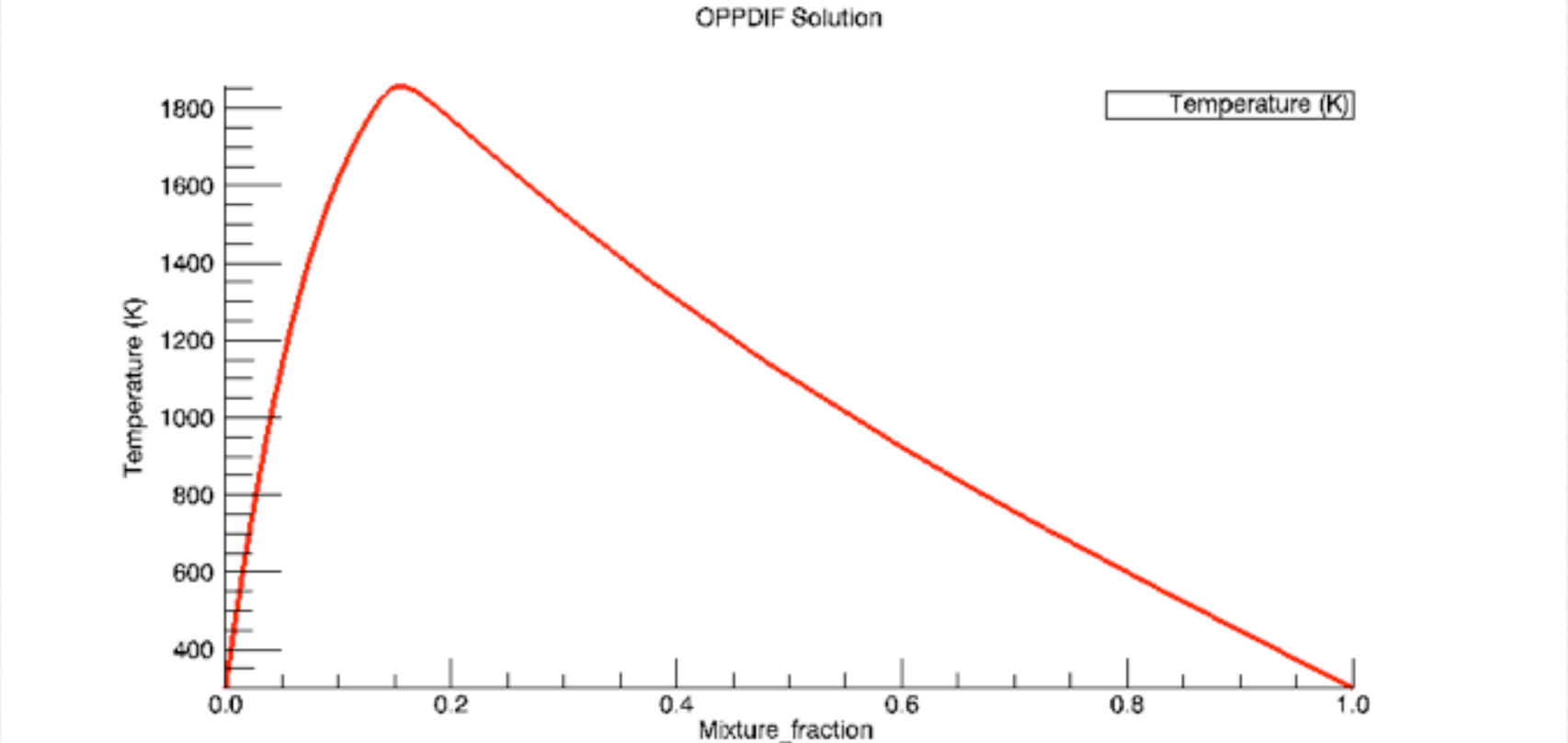


Results....

OppDif

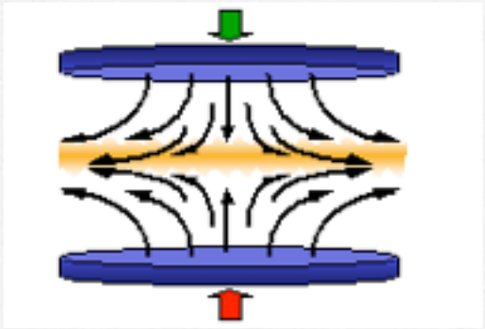


Temperature profile versus Mixture Fraction

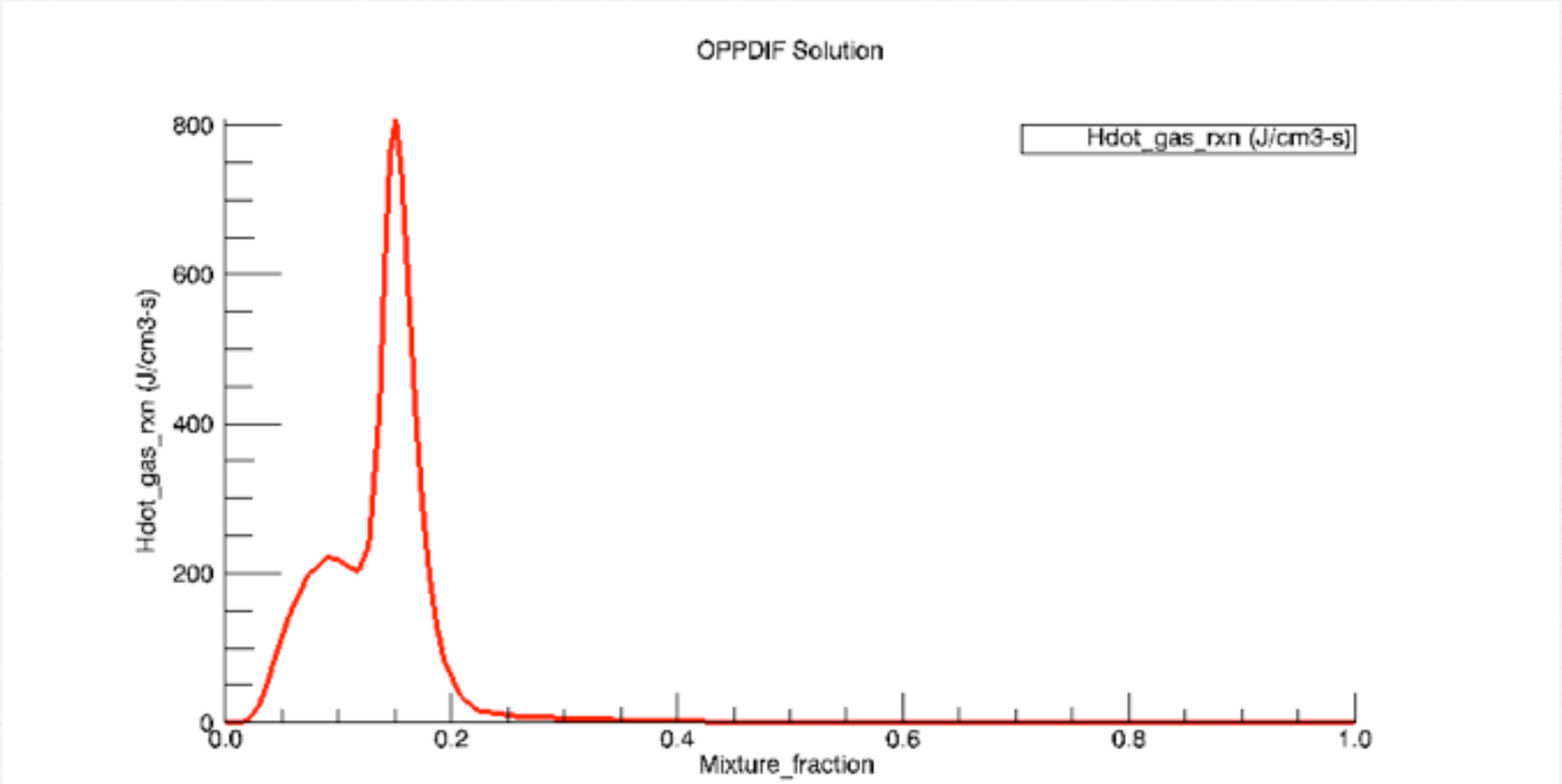


Results....

OppDif

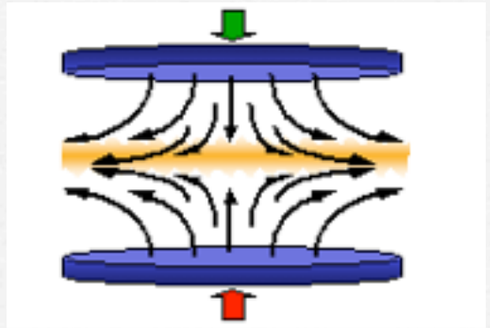


Heat release Rate profile versus Mixture Fraction

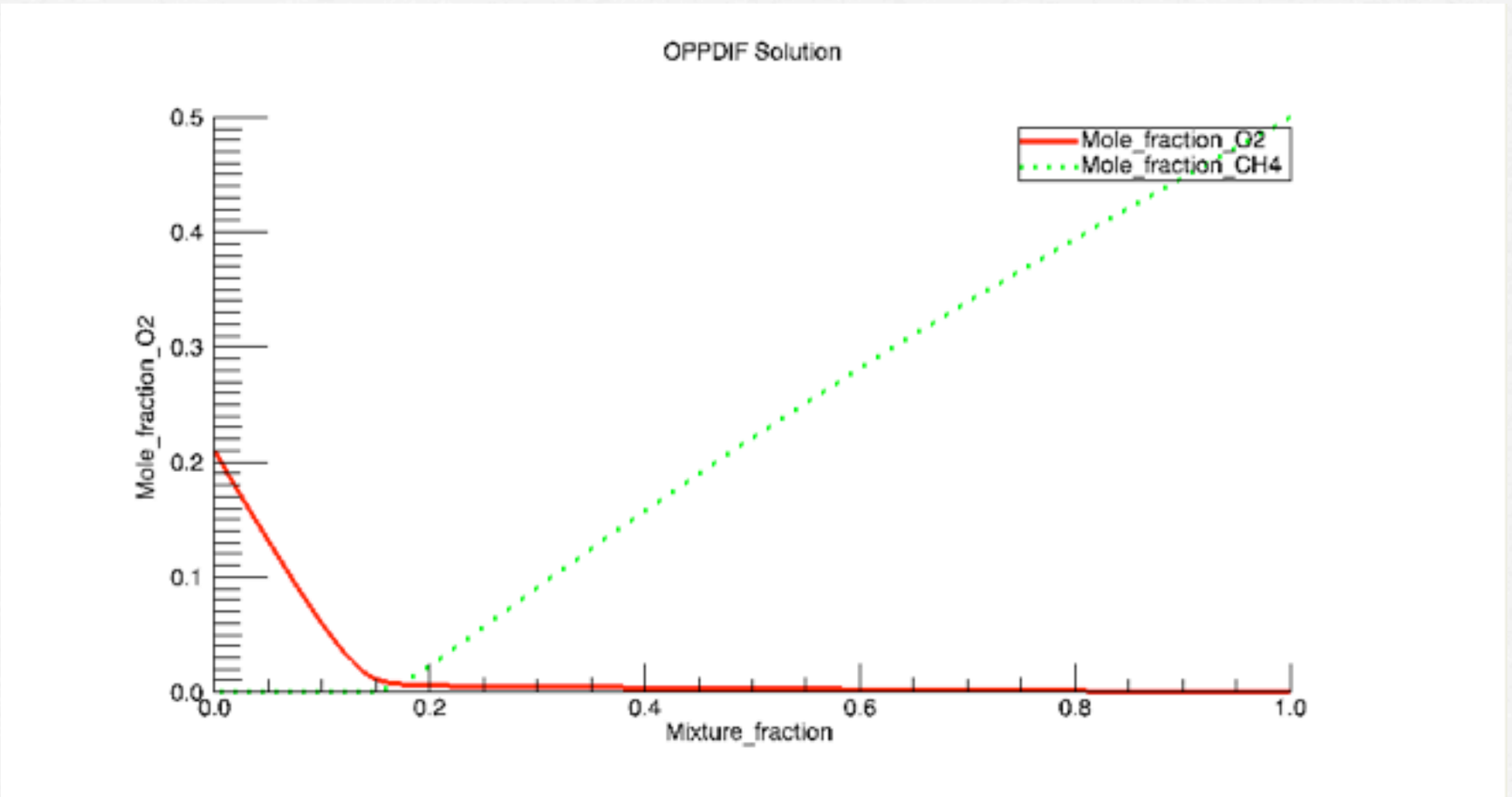


Results....

OppDif

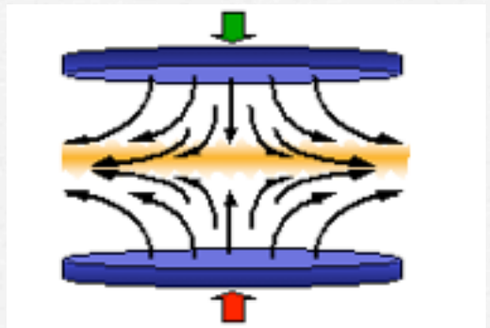


Species profiles versus Mixture Fraction

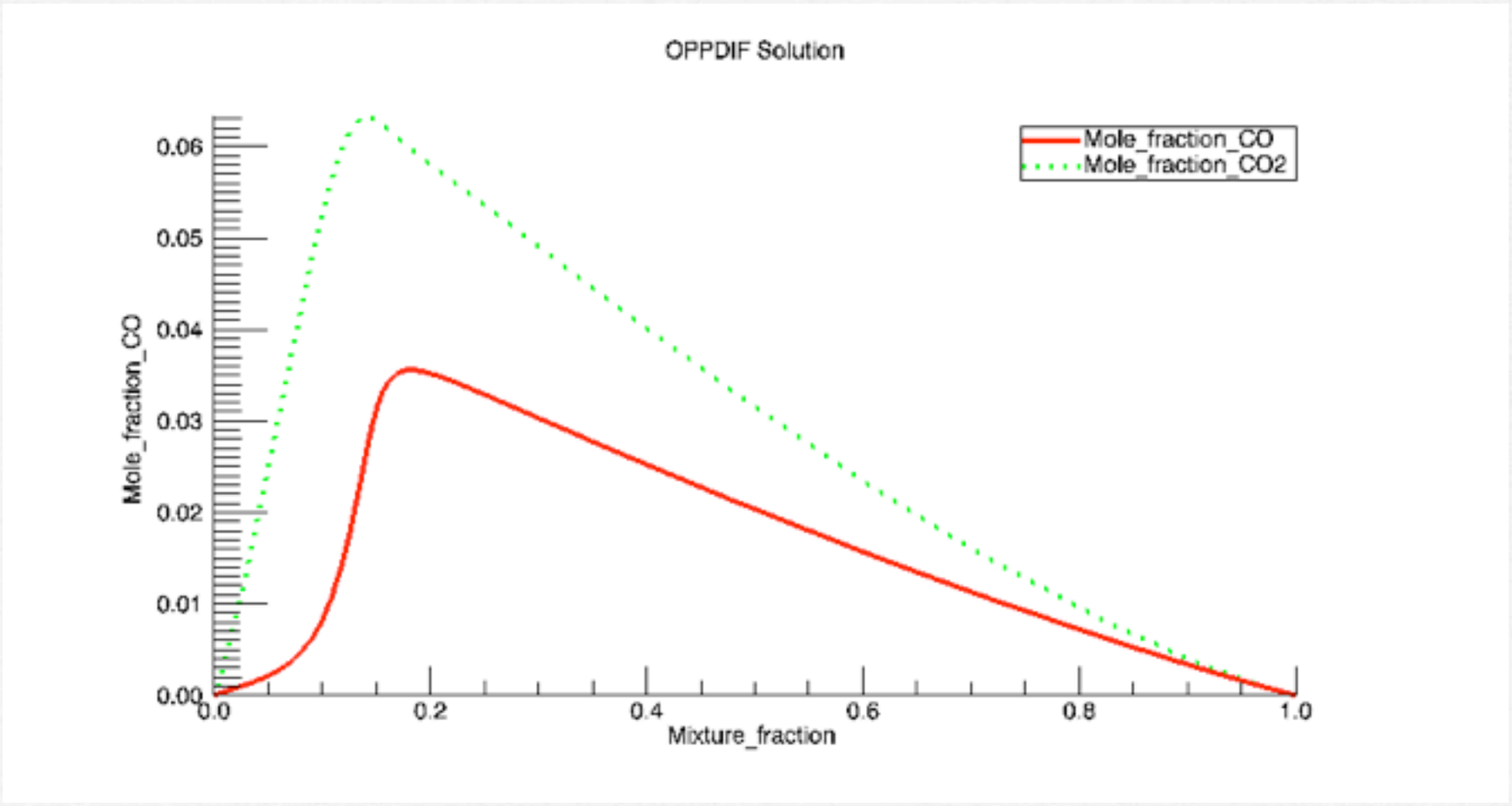


Results....

OppDif



Species profiles versus Mixture Fraction



References

1. http://www.reactiondesign.com/lobby/open/index.html (sito di riferimento CHEMKIN)
2. http://maeweb.ucsd.edu/~combustion/cermech/ (SANDIEGO mechanism)
3. http://www.me.berkeley.edu/gri-mech/ (GRI mechanism)
4. http://creckmodeling.chem.polimi.it/kinetic.html (Ranzi mechanism)