Combustion Summer School 2018

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## **Course Overview**



## Part I: Fundamentals and Laminar Flames

- Introduction
- Fundamentals and mass balances of combustion systems
- Thermodynamics, flame temperature, and equilibrium
- Governing equations
- Laminar premixed flames:
   Kinematics and Burning Velocity
- Laminar premixed flames:
   Flame structure
- Laminar diffusion flames
- FlameMaster flame calculator

- Introduction
- Counterflow diffusion flame
- Flamelet structure of diffusion flames
- FlameMaster flame calculator
- Single droplet combustion

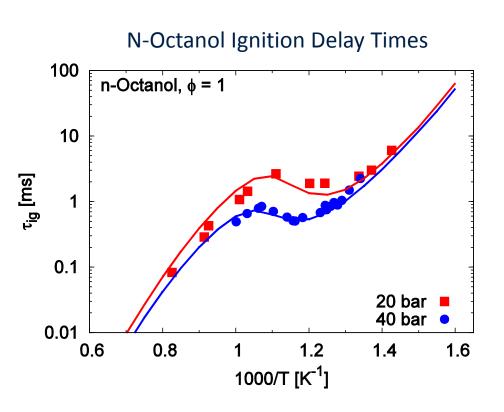


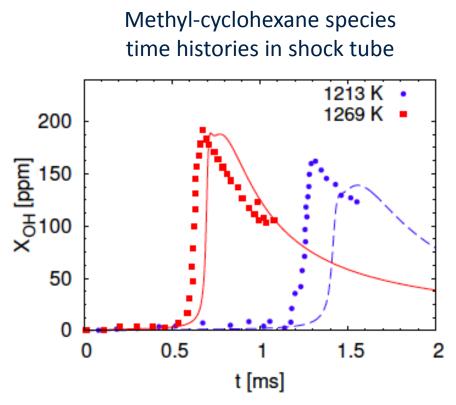
- FlameMaster: A C++ Computer Program for 0D Combustion and 1D Laminar Flame Calculations
  - Premixed and non-premixed
  - Steady and unsteady
  - Emphasis on pre- and post-processing
    - Sensitivity analysis
    - Reaction flux analysis
- At request, available online at

https://itv.rwth-aachen.de/index.php?id=13



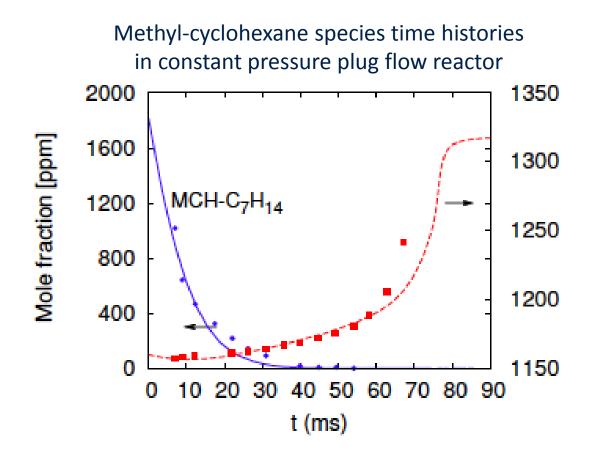
Example: Shock tube, homogeneous reactor







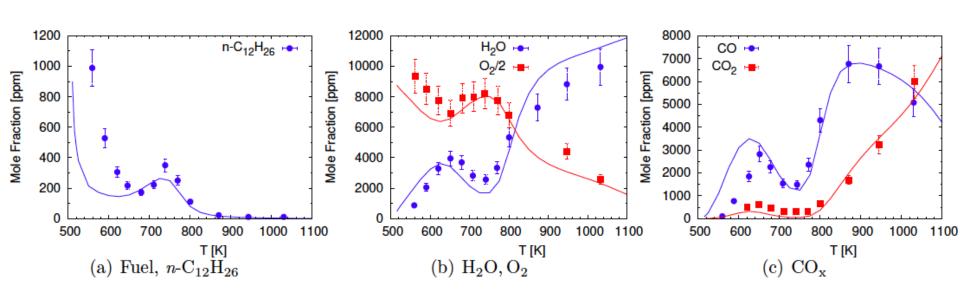
Example: Flow reactor





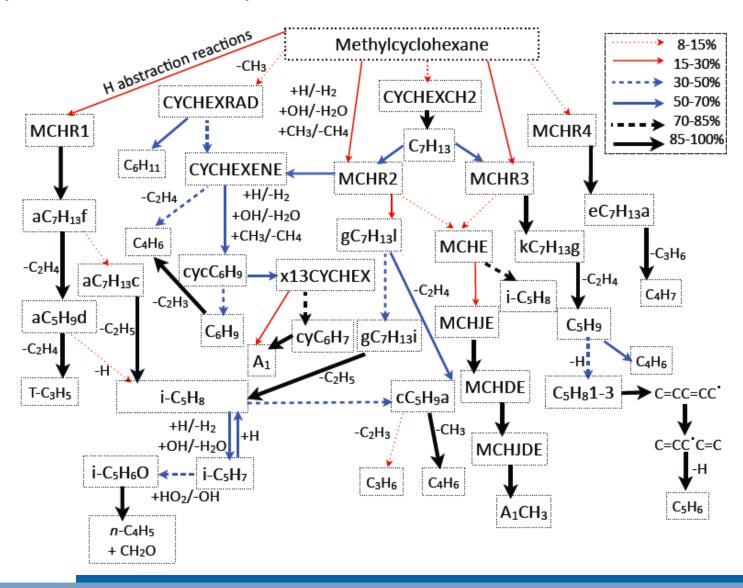
Example: Jet stirred reactor

#### N-Dodecane oxidation in jet stirred reactor



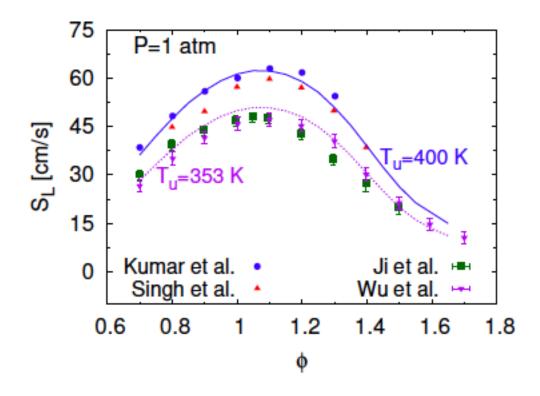


Example: Reaction flux analysis



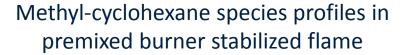


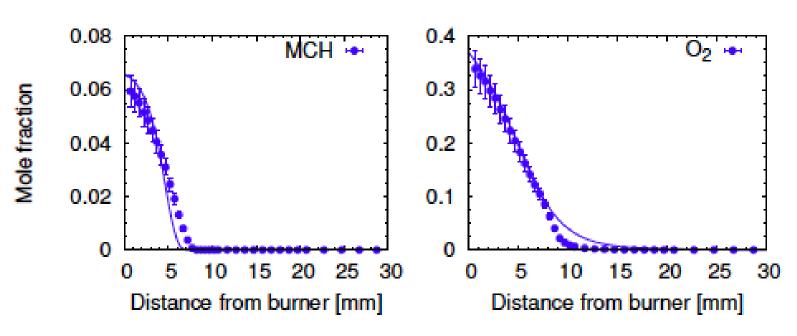
Example: Laminar burning velocities





Example: Premixed flame structure

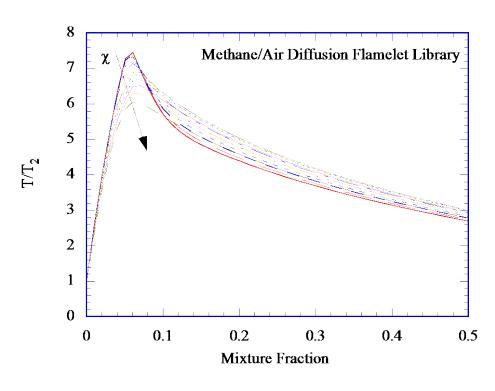


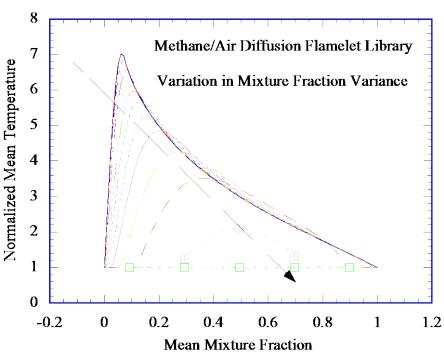




Example: Flamelet libraries

#### Flamelet library for methane/air non-premixed combustion





## FlameMaster Tutorial



- Distribution and installation
- Code structure
- Pre-processing
- Examples:
  - Homogeneous reactor
  - Premixed flames
  - Diffusion flames
  - Unsteady flamelet

## FlameMaster Tutorial: Distribution and Installation



- Code available at request, available online at https://itv.rwth-aachen.de/index.php?id=13
- Distribution for Linux, MacOS, and Windows systems
- Prerequisites
  - C and C++ compiler (C11/C++11 compliant)
  - 2. **CMake**
  - 3. Flex, Bison
  - Sundials (optionally installed by FlameMaster)
- Installation on Linux/MacOS

```
tar -xf FlameMaster.zip
cd FlameMaster
mkdir Build && cd Build
cmake ../Repository -DCMAKE BUILD TYPE=Release -DINSTALL SUNDIALS=ON
make install -j4
```

Set up environment

cd .. && source Bin/bin/Source.bash

Create Mechanisms

cd Run/ScanMan && bash CreateAllMechanisms.bash

#### **Further information:**

Repository/README.md

**Operating System** specific instructions:

Repository/doc/

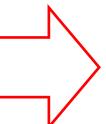
**Consider using your** package manager

## FlameMaster Tutorial: Installation on Windows I



- Multiple options
- Avoid spaces or special characters in directories and file names

- Option 1: Install Cygwin including all prerequisites (http://cygwin.org/)
- Option 2: Install Linux in a Virtual Box (https://www.virtualbox.org/)



Use Linux-instructions

**Option 1/2 are the recommended options** 

## FlameMaster Tutorial: Installation on Windows II



- Option 3: Install FlameMaster natively without Cygwin
  - Install only Compilers, CMake, and Python
  - FlameMaster installs flex, bison, and sundials
  - During the installation of CMake and Python
    - Choose to add the executables to the PATH
  - Extract FlameMaster to C:\FlameMaster
  - Commands for the installation

```
cd C:\FlameMaster
mkdir Build && cd Build
cmake ../Repository -DCMAKE_BUILD_TYPE=Release
-DINSTALL_SUNDIALS=ON
cmake --build . --config Release --target
install
```

- Option 4: Install FlameMaster from a binary installer
  - Install FlameMaster to C:\FlameMaster
- Set up environment
  - Double click: C:\FlameMaster\Bin\bin\Source.bat
- Create Mechanisms

cd Run\ScanMan && CreateAllMechanisms.bat

## Option 3/4 are in beta

#### Possible issues:

Fixing requires solid understanding of C++ and CMake

#### **Further instructions:**

Repository/doc/ Windows.md

## FlameMaster Tutorial: Directory layout



Directory	Purpose
Repository/	Permanent directory for the source code. Do all changes here.
Build/*	Intermediate directory containing configuration information ("CMake cache") and object files
Bin/*	Installation directory containing binaries and scripts that set up your environment (for bash, csh, zsh, bat)
Run/*	Directory containing examples
Data/*	Directory checked by ScanMan and FlameMan via the shell variable FM_DATA to find binary input files

\*Do not modify automatically generated files. Changes are overwritten if you rerun the installation. Instead, modify the respective template files in Repository/

## FlameMaster Tutorial: Code Structure



Four different parts (main executables):

1. Preprocessing of thermo- and transport data: CreateBinFile

2. Preprocessing of chemical mechanism: ScanMan

3. Simulation: FlameMan

4. Post-processing tools: e.g. ListTool

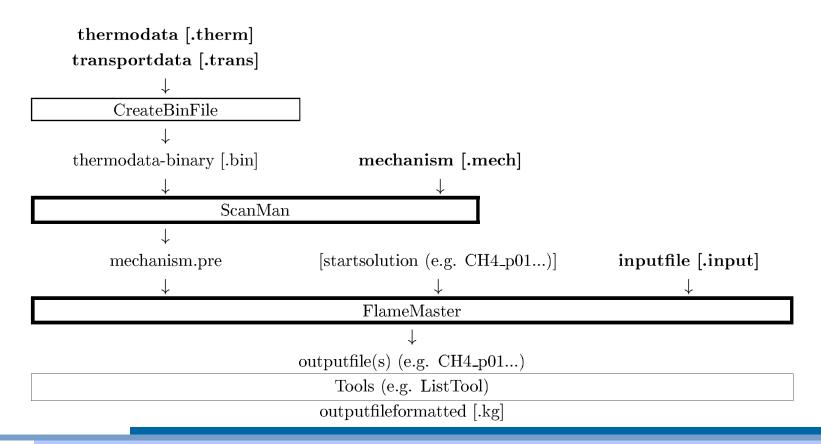
All tools have help function: Type <Executable> -h

- Main input files
  - Mechanism
    - Thermodata file
    - Transport data file
    - Mechanism file
  - 2. FlameMaster input file
    - Information about configuration, boundary and initial conditions, post-processing options, ...

## FlameMaster Tutorial: Code Structure



- Four different parts (main executables):
  - 1. Preprocessing of thermo- and transport data: CreateBinFile
  - 2. Preprocessing of chemical mechanism: ScanMan
  - 3. Simulation: FlameMan
  - 4. Post-processing tools: e.g. ListTool



## FlameMaster Tutorial: Proproc. Thermo/Trans



- CreateBinFile
  - Creates a binary file
     thermotransout to be
     used by ScanMan including
     all thermodata and transport data
  - Input files are thermodata file and transport data file
  - Reads Chemkin II format

#### Example: Thermodata file

- Syntax:

CreateBinFile -i <thermo> -m <transport> -o <thermotransout>

- Example:

```
cd Run/ScanMan/GRI3.0
CreateBinFile -i gri.30.therm -m gri.30.trans -o gri.30.bin
```

## FlameMaster Tutorial: Proproc. Mechanism File



#### ScanMan

- Creates a binary file to be used by FlameMan including all thermodata, transport data, and reaction mechanism data
   <mechanism>.mech
- Input files are binary file thermotransout created by CreateBinFile and reaction mechanism file
- ScanMan has its own format for mechanism file, but also reads Chemkin II format
- Resulting output file should typically be copied to directory Data

```
Let allowed atoms be C, H, O, N, He, AR.
Let additional species be N2,C0,C02.
Let temperature exponent be n k.
Let order of reaction be n.
Let units for A be [ cm^{(3(n-1))} / ( s * mole^{(n-1)} * K^n_k ) ].
Let units for E be [ kJ / mole ].
                          H2/CO Chemistry from
             "An optimized kinetic model of H2/CO combustion"
                   Davis, Joshi, Wang, and Egolfopoulos
                   Proc. Comb. Inst. 30 (2005) 1283-1292
# Reactions of H2/02
                        { a = 1.040E+14 n = 0.000 E = 63.957 }
                       { a = 3.818E+12 n = 0.000 E = 33.254 }
                        { a = 8.792E+14 n = 0.000 E = 80.207 }
4f: H2 + OH -> H2O + H { a = 2.160E+08 n = 1.510 E = 14.351 }
5f: OH + OH -> O + H2O { a = 3.340E+04 n = 2.420 E = -8.075 }
6f: H2 + M41 -> H + H + M41 { a = 4.577E+19 n = -1.400 E = 436.726 }
7f: H2 + AR -> H + H + AR { a = 5.840E+18 n = -1.100 E = 436.726 }
8f: H2 + HE -> H + H + HE { a = 5.840E+18 n = -1.100 E = 436.726 }
```

Example: Mechanism file

## FlameMaster Tutorial: Proproc. Mechanism File



- ScanMan (Mechanism file in FlameMaster format)
  - Syntax:

```
ScanMan -i <Mechanismfile>.mech -t <thermotransportoutput>
<mechanismbinfile>.pre
```

- Example:

```
cd Run/ScanMan/GRI3.0
ScanMan -i gri.30.mech -t gri.30.bin -rs3 > gri.out
mv gri.30.pre ../../Data
```

- ScanMan (Mechanism file in Chemkin format)
  - CreateBinFile not required
  - Syntax:

```
ScanMan -i <Mechanismfile>.chmech -t <thermodata> -m
<transportdata> -f chemkin
```

- Example:

```
cd Run/ScanMan/GRI3.0_CK
ScanMan -i grimech30.dat -t thermo30.dat -m transport.dat -f
chemkin -rs3 > gri.out
```



- FlameMan performs simulations for different configurations
- Main input file called
   FlameMaster.input (default name)
   or name specified on command line using
   -i option
- All parameters and inputs are provided in FlameMaster.input file
- Some parameters can be specified by command line options, which overwrite input file values

```
#######
# I/O #
#######
WriteEverySolution is TRUE
OutputPath is ./Output
NOutputs = 50
##################
# Chemistrv #
##############
MechanismFile is Base.pre
globalReaction is 2H2 + 02 == 2H2O;
fuel is H2
oxidizer is o2
#########
# Flame #
#########
Flame is Isochor Homo Reactor
#Flame is Isobar Homo Reactor
#phi = 0.5
phi = 1.0
#phi = 2.0
Pressure = 13e5
Pressure = 1e5
# Boundary conditions #
********************
ContInc = -0.1
ContType is Temperature
ContBound = 0.7
InitialCond {
   X->N2 = 0.79
   X -> 02 = 0.21
```



## Typical input file (part 1)

- Comments start with #
- Typical statement is <Keyword> = <value>Keyword> is <value>
- Most <Keywords> have default values, usually FALSE, if applicable
- I/O
  - Outputpath
- Chemistry
  - Mechanism input file
  - Global reaction (for equivalence ratio)
  - Fuel and oxidizer (for equivalence ratio)

```
#######
# I/O #
WriteEverySolution is TRUE
OutputPath is ./Output
NOutputs = 50
##############
# Chemistry #
##############
MechanismFile is Base.pre
globalReaction is 2H2 + 02 == 2H2O ;
fuel is H2
oxidizer is o2
```



## Typical input file (part 2)

- Configuration
  - Flame is ...
  - phi is equivalence ratio
  - Several phi and pressure can be specified
  - If no phi is specified, it will be computed from initial composition

```
# Flame #
Flame is Isochor Homo Reactor
#Flame is Isobar Homo Reactor
#phi = 0.5
phi = 1.0
#phi = 2.0
Pressure = 13e5
Pressure = 1e5
# Boundary conditions #
*****************
ContInc = -0.1
ContType is Temperature
ContBound = 0.7
InitialCond {
   t = 1.7
   X->N2 = 0.79
   X -> 02 = 0.21
```



## Typical input file (part 2)

- Boundary and initial conditions (here initial condition for homogeneous reactor)
  - Initial composition either from phi and global reaction or specification in InitialCond
  - X->N2 is mole fraction
  - Y->N2 is mass fraction
  - T or t is temperature
    - If T < 10, then value is 1000/T
  - Continuation in temperature, if Continc is non-zero
    - ContType is Temperature means continuation in temperature
    - Continuation ends, if ContBound is reached
    - Continc is increment between two simulations. If Continc < 10, then increment is applied to 1000/T</li>
    - In the example, temperature is varied from 1000/T = 1/1.7 to 1/0.7 corresponding to 588 to 1000

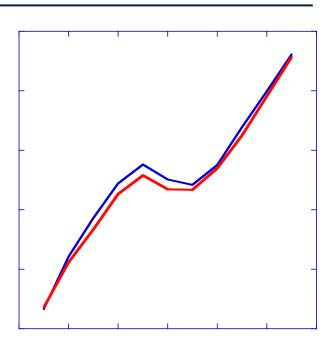
```
# Flame #
Flame is Isochor Homo Reactor
#Flame is Isobar Homo Reactor
#phi = 0.5
phi = 1.0
#phi = 2.0
Pressure = 13e5
Pressure = 1e5
# Boundary conditions #
******************
ContInc = -0.1
ContType is Temperature
ContBound = 0.7
InitialCond {
   X->N2 = 0.79
   X -> 02 = 0.21
```

## FlameMaster Tutorial: Homogeneous Reactor



Constant volume homogeneous reactor computing ignition delay times for *n*-heptane/air mixtures

- Example: cd Run/FlameMan/Prem/OD/nHeptane FlameMan
- This will create a file Output/N-C7H16\_IgniDelTimes.dout which has the values of ignition delay times for all computed conditions as tab-separated list



- If the flag WriteEverySolution is TRUE is added to the input file, then mass fractions and temperatures as function of time are given in files like Y1\_N-C7H16\_p13phi100to0833.dout
- File names include information on fuel, pressure, equivalence ratio, and initial temperature

## FlameMaster Tutorial: Homogeneous Reactor



02 + H202 = 2 H02

```
Constant volume homogeneous
                                                   Tig:
                                                              -0.429595
                                                                                 02 + H = 0H + 0
                                                                         1f:
reactor performing sensitivity
                                                              0.417076
                                                                         8f:
                                                                                 H + 02 + M1 = H02 + M1
                                                              -0.31854
                                                                         16b:
                                                                                 H02 + H2 = H + H202
analysis for hydrogen/air mixtures
                                                              0.156775
                                                                         13f:
                                                                                 H02 + 0H = H20 + 02
                                                              -0.151255
                                                                         10b:
                                                                                 02 + H2 = H + H02
                                                              -0.132167
                                                                         14f:
                                                                                 2 H02 = H202 + 02
                                                              0.114924
                                                                         10f:
                                                                                 H02 + H = H2 + 02
   Example:
                                                             -0.0911612
                                                                         9f:
                                                                                 H02 + H = 2 OH
                                                                          3f:
                                                             -0.0679557
                                                                                 H2 + OH = H2O + H
   cd Run/FlameMan/Prem/0D/H2
                                                             -0.0349418
                                                                          8b:
                                                                                 H02 + M1 = 02 + H + M1
   FlameMan
                                                             -0.0227425
                                                                         15b:
                                                                                 H202 + M1 = 2 OH + M1
                                                                         12f:
                                                             0.0197566
                                                                                 H02 + 0 = 0H + 02
                                                                         11f:
                                                                                 H02 + H = H20 + 0
                                                             -0.0157099
                                                             -0.0111745
                                                                         2f:
                                                                                 H2 + 0 = 0H + H
   If the flag SensAnalReac is TRUE is
                                                                         17f:
                                                                                 H202 + H = H20 + OH
                                                            0.000484599
                                                                         19f:
                                                                                 H202 + OH = H20 + H02
                                                            0.000372708
   added to the input file, then
                                                           -0.000190179
                                                                         19b:
                                                                                 H02 + H20 = OH + H202
                                                            9.88041e-05
                                                                          3b:
                                                                                 H + H20 = OH + H2
       Reaction sensitivity analysis is performed
                                                            8.04196e-05
                                                                         7f:
                                                                                 H + OH + M1 = H2O + M1
                                                            8.00509e-05
                                                                         16f:
                                                                                 H202 + H = H2 + H02
       Sensitivity coefficients for ignition delay
                                                            7.48334e-05
                                                                         18f:
                                                                                 H202 + 0 = 0H + H02
                                                            -3.5944e-05
                                                                         2b:
                                                                                 H + OH = O + H2
       times or chosen species are given in files
                                                            3.00888e-05
                                                                         1b:
                                                                                 0 + 0H = H + 02
       like
                                                            -2.5005e-05
                                                                         4b:
                                                                                 0 + H20 = 2 OH
       MAXSorted Reac SC H2 p01phi1
                                                            1.00366e-05
                                                                         15f:
                                                                                 2 \text{ OH} + \text{M1} = \text{H2O2} + \text{M1}
                                                           -8.63985e-06
                                                                         18b:
                                                                                 H02 + 0H = 0 + H202
        00to1000.tout
                                                                          5b:
                                                           -7.61168e-06
                                                                                 H2 + M1 = 2 H + M1
                                                                         4f:
                                                           -6.10434e-06
                                                                                 2 \text{ OH} = H20 + 0
   More details are found in
                                                           -3.61813e-06
                                                                          6b:
                                                                                 02 + M1 = 20 + M1
```

2.97311e-06

14b:

.pdf

Run/FlameManPrem/OD/SensAnalOD

## FlameMaster Tutorial: Homogeneous Reactor

H:

0H:

-0.00130305



```
Constant volume homogeneous reactor performing reaction flux analysis for hydrogen/air mixtures
```

- Example: cd Run/FlameMan/Prem/0D/H2 FlameMan
- If the flag ReactionFluxAnal is TRUE is added to the input file, then reaction pathway analysis is performed, and production and consumption channels of species are given in files like Output/IntProRa\_H2\_p30phil 0: 00to1000.tout (requires

also AdditionalOutput is

TRUE)

```
0.776747
                 3f:
                          H2 + OH = H2O + H
                 8f:
   -0.377077
                          H + 02 + M1 = H02 + M1
                 1f:
                          02 + H = 0H + 0
   -0.271011
    0.253203
                 2f:
                          H2 + 0 = 0H + H
   -0.163056
                 9f:
                          H02 + H = 2 OH
  -0.0965657
                 7f:
                          H + OH + M1 = H2O + M1
  -0.0352961
                 5f:
                          2 H + M1 = H2 + M1
  -0.0293398
                 10f:
                          H02 + H = H2 + 02
                 11f:
                          H02 + H = H20 + 0
  -0.0268207
                 16f:
  0.00500216
                          H202 + H = H2 + H02
-0.000833782
                 17f:
                          H202 + H = H20 + OH
   -0.834354
                 3f:
                          H2 + OH = H2O + H
    0.350298
                 9f:
                          H02 + H = 2 OH
     0.29111
                          02 + H = 0H + 0
                 1f:
                          H2 + 0 = OH + H
    0.271982
                 2f:
                 7f:
   -0.103727
                          H + OH + M1 = H2O + M1
                 15f:
    0.103051
                          2 \text{ OH} + \text{M1} = \text{H2O2} + \text{M1}
  -0.0611793
                 13f:
                          H02 + 0H = H20 + 02
                 4f:
    0.053952
                          2 \text{ OH} = \text{H2O} + \text{O}
  0.00727006
                 12f:
                          H02 + 0 = 0H + 02
                 17f:
0.000895619
                          H202 + H = H20 + OH
                 19f:
                          H202 + OH = H20 + H02
-0.000739134
                 18f:
0.000400465
                          H202 + 0 = 0H + H02
    0.947228
                 1f:
                          02 + H = 0H + 0
   -0.884988
                 2f:
                          H2 + 0 = 0H + H
  0.0937429
                 11f:
                          H02 + H = H20 + 0
  -0.0877758
                 4f:
                          2 \text{ OH} = \text{H2O} + \text{O}
                 12f:
  -0.0236557
                          H02 + 0 = 0H + 02
 -0.00227764
                 6f:
                          2 0 + M1 = 02 + M1
```

18f:

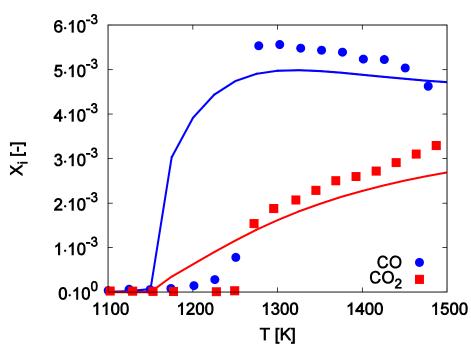
H202 + 0 = 0H + H02

## FlameMaster Tutorial: Perfectly Stirred Reactor



Perfectly stirred reactor (PSR) computing stable species profiles for methane/air mixtures

Example: cd Run/FlameMan/Prem/PSR FlameMan

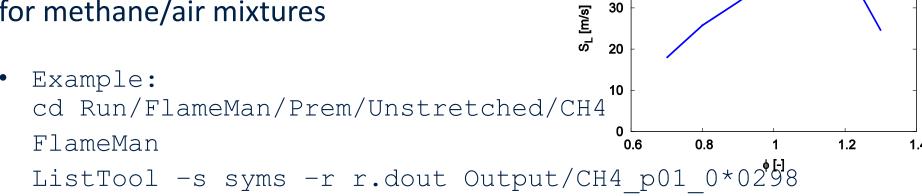


- This will create a file Output/PSR\_X\_CH4\_p01phi128tau00.14.dout which has mole fractions of species for all computed initial temperatures as tab-separated list
- More details are found in Run/Prem/PSR/README.md

## FlameMaster Tutorial: Unstretched Premixed Flame



Unstretched premixed flame computing laminar burning velocities for methane/air mixtures



50

40

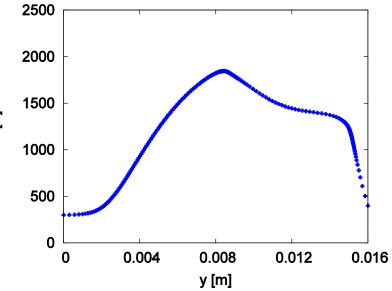
- FlameMan will create files like Output/CH4\_p01\_0phi1\_0000tu0298 containing the spatial distribution of all scalar fields at all computed conditions
  - With PrintMoleFractions is TRUE, also mole fractions are printed
- ListTool generates a file r.dout, which has the values of burning velocities or other scalar quantities specified in syms and maximum values of all vector quantities for all computed conditions as tab-separated list
  - Specified symbols are from the header of FlameMaster output files

## FlameMaster Tutorial: Counterflow Diffusion Flame



Counterflow diffusion flame with plug flow boundary condition on physical coordinate for acetylene/air mixtures

Example: cd Run/FlameMan/Diff/SteadyPlugFlow FlameMan



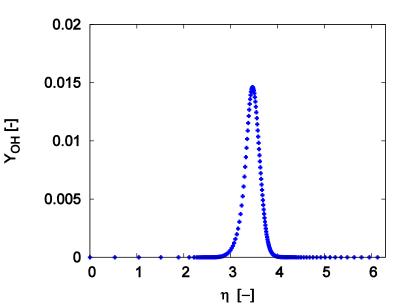
- This will create a file Output/C2H2\_p01a00018tf0300to0400 containing the spatial distribution of all scalar fields at all computed conditions
- Different forms of continuation can be used
  - E.g., if the flag ContType is velocity is added to the input file, then critical conditions (e.g. strain rates) of extinction or autoignition can be determined.

## FlameMaster Tutorial: Counterflow Diffusion Flame



Counterflow diffusion flame with potential flow boundary condition on similarity coordinate for hydrogen/air mixtures

• Example: cd Run/FlameMan/Diff/Steady/H2 FlameMan -i H2.count.in



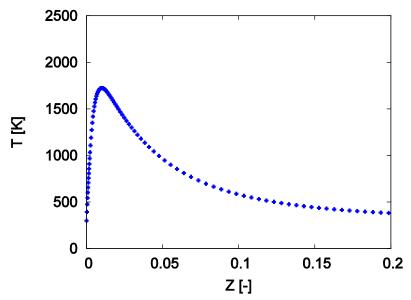
- This will create a file
   OutCount/H2\_p01\_0a00100\_0tf0300to0300
   containing the spatial distribution of all scalar fields at all computed conditions
- More details are found in Repository/doc/FlameManMan.pdf Repository/doc/MThesisGer.pdf

## FlameMaster Tutorial: Flamelet Equations



Diffusion flames solving flamelet equations using mixture fraction coordinate for hydrogen/air mixtures

• Example: cd Run/FlameMan/Diff/Steady/H2 FlameMan -i H2.mixfrac.in



• This will create a file OutMixFrac/H2\_p01\_0chi1.734tf0300to0300 containing the spatial distribution of all scalar fields at all computed conditions

## FlameMaster Tutorial: Flamelet Equations



# Solving flamelet equations with continuation for methane/air mixtures

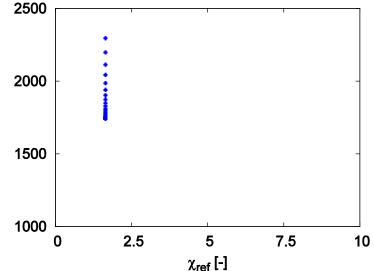
- Example:
   cd Run/FlameMan/Diff/Steady/CH4
   FlameMan -i FlameMasterCont.input
- If the flag ArclengthCont is TRUE is added to the input file, FlameMaster computes solutions along S-shaped curve
- ListTool -s syms -r r.dout OutMethaneCont/CH4\_p01\_0chi\*st\* creates a file r.out containing data for scalar quantities specified in syms and maximum values of all vector quantities for all computed flamelets
- More details are found in Run/FlameMan/Diff/Steady/CH4/README.md

## FlameMaster Tutorial: Transient flamelet



## Transient flamelet for hydrogen/air mixtures

• Example: cd Run/FlameMan/Diff/Unsteady/H2 FlameMan



This will create output files

Lib\_Chi01.64\_T1742t00014.tout Lib\_Chi01.64\_T1742t00015.tout Lib\_Chi01.64\_T1742t00016.tout

•••

which has the values of temperature, species mass and mole fractions, velocity, heat release, density ... as function of mixture fraction at the computed condition



- FlameMaster: A C++ Computer Program for 0D Combustion and 1D Laminar Flame Calculations
  - Premixed and non-premixed
  - Steady and unsteady
  - Emphasis on pre- and post-processing
    - Sensitivity analysis
    - Reaction flux analysis
- At request, available online at https://itv.rwth-aachen.de/index.php?id=13

## Summary



## Part I: Fundamentals and Laminar Flames

- Introduction
- Fundamentals and mass balances of combustion systems
- Thermodynamics, flame temperature, and equilibrium
- Governing equations
- Laminar premixed flames:
   Kinematics and Burning Velocity
- Laminar premixed flames:
   Flame structure
- Laminar diffusion flames
- FlameMaster flame calculator

- Introduction
- Counterflow diffusion flame
- Flamelet structure of diffusion flames
- FlameMaster flame calculator
- Single droplet combustion