

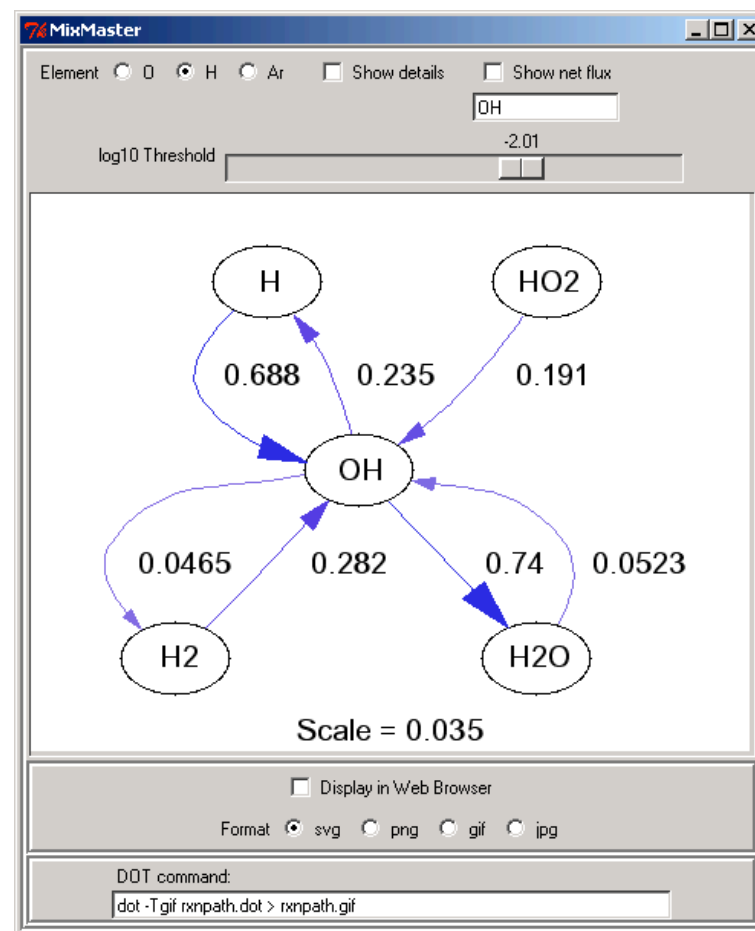


# MixMaster

A Cantera Application

# MixMaster is a Cantera-based graphical tool that allows you to...

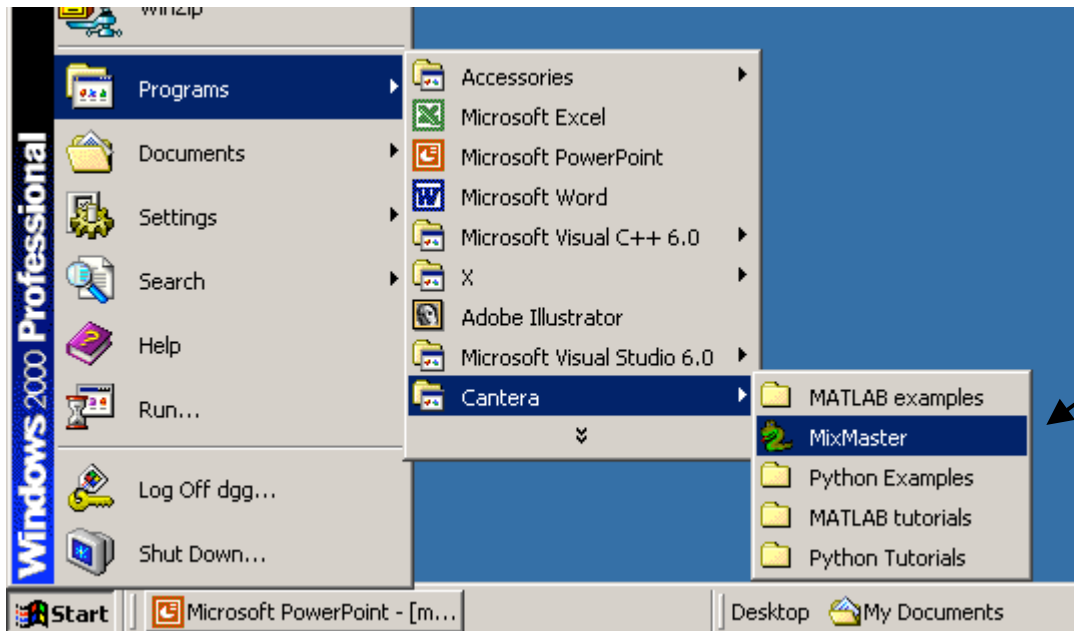
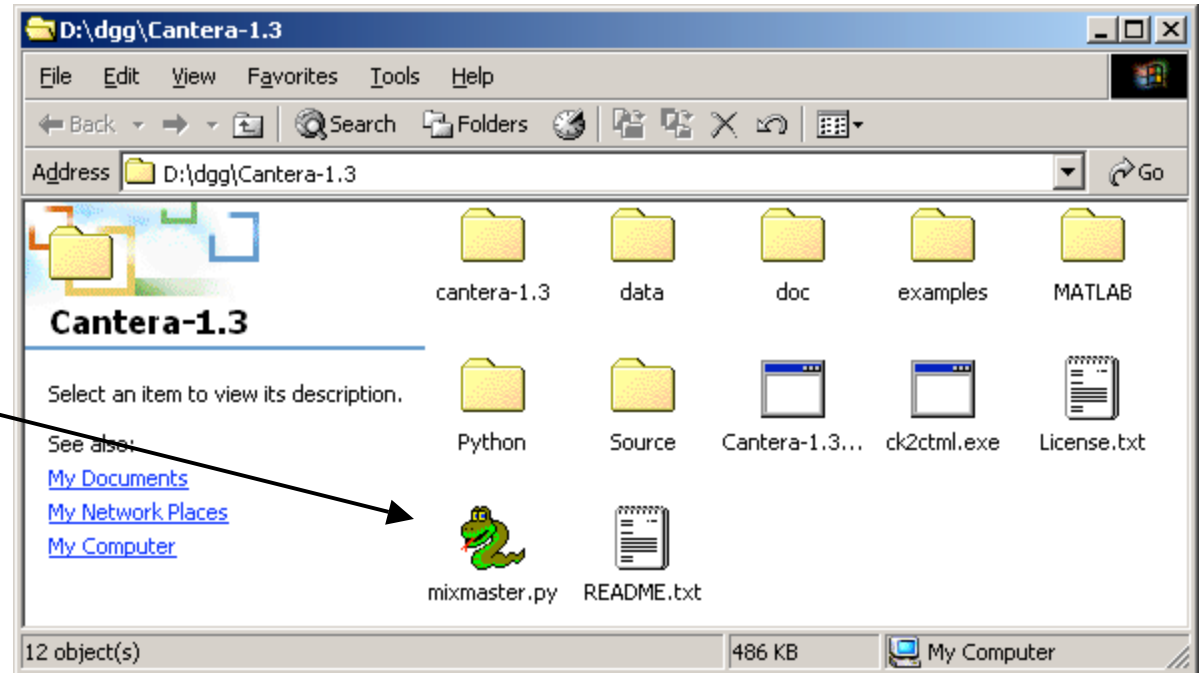
- import reaction mechanisms in standard file formats
- view/set the state of mixtures
- carry out thermodynamic processes
- compute chemical equilibrium
- view species properties
- view reaction data
- postprocess simulation data
- view reaction paths



MixMaster 2003

# Getting Started

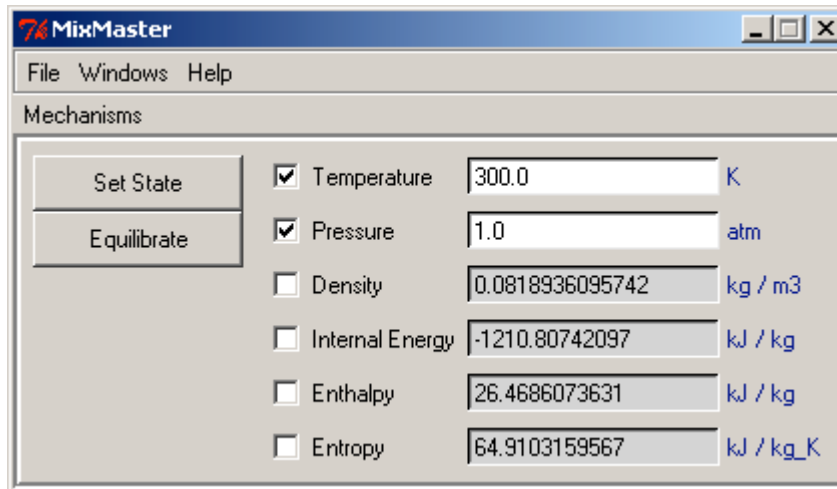
double-click the MixMaster icon in the Cantera folder



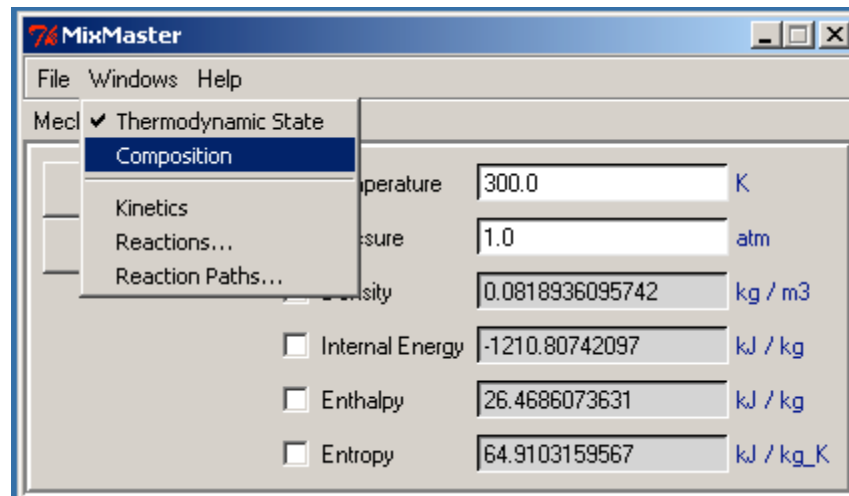
or select it from the Start menu

# The Thermodynamic Properties Window

- When MixMaster starts, you will see a window that looks like this



- To view the mixture composition, select the 'Composition' window



# Setting the Mixture State

The state updates automatically whenever a property value or the composition is changed

specify two property values  
(check the box to activate a property)

The screenshot shows the MixMaster software interface. The top menu bar includes 'File', 'Windows', and 'Help'. Below the menu bar is the 'Mechanisms' section. The main area is divided into two panels. The upper panel contains a 'Set State' button and a list of properties with checkboxes and input fields. The lower panel contains a table of species and moles, along with radio buttons for 'Moles', 'Mass', and 'Concentration', and a 'Hide Missing Species' checkbox. Two arrows point from the text above to the 'Pressure' and 'Enthalpy' input fields. A third arrow points from the text 'specify the composition' to the 'Moles' radio button.

Property	Value	Unit
Temperature	574.070222287	K
Pressure	1.0	atm
Density	0.0427963024705	kg / m <sup>3</sup>
Internal Energy	1632.38891795	kJ / kg
Enthalpy	4000.0	kJ / kg
Entropy	74.3135304698	kJ / kg_K

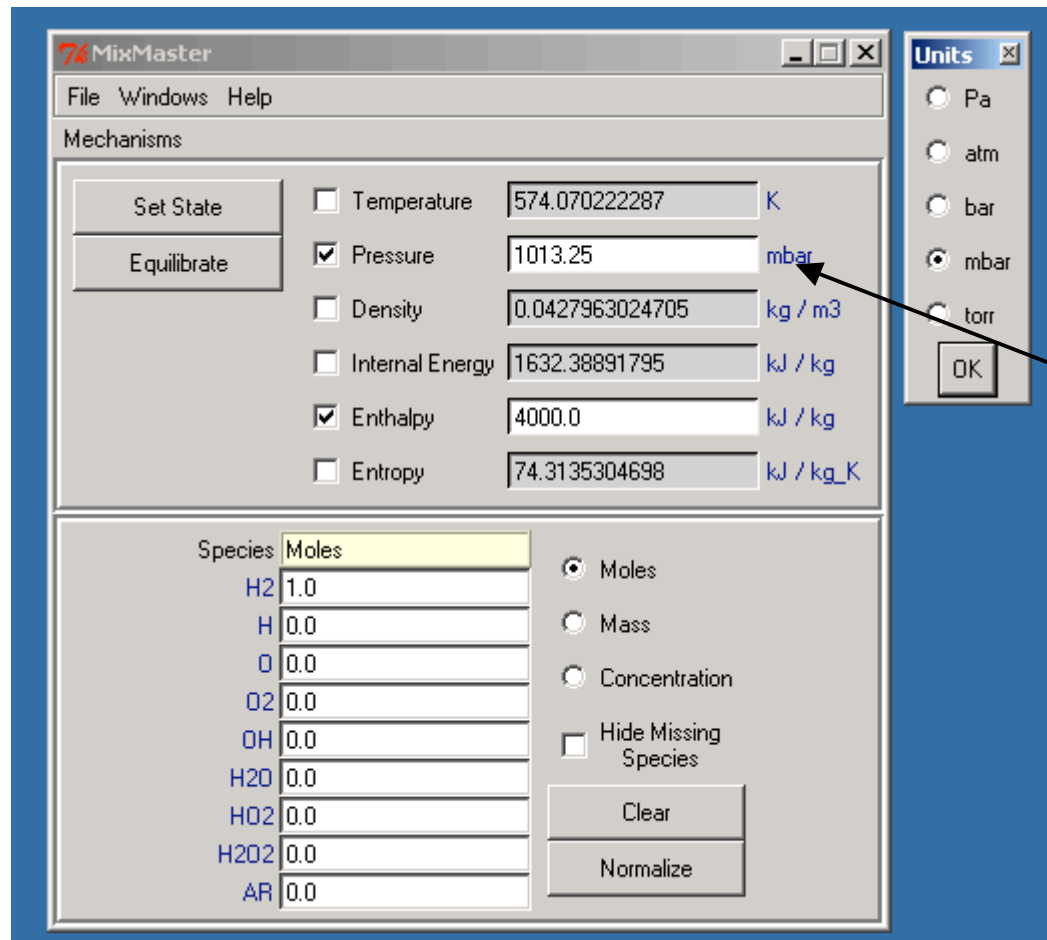
  

Species	Moles
H <sub>2</sub>	1.0
H	0.0
O	0.0
O <sub>2</sub>	0.0
OH	0.0
H <sub>2</sub> O	0.0
HO <sub>2</sub>	0.0
H <sub>2</sub> O <sub>2</sub>	0.0
AR	0.0

specify the composition

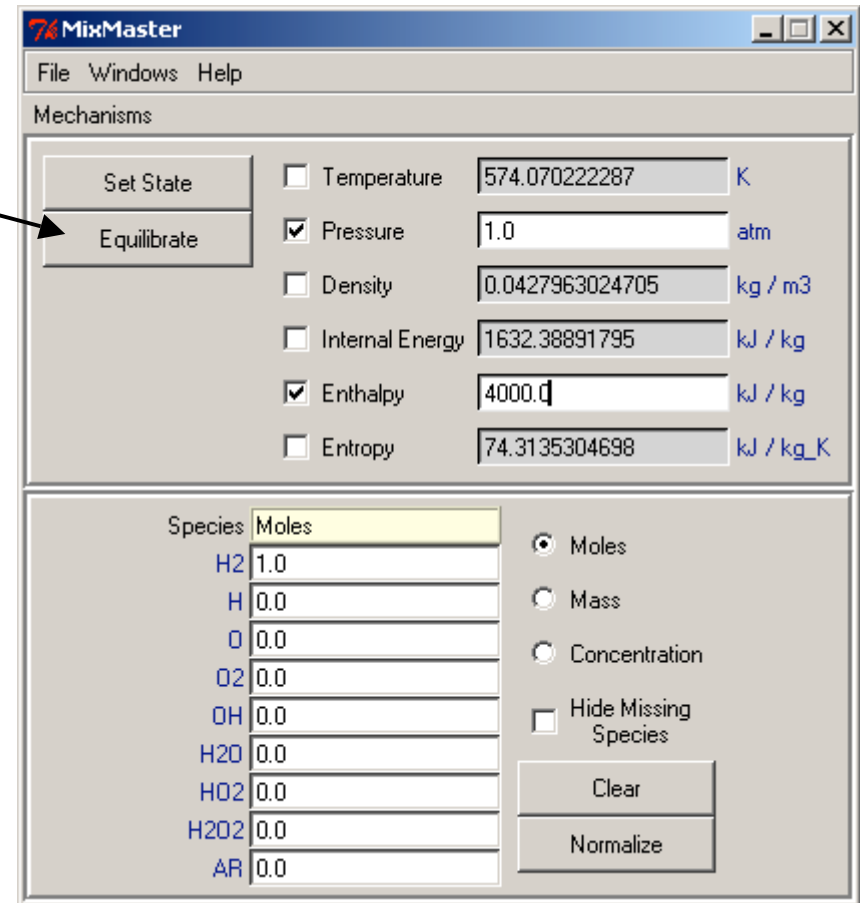
# Units

- Double-click on a unit string to change units



# Chemical Equilibrium

- Press the 'Equilibrate' button to set the mixture to a state of chemical equilibrium
- Specified property values held fixed
- Mixture elemental composition held fixed



The screenshot shows the 'MixMaster' software interface. The 'Mechanisms' panel is active, displaying a list of properties with checkboxes and input fields. The 'Equilibrate' button is highlighted by an arrow. Below the properties panel, there is a table for species moles and a set of radio buttons for units.

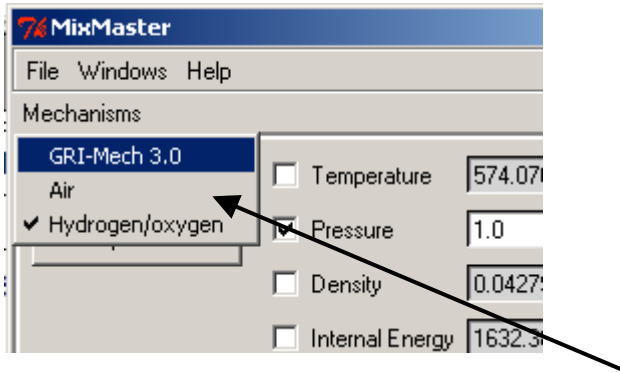
Species	Moles
H2	1.0
H	0.0
O	0.0
O2	0.0
OH	0.0
H2O	0.0
HO2	0.0
H2O2	0.0
AR	0.0

Units:  Moles,  Mass,  Concentration

Hide Missing Species

Buttons: Clear, Normalize

# Pre-Loaded Mixtures



- When MixMaster starts up, it loads three mixtures, each corresponding to a different reaction mechanism
- The H/O/Ar mixture is initially selected
- Switch between loaded mixtures using the 'Mixtures' menu

Mechanism	Description	Elements	Species	Rxns
GRI-Mech 3.0*	natural gas combustion	H C O N Ar	53	325
Air	subset of GRI-Mech 3.0	N O Ar		
H/O/Ar	subset of GRI-Mech 3.0	H O Ar		

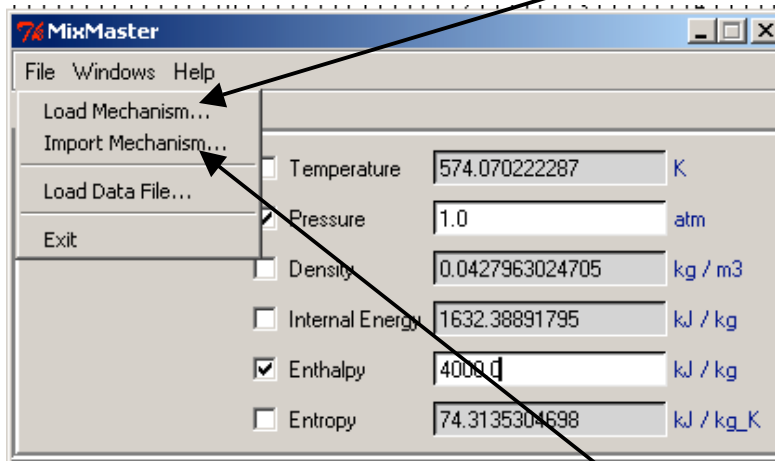
\*[http://www.me.berkeley.edu/gri\\_mech](http://www.me.berkeley.edu/gri_mech)



# Loading Reaction Mechanisms from Files

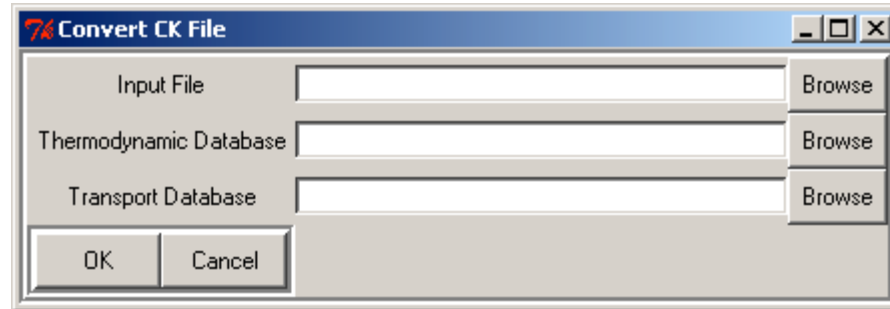
Select 'File' then...

select 'Load Mechanism' to load a reaction mechanism from a file in CTML format



select 'Import Mechanism' to convert a Chemkin™-format mechanism file to CTML and then load it

# Importing Chemkin™-Format Files



- Enter the input file name
- If the input file is missing some or all species data, enter the name of the file where the data may be found. This may be any other Chemkin™-format mechanism file containing a THERMO section, or a special thermodynamic database file
- If you want transport properties in the CTML file that is generated, enter the transport database name

# Viewing Species Properties

The screenshot displays the MixMaster software interface. On the left, the 'Mixtures' panel shows state settings: Temperature (300.0), Pressure (1.0), Density (0.08189), Internal Energy (-1210.8), Enthalpy (26.4686), and Entropy (64.9103). Below this is a species list with moles for H2 (1.0), H (0.0), O (0.0), O2 (0.0), OH (0.0), H2O (0.0), HO (0.0), H2O2 (0.0), and AR (0.0). The 'H2O' species is highlighted. The main window shows the 'H2O' properties for 1 O 2 H atoms. The standard heat of formation at 298 K is -241.81 kJ/mol, and the molar mass is 18.01528. The current temperature is 1690.000 K. The specific heat capacity (c\_p) is 49.1621788458 kJ/kg\_K, the enthalpy is -184434.522526 kJ/kg, and the entropy is 433318.493053 kJ/kg\_K. Three graphs show c\_p/R (5.9132), enthalpy/RT (-13.1264), and entropy/R (30.8397) versus temperature. A slider at the bottom is set to 1690.000 K.

Property	Value	Units
Standard Heat of Formation at 298 K	-241.81	kJ/mol
Molar Mass	18.01528	
Temperature	1690.000	K
c_p	49.1621788458	kJ / kg_K
Enthalpy	-184434.522526	kJ / kg
Entropy	433318.493053	kJ / kg_K

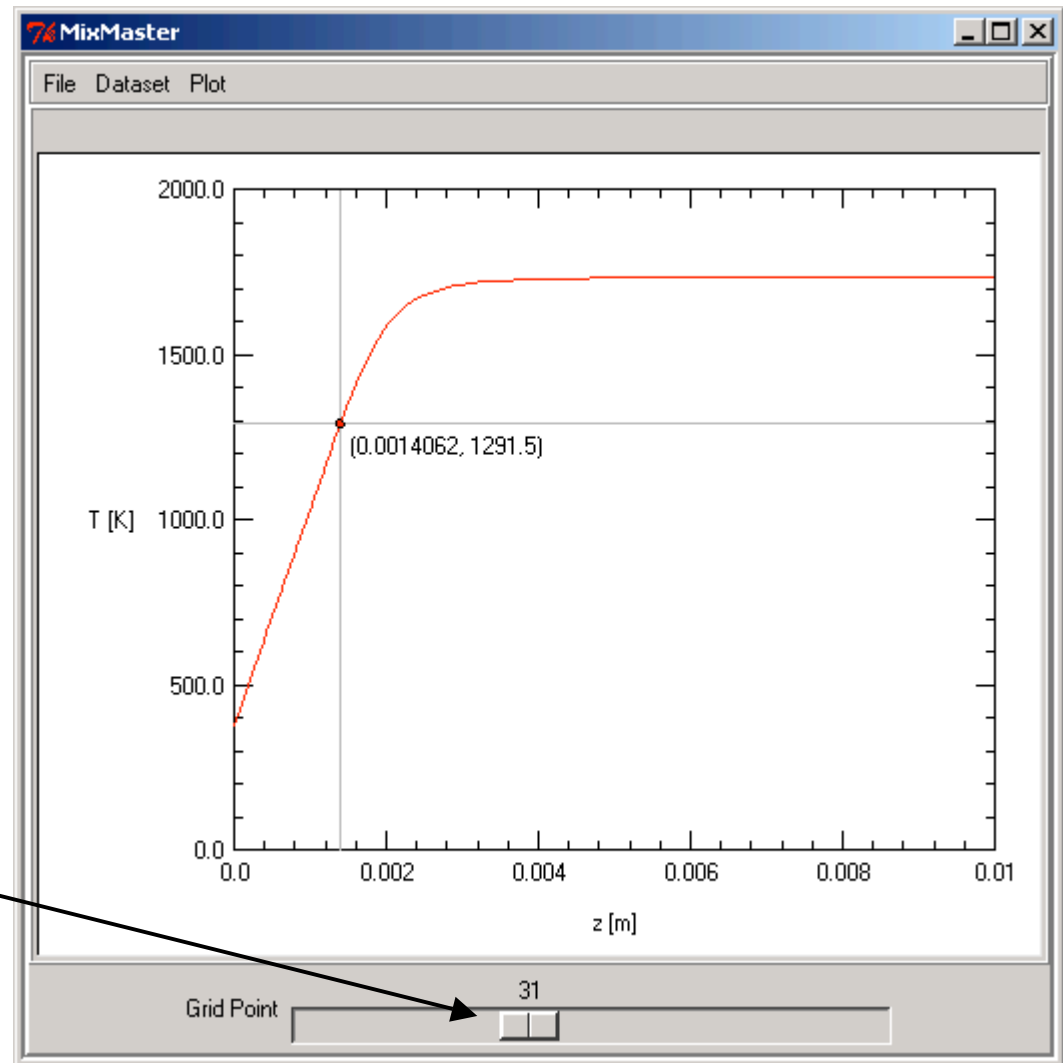
Property	Value
c_p/R	5.9132
enthalpy/RT	-13.1264
entropy/R	30.8397

double-click on species name to view properties

slider changes temperature

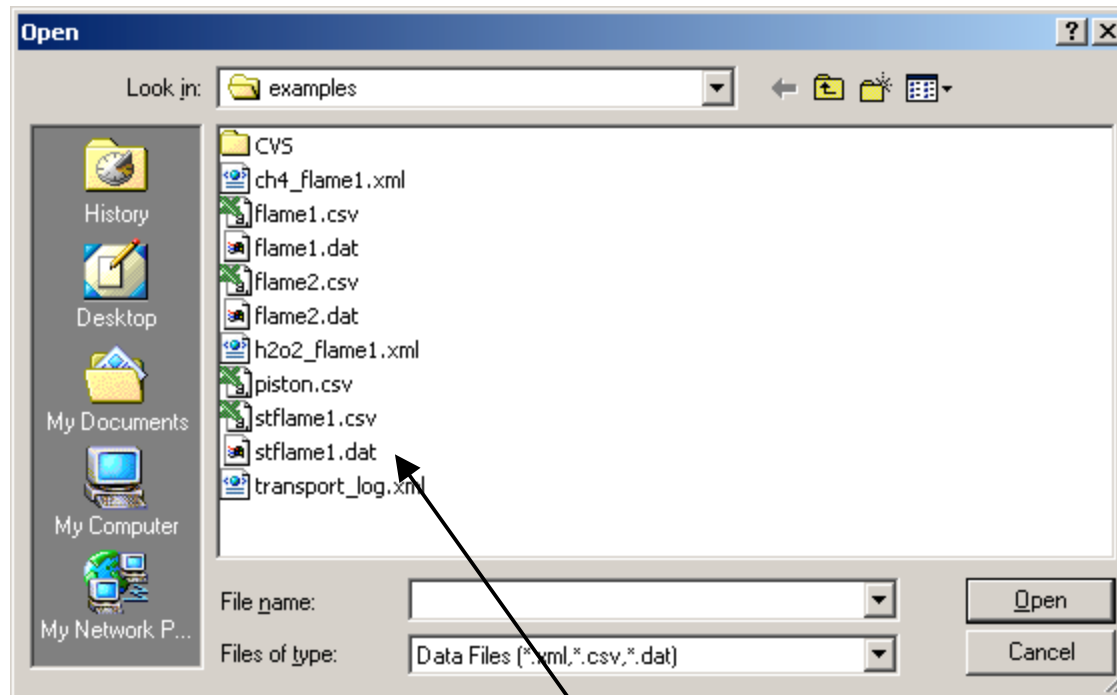
# Postprocessing Simulation Data

- MixMaster can be used to view / postprocess simulation output
- Simulation data can be generated by any program that can write a text file, whether it uses Cantera or not
- Moving the slider sets the mixture state to the T, P, and mass fractions at a specific grid point



# Loading a Data File

- On the **File** menu, select **Load Data File**



select the desired file

# Creating a Data File

- Create an Excel spreadsheet and save it in CSV format, or create a text file with comma-separated columns

Temperature in K

Pressure in Pa

Species mass fractions  
(not mole fractions)

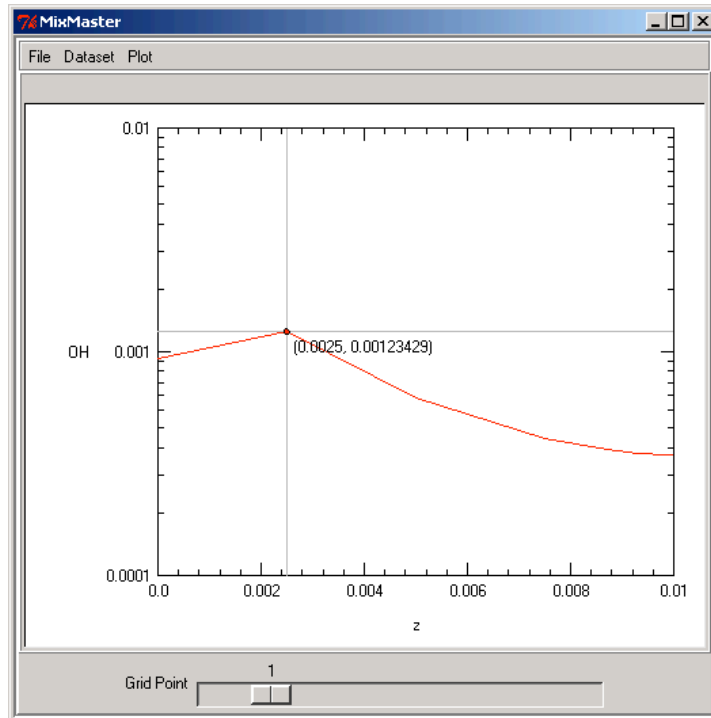
z (cm)	T	P	H2	H	O	OH
0.1	1200	1.00E+05	0.1	0.0056	0.000007	0.00044
0.15	1246	1.01E+05	0.098	0.006	0.000006	0.00034
0.2	1292	1.02E+05	0.096	0.0064	0.000005	0.00024

↑  
Independent variable  
must be in first column

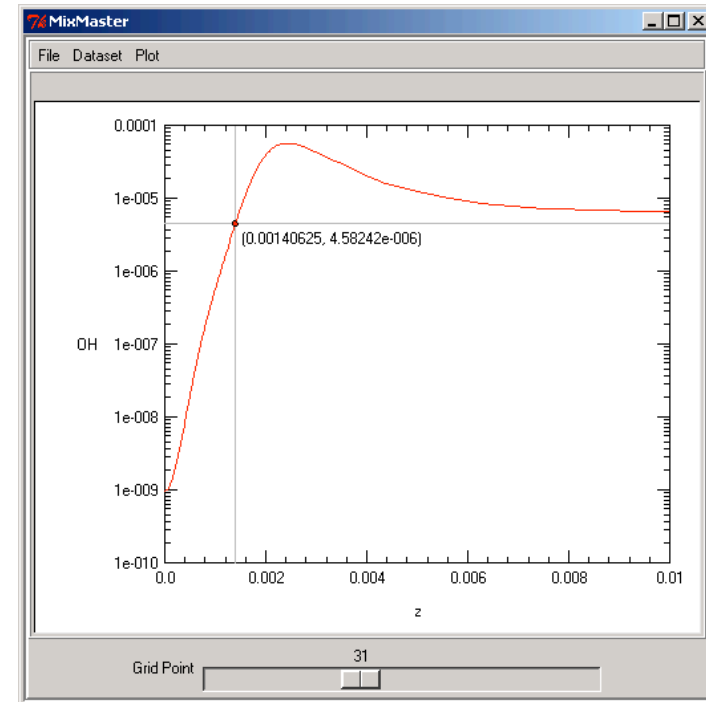
- First row must contain variable names
- columns labeled 'T' and 'P' are required
- columns labeled 'u' and 'V' may optionally be included
- additional column headings are matched against species names in the current mechanism
- missing species are set to zero, and unrecognized ones are ignored

# Postprocessing Flame Simulations

- MixMaster can also read the CTML output files produced in 1D flame simulations with Cantera
- Output files may contain multiple solutions

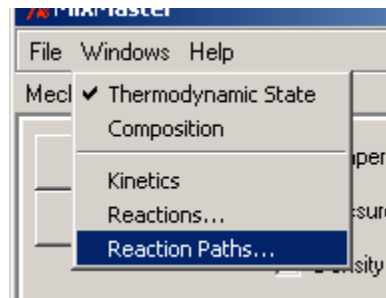


8-point solution with fixed temperature profile

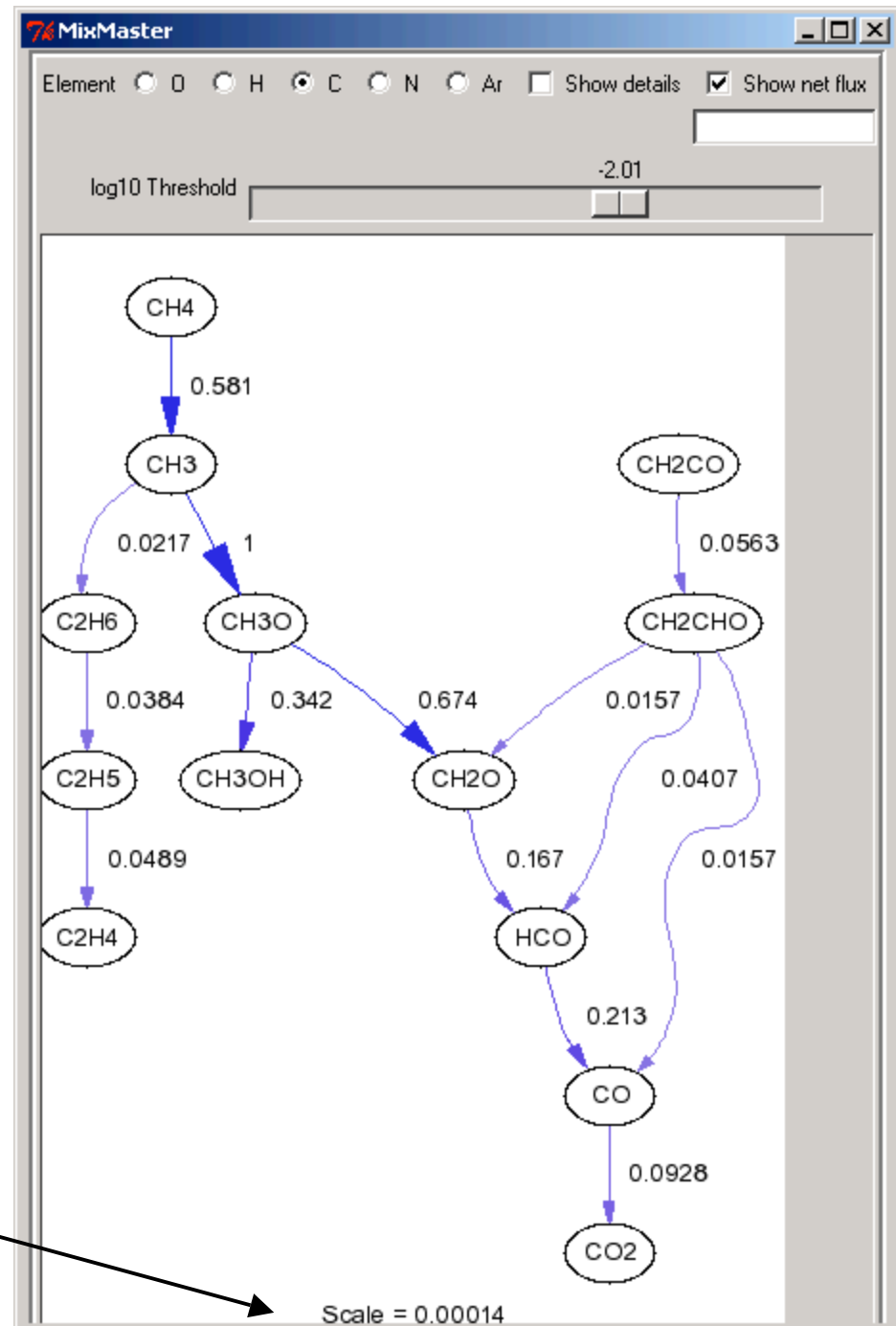


82-point solution with the energy equation enabled

# Reaction Path Diagrams



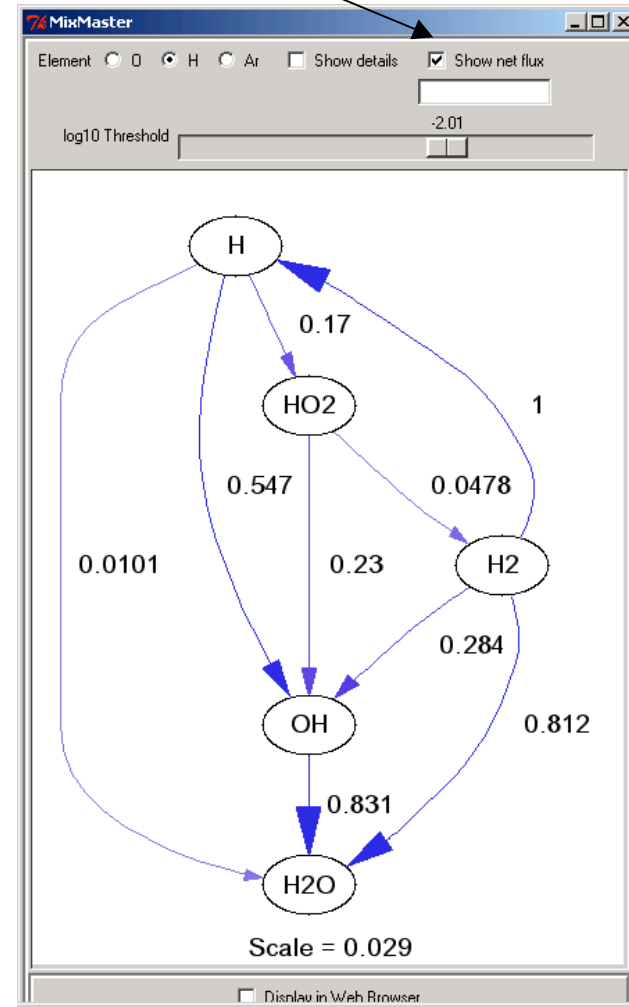
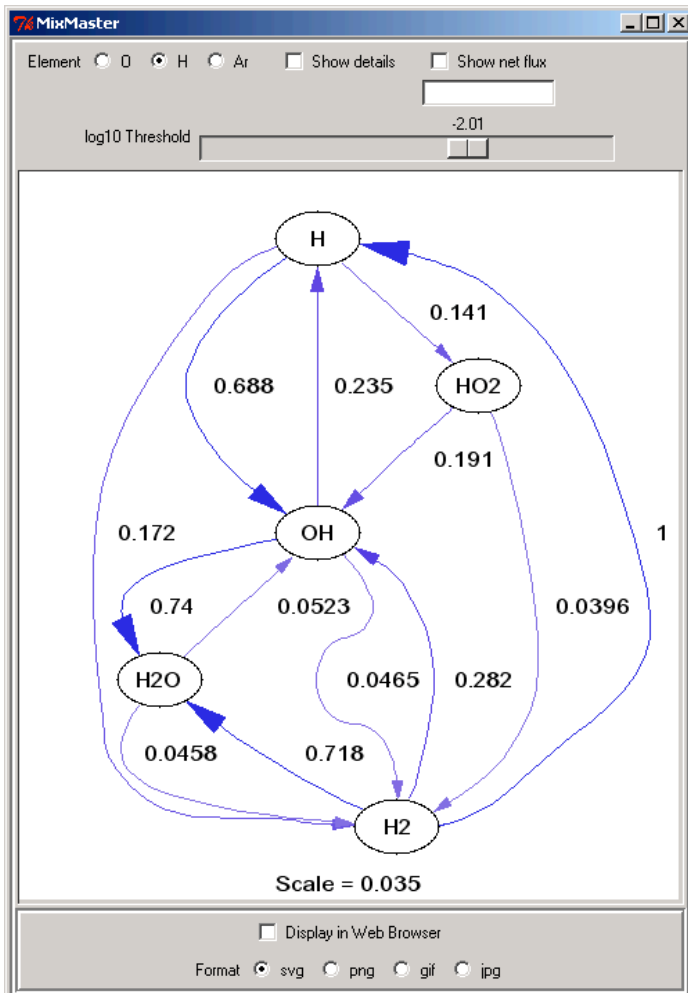
- View 'flow' of a conserved element through species due to reactions
- Diagram updates automatically if states changes
- Path strengths are relative to maximum
- Absolute scale shown at bottom





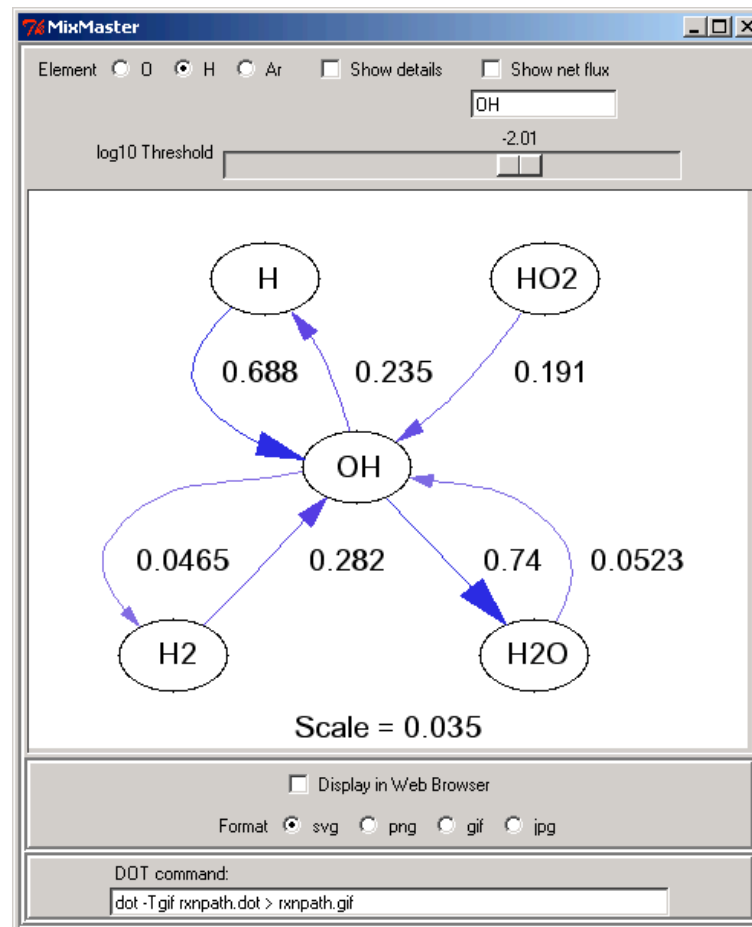
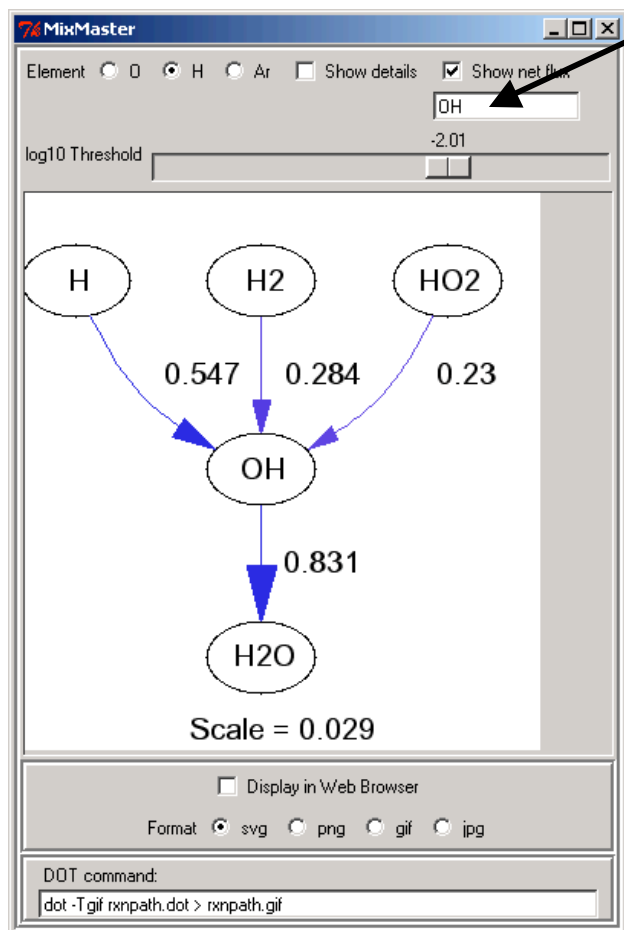
# View bi-directional or net fluxes

check box for net flux

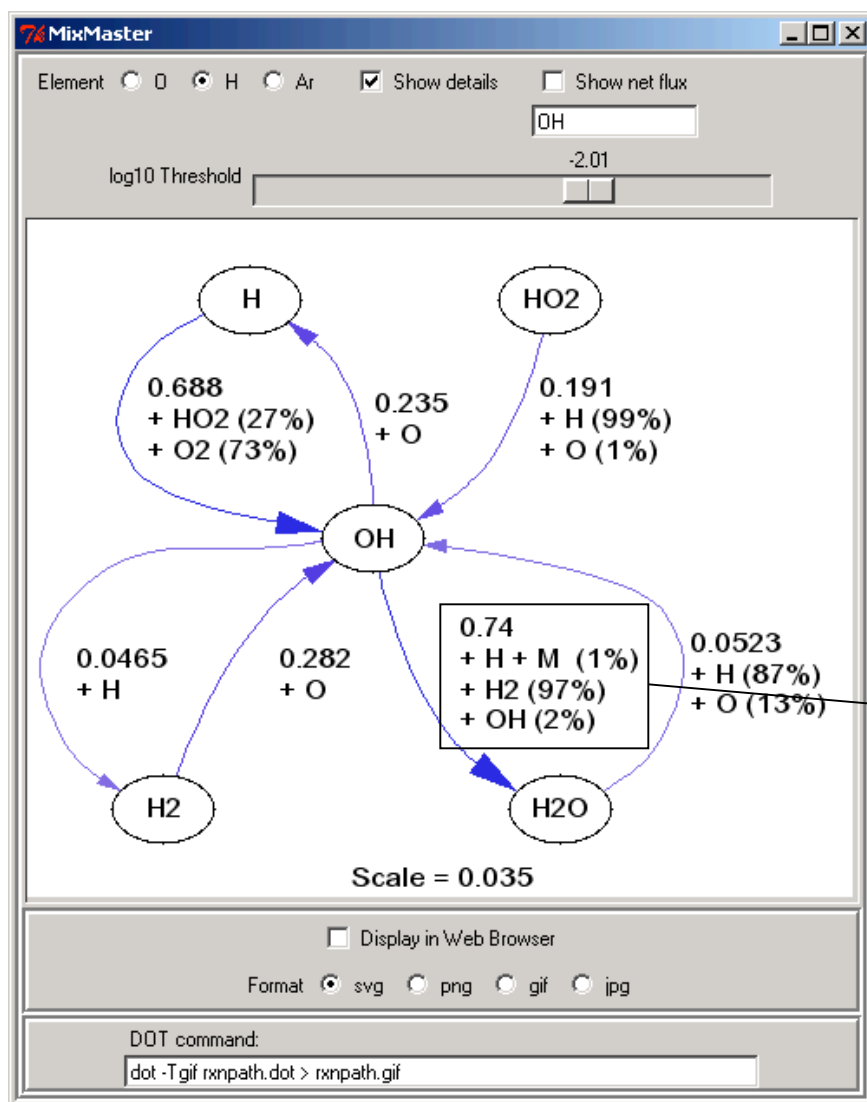


# View the fluxes to and from one species

enter species name here



# View Details



- If more than one reaction contributes to a path, the other reactant(s) are listed, along with the relative contribution of each reaction

$\text{OH} + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$   
is responsible for 97% of the flux of elemental H from OH to  $\text{H}_2\text{O}$ , and  $\text{OH} + \text{H} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M}$  is only responsible for 1%