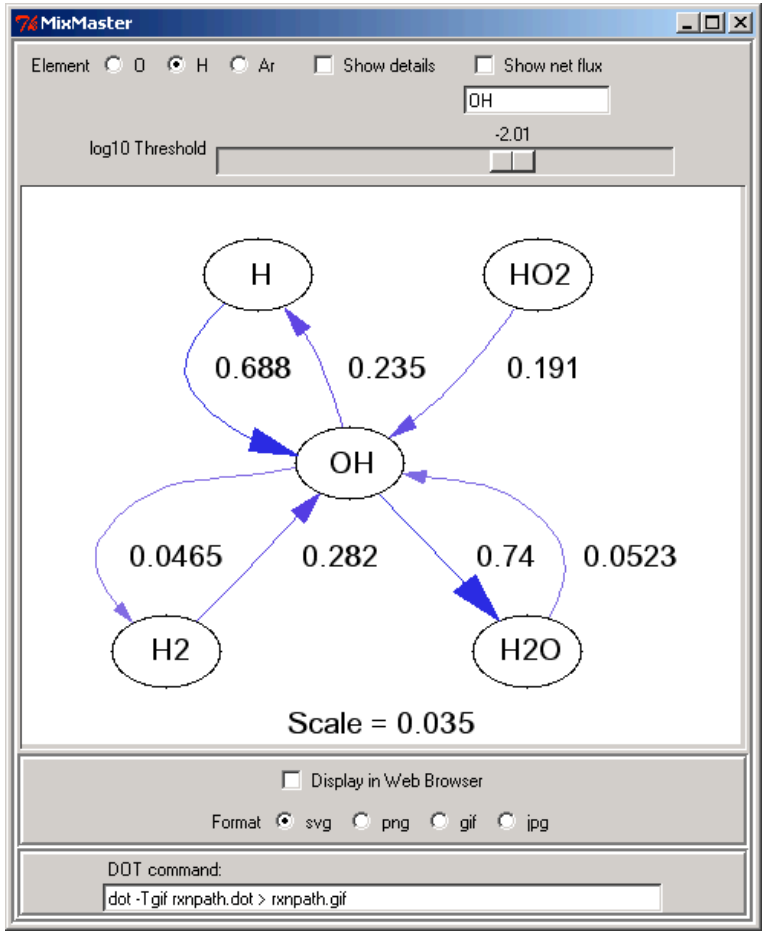
MixMaster

A Cantera Application

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

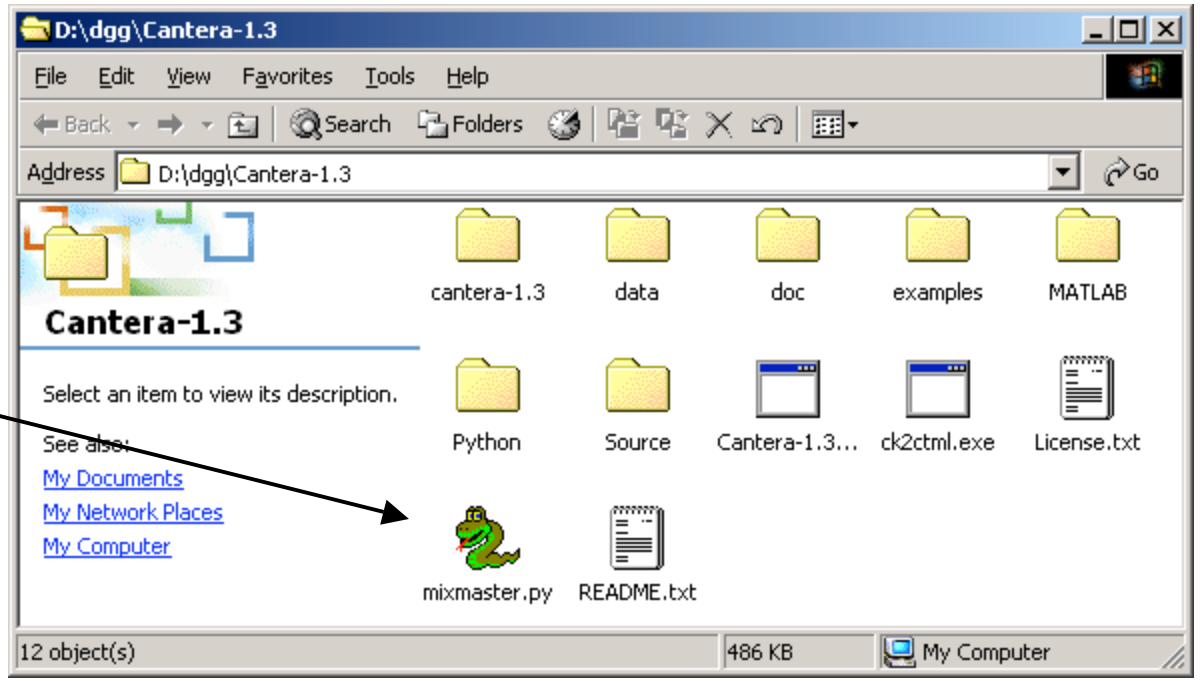
- import reaction mechanisms in standard file formats
- view/set the state of mixtures
- carry out thermodynamic processes
- compute chemical equilibrium
- view species properties
- view reaction data
- postprocess simulation data
- view reaction paths

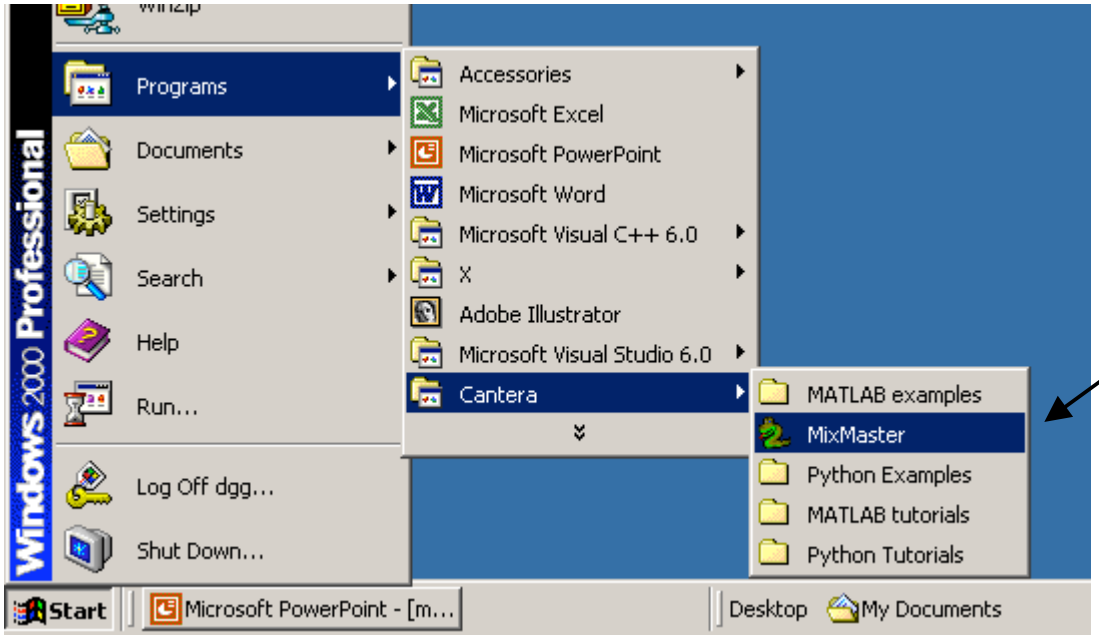


MixMaster 2003

Getting Started

double-click the MixMaster icon in the Cantera folder

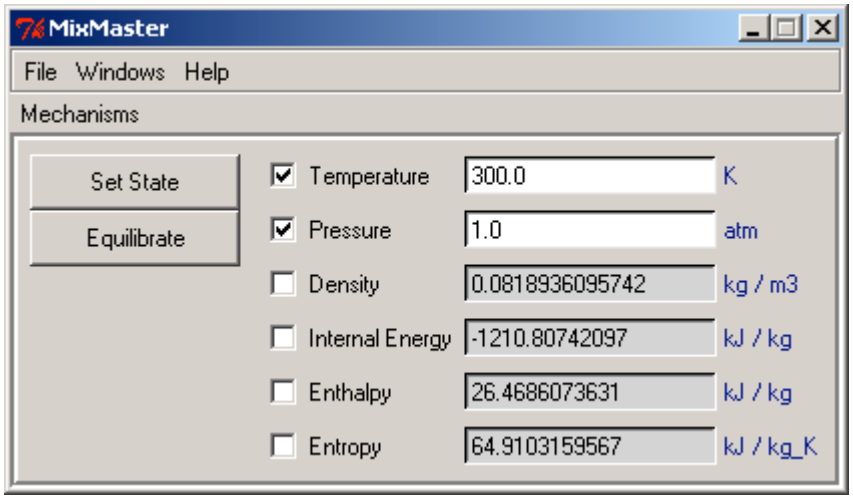




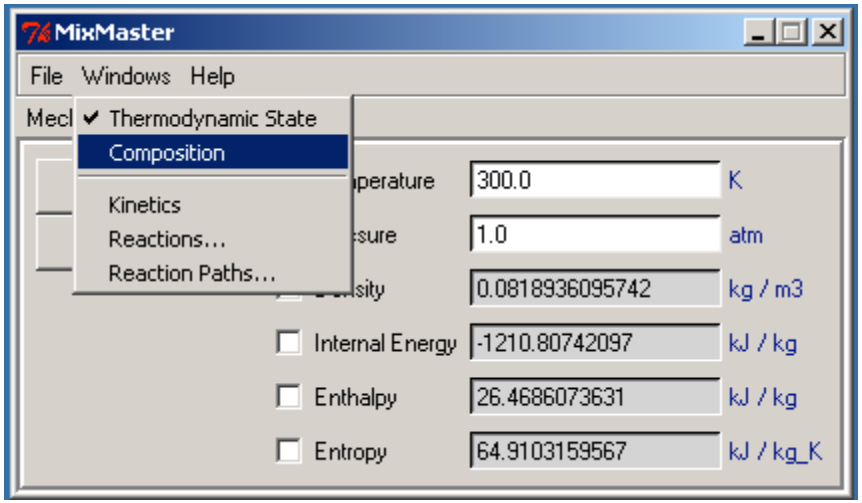
or select it from the Start menu

The Thermodynamic Properties Window

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



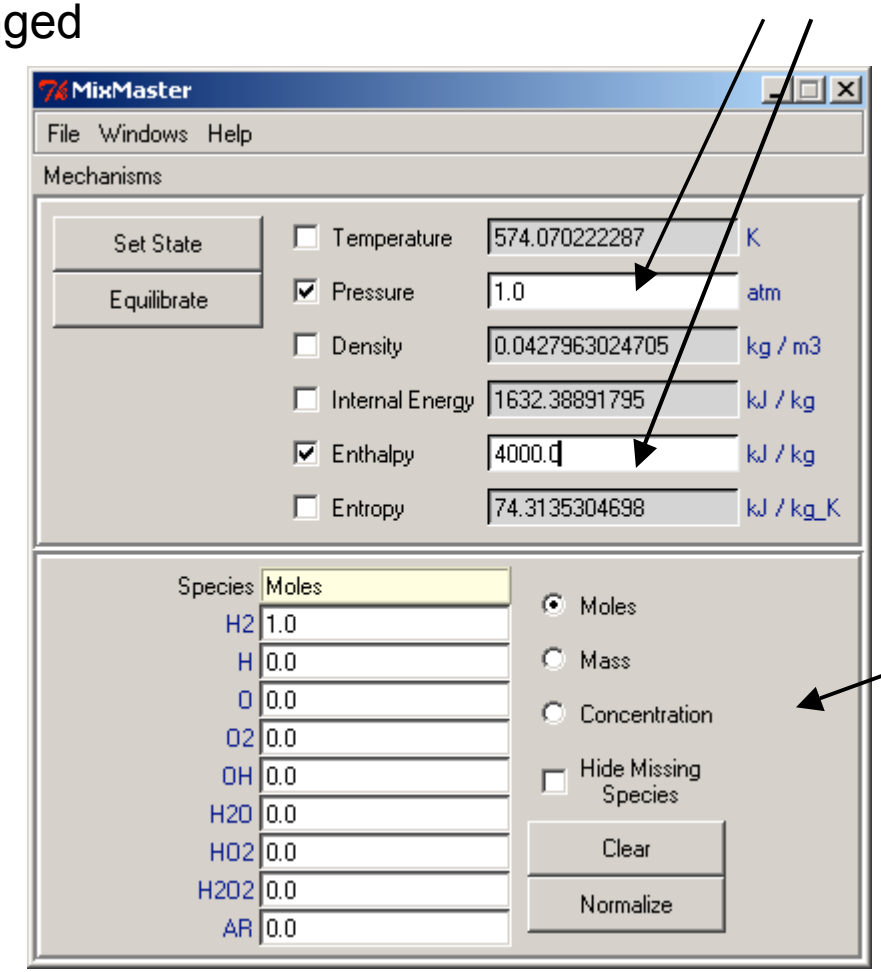
- To view the mixture composition, select the 'Composition' window



Setting the Mixture State

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

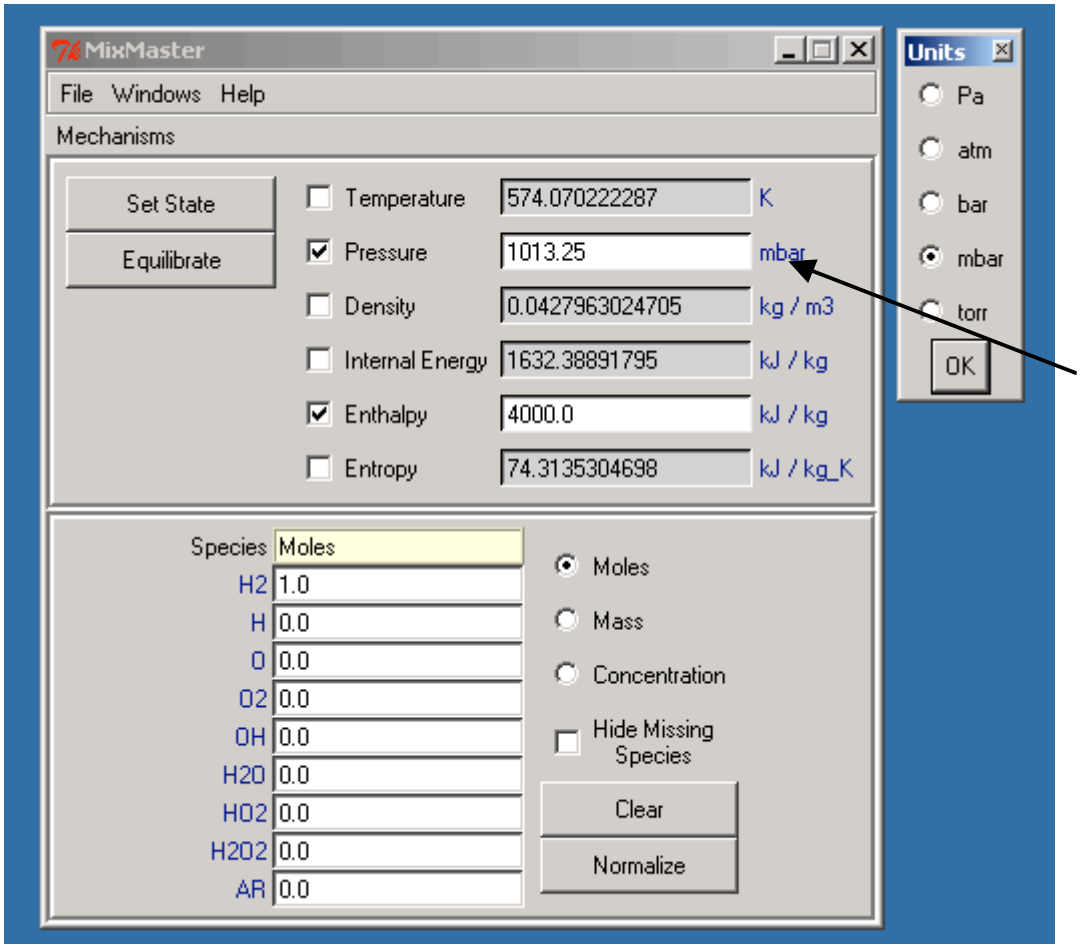
specify two property values (check the box to activate a property)



specify the composition

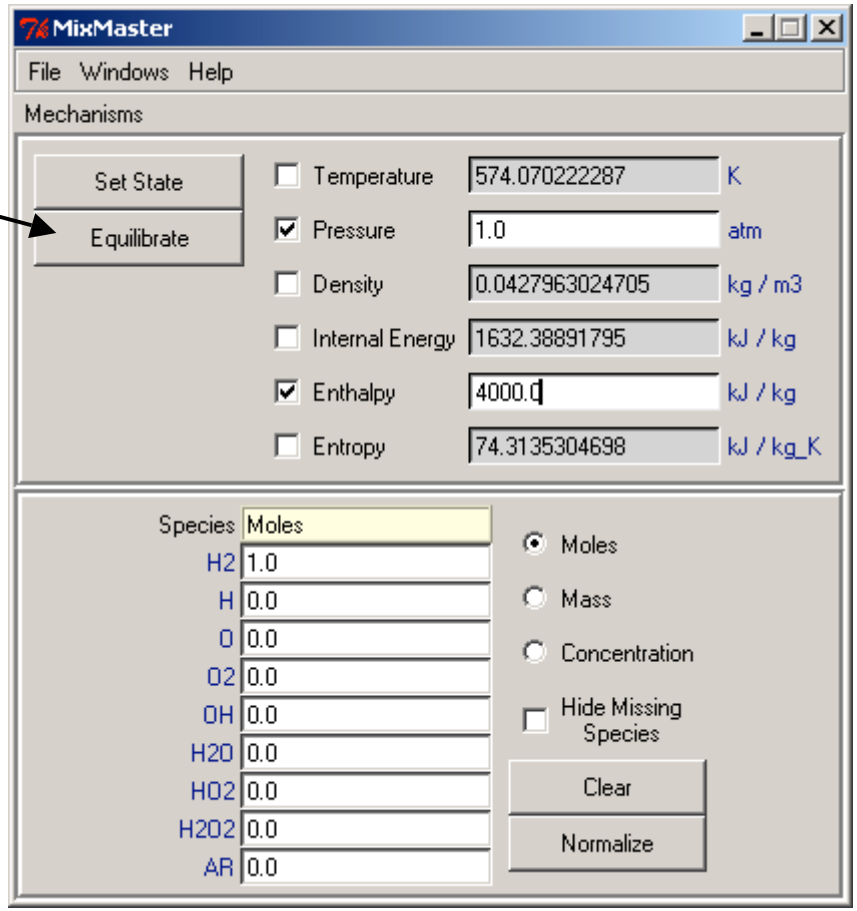
Units

- Double-click on a unit string to change units

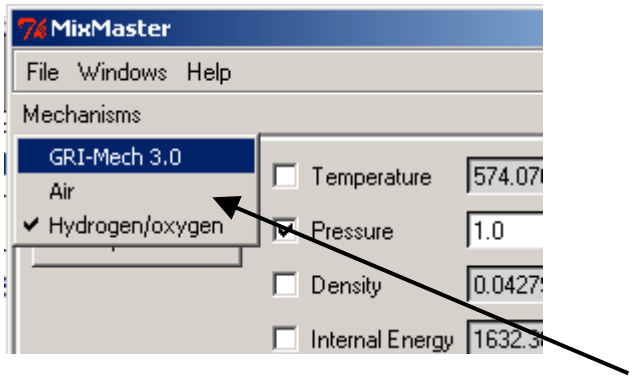


Chemical Equilibrium

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



Pre-Loaded Mixtures



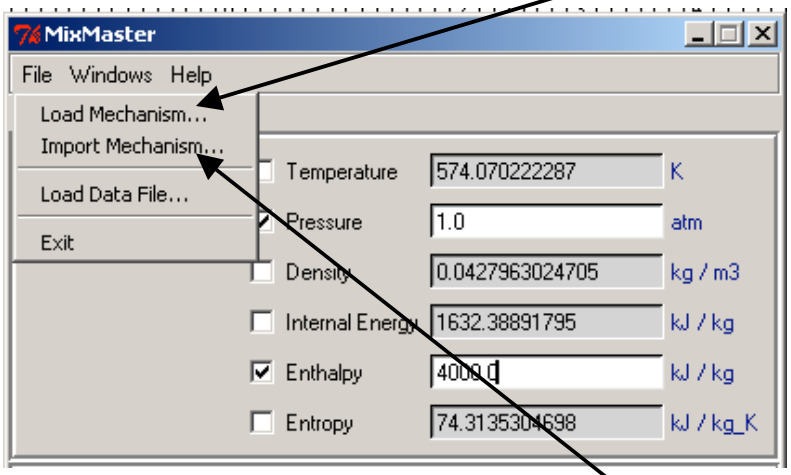
- When MixMaster starts up, it loads three mixtures, each corresponding to a different reaction mechanism
- The H/O/Ar mixture is initially selected
- Switch between loaded mixtures using the 'Mixtures' menu

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

Loading Reaction Mechanisms from Files

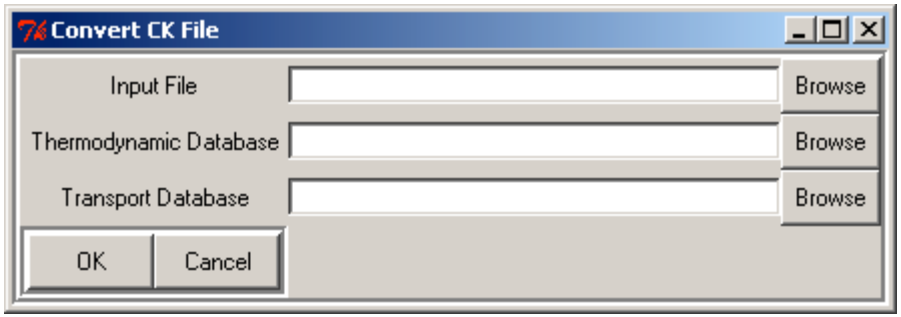
Select ‘File’ then…



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

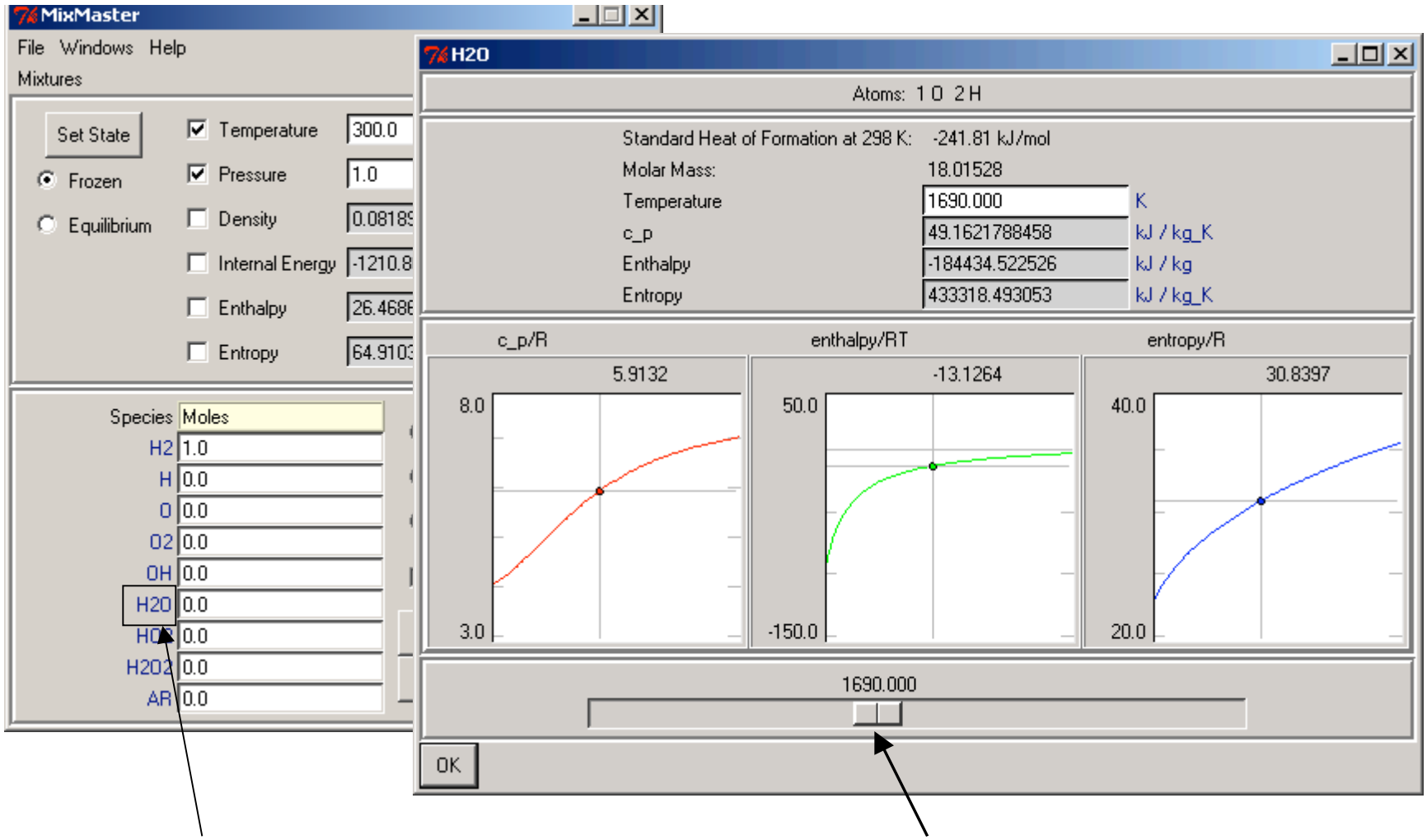
select ‘Import Mechanism’ to convert a Chemkin™-format mechanism file to CTML and then load it

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

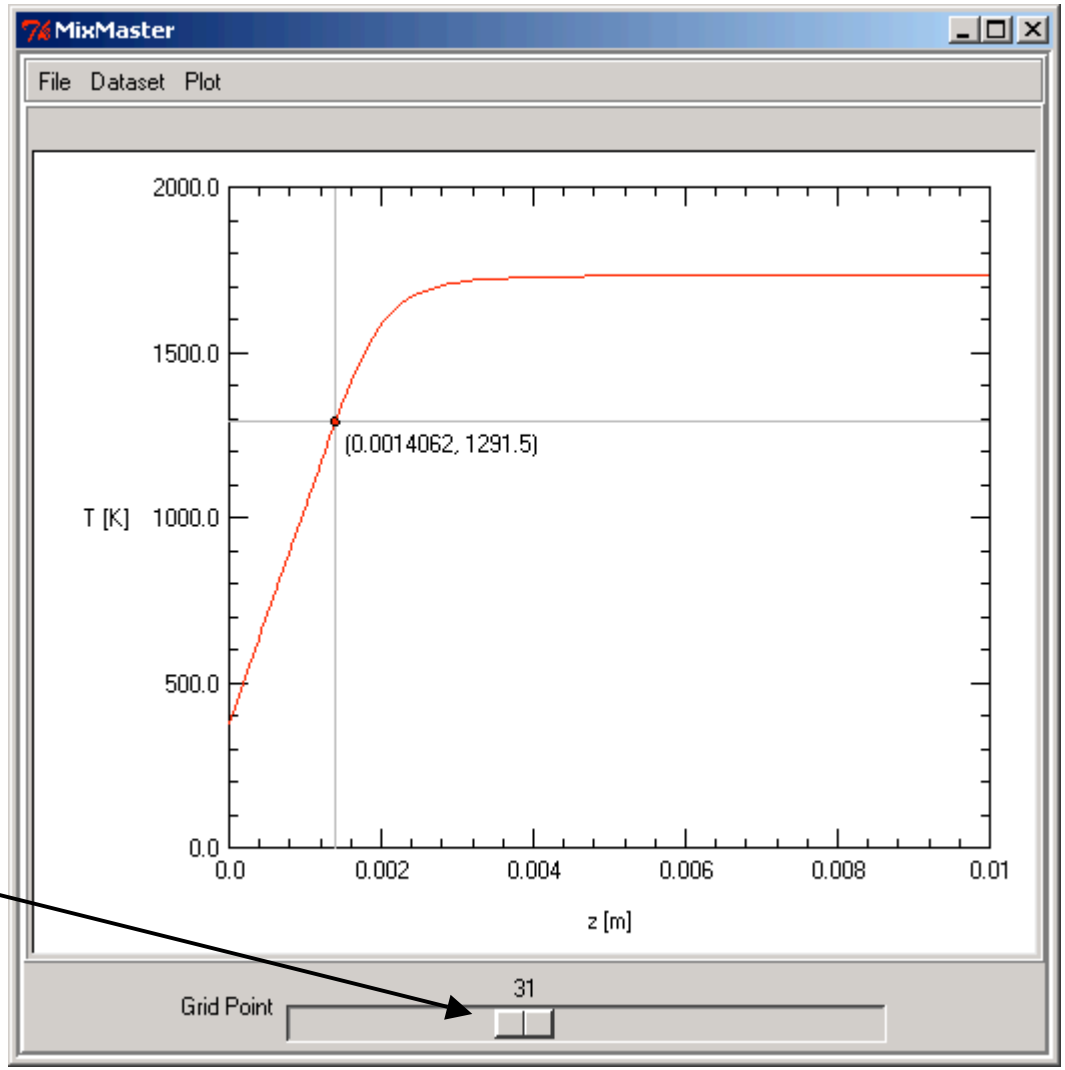


double-click on species name to view properties

slider changes temperature

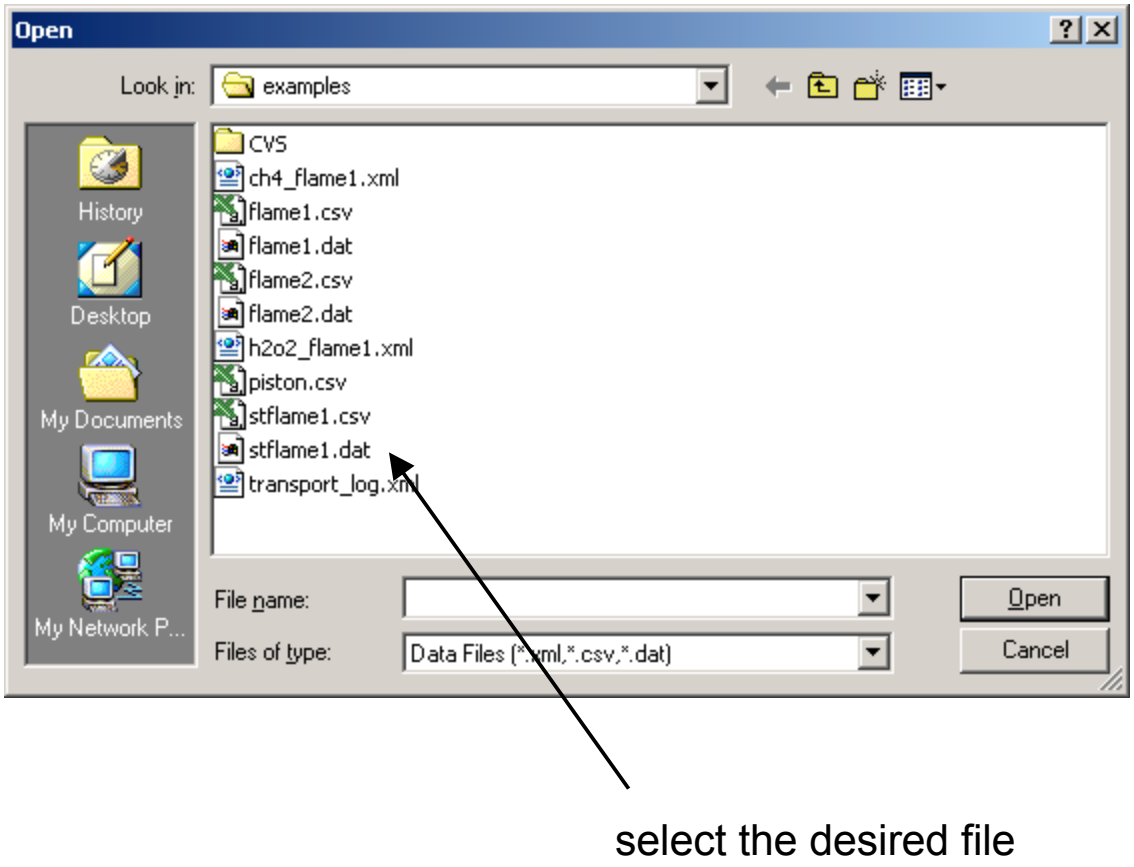
Postprocessing Simulation Data

- 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



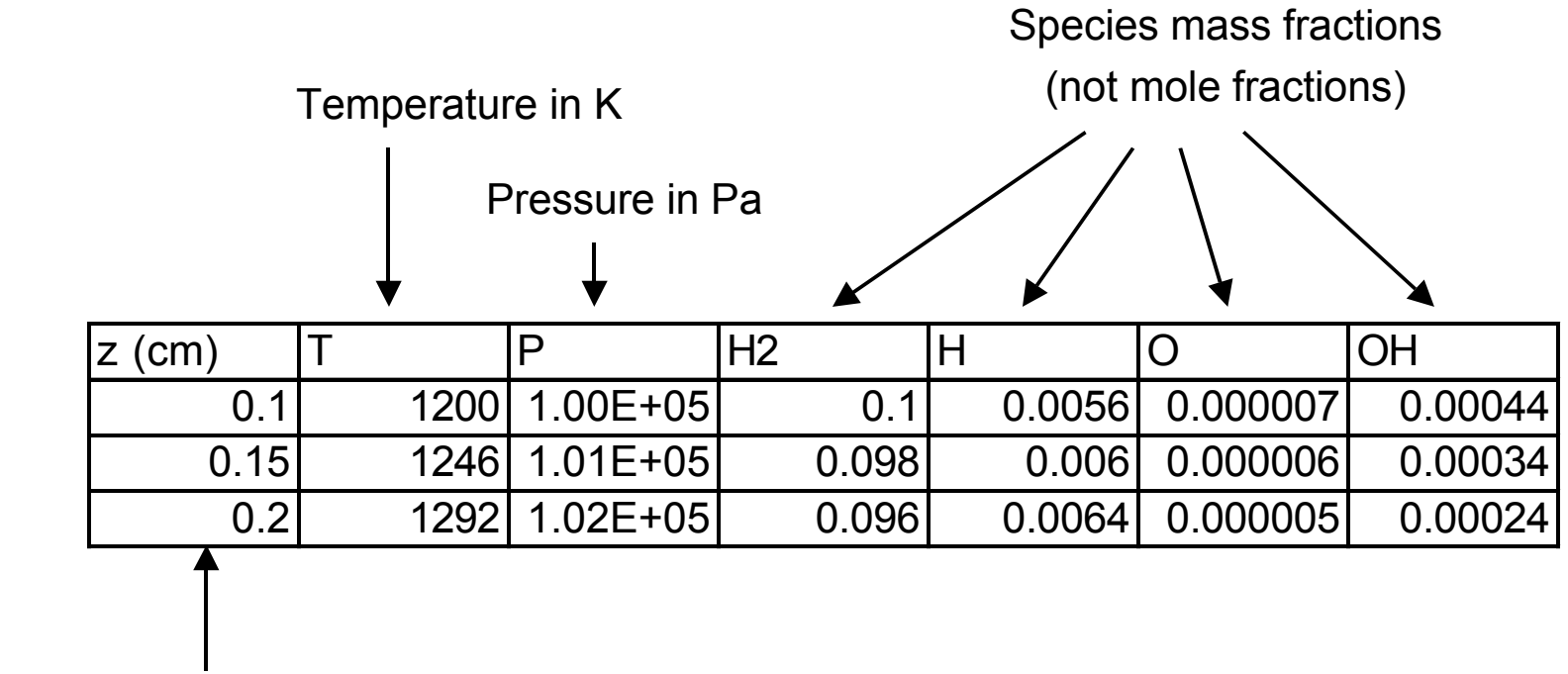
Loading a Data File

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



Creating a Data File

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



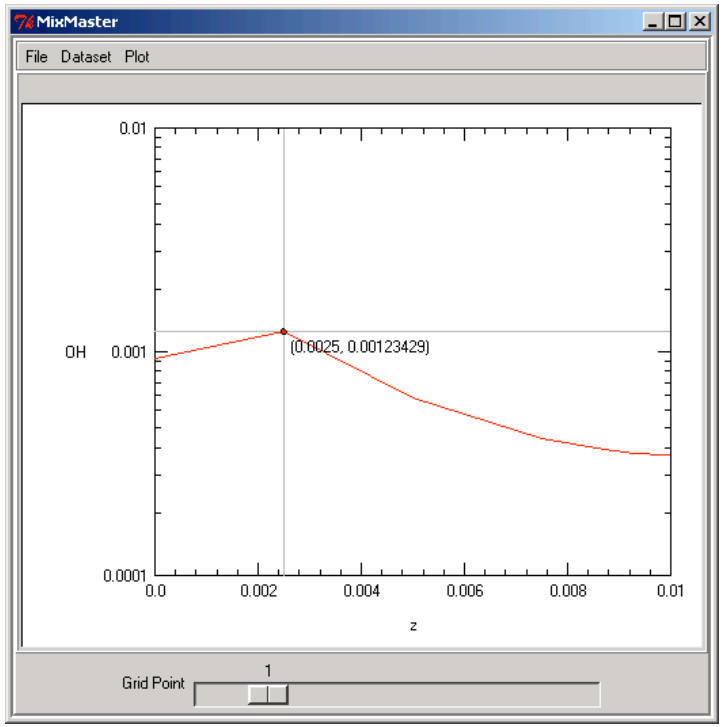
z (cm)	T	P	H2	H	O	OH
0.1	1200	1.00E+05	0.1	0.0056	0.000007	0.00044
0.15	1246	1.01E+05	0.098	0.006	0.000006	0.00034
0.2	1292	1.02E+05	0.096	0.0064	0.000005	0.00024

Independent variable must be in first column

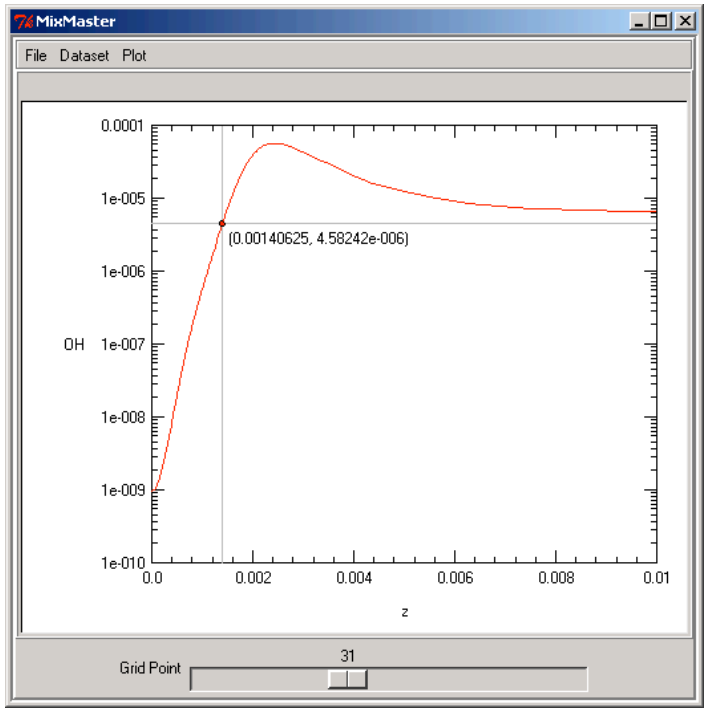
- First row must contain variable names
- columns labeled ‘T’ and ‘P’ are required
- columns labeled ‘u’ and ‘V’ may optionally be included
- additional column headings are matched against species names in the current mechanism
- missing species are set to zero, and unrecognized ones are ignored

Postprocessing Flame Simulations

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

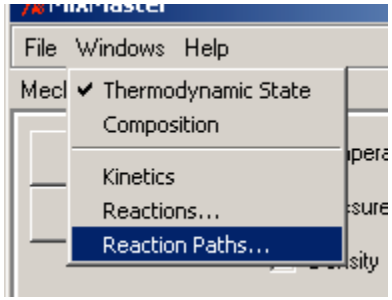


8-point solution with fixed temperature profile

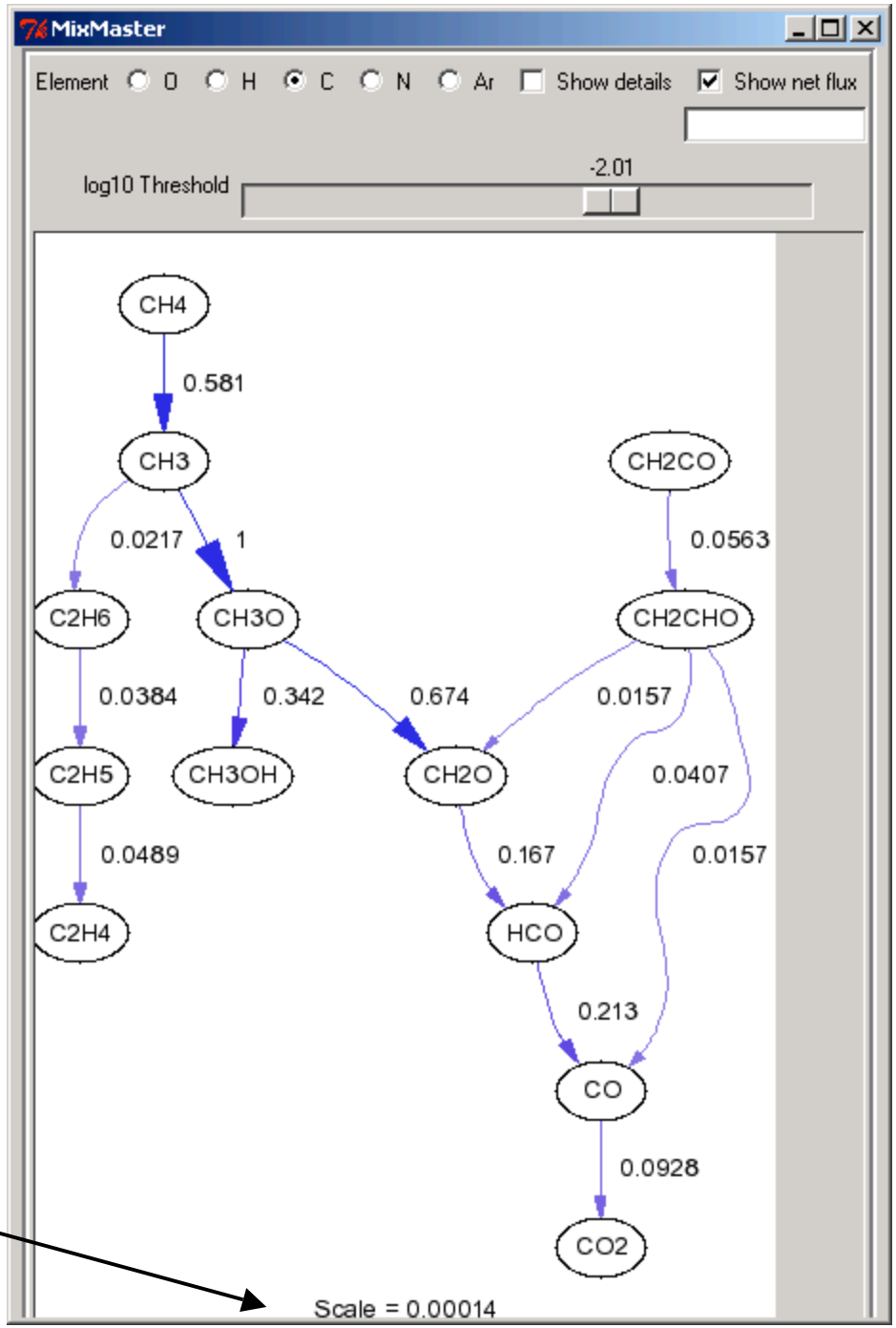


82-point solution with the energy equation enabled

Reaction Path Diagrams

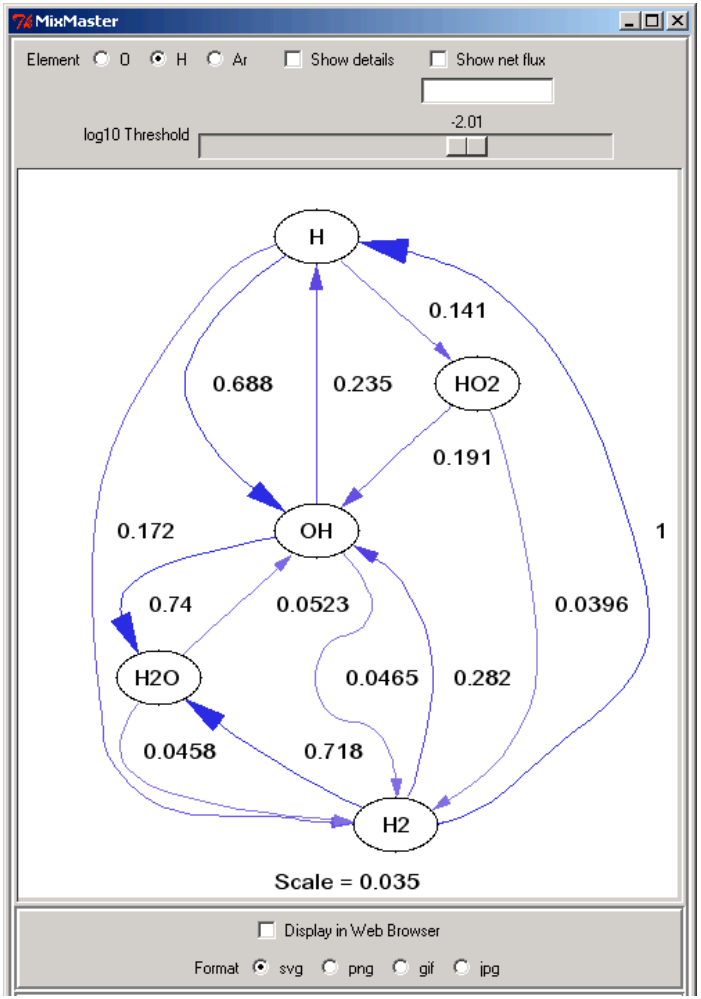


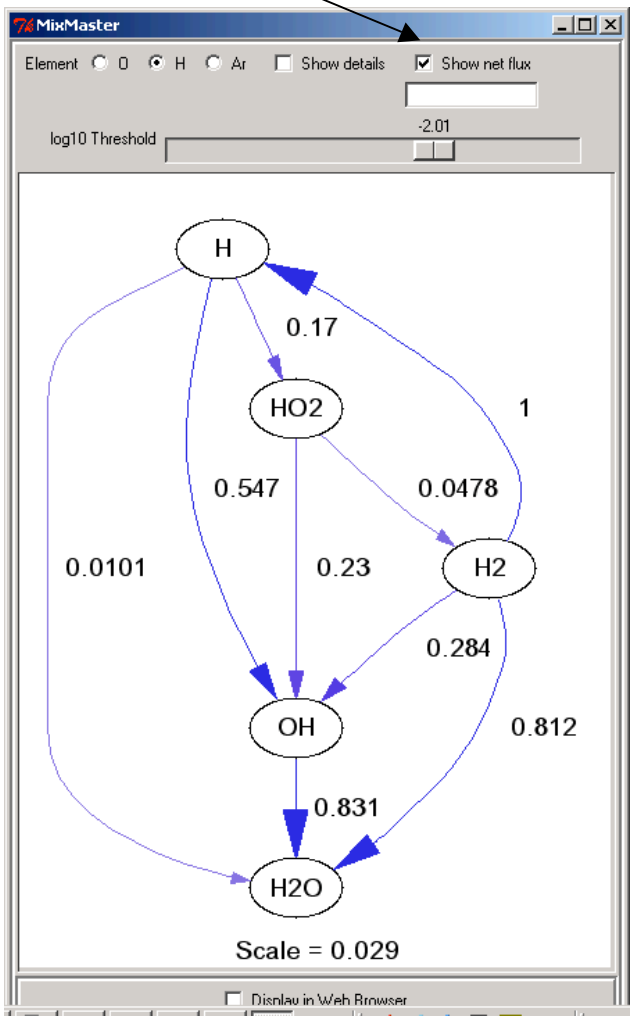
- View ‘flow’ of a conserved element through species due to reactions
- Diagram updates automatically if states changes
- Path strengths are relative to maximum
- Absolute scale shown at bottom



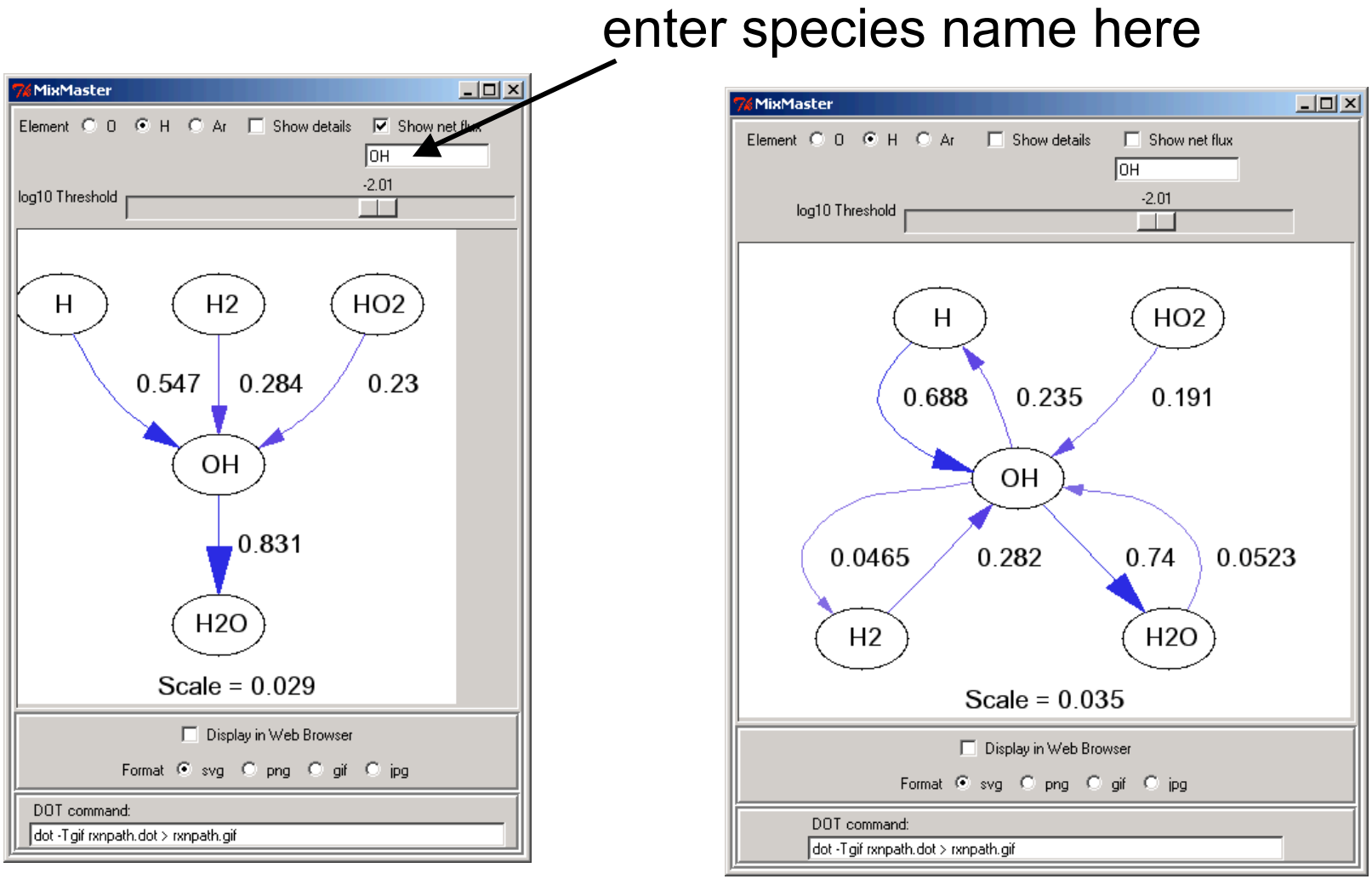
View bi-directional or net fluxes

check box for net flux

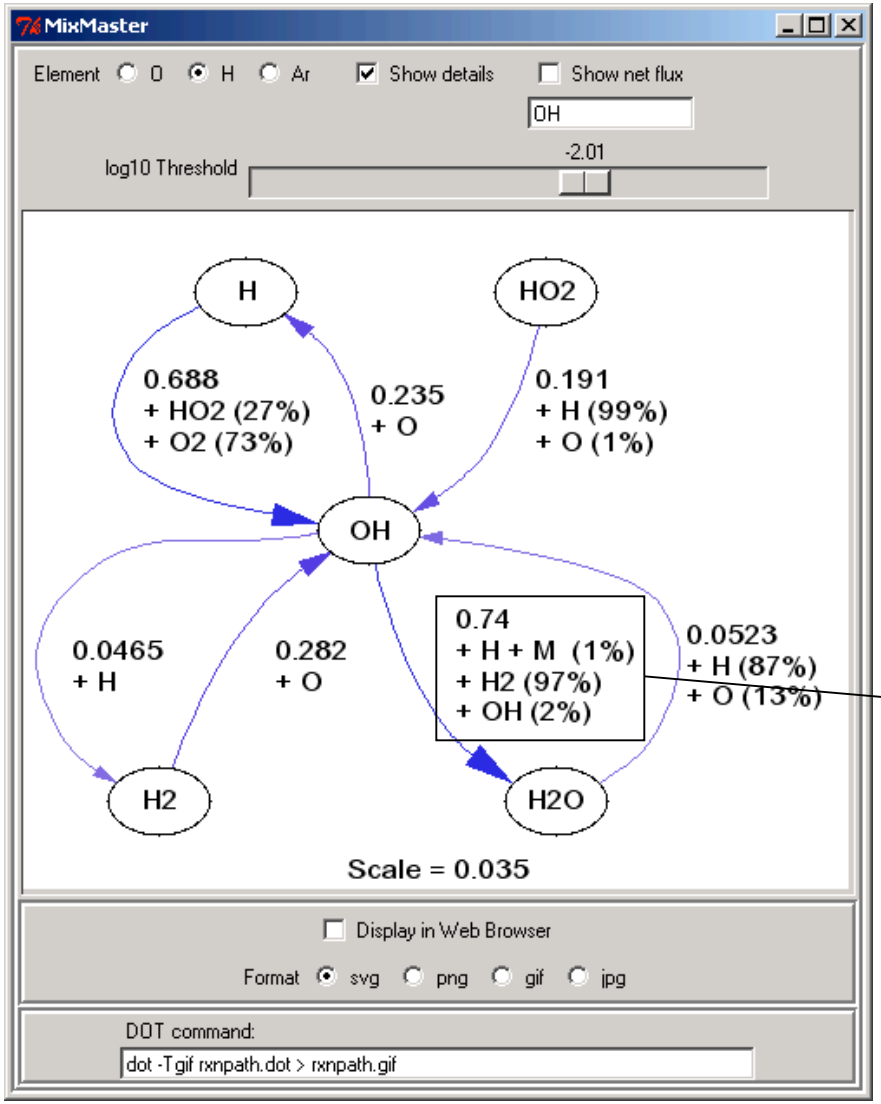




View the fluxes to and from one species



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

$OH + H_2 \rightarrow H + H_2O$ is responsible for 97% of the flux of elemental H from OH to H_2O, and $OH + H + M \rightarrow H_2O + M$ is only responsible for 1%