

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

double-click the MixMaster icon in the Cantera folder Select an Rem to view its description. Set The Methods Places My Computer Python Source Cartera-1.3 di2ctml.exe License.txt My Computer Python Source Cartera-1.3 di2ctml.exe License.txt My Computer Microsoft Visual Cit+ 6.0 Settings Microsoft Visual Cit+ 6.0 Settings Microsoft Visual Cit+ 6.0 Microsoft Visual Cit+ 6.0 Mi	etting Started	D:\dgg\Cantera-1.3	_ 🗆 🗙
double-click the MixMaster icon in the Cantera folder Select an item to view its description. Select an item to view its description. Python Source Cantera-1.3 d22tml.exe License.txt thy Documents Wy Computer I2 object(s) Nature Picture Select an item to view its description. Python Source Cantera-1.3 d22tml.exe License.txt thy Documents Wy Computer Normaster.py README.txt Select an item to view its description. Second to the Normatic Python Source Cantera-1.3 d22tml.exe License.txt thy Documents Microsoft Programs Settings Seti	g etaited	<u>File E</u> dit <u>V</u> iew F <u>a</u> vorites <u>T</u> ools <u>H</u> elp	1
double-click the MixMaster icon in the Cantera folder Cantera-1.3 data doc examples MATLAB Select an item to view its description. See The View its descript		$\leftarrow Back \checkmark \Rightarrow \checkmark \boxdot \bigcirc Search \land \boxdot Folders \bigcirc \overset{\otimes}{=} \overset$	
double-click the MixMaster icon in the Cantera folder Cantera-1.3 data doc examples MATLAB Select an item to view its description. Python Source Cantera-1.3 cl2ctml.exe License.txt My Documents My Documents My Documents Microsoft Excel Microsoft Word Microsoft Word Microsoft Visual Studio 6.0 Microsoft Visual Studio 6.0		Address D:\dgg\Cantera-1.3	▼ @Go
Canter a -1.3 Use a use use with description. Select an item to view its description. Wy Documents My Network Places My Computer With Computer	ouble-click the MixMaster		MATLOP
Select an item to view its description. Python Source Cantera-1.3, ck2ctml.exe License.txt Wy Documents Wy Computer Wicrosoft Bixel Wy Computer Image: Cantera Computer <t< td=""><td>con in the Cantera folder</td><td>Cantera-1.3 data dot examples</td><td>MATLAD</td></t<>	con in the Cantera folder	Cantera-1.3 data dot examples	MATLAD
Python Source Cantera-1.3 ck2ctmil.exe License.txt		Select an item to view its description.	
My Documents My Computer My Computer Imixmaster.py I2 object(s) 486 KB My Computer I2 object(s) 486 KB My Computer II object(s) 486 KB My Computer III object(s) 486 KB My Computer III object(s) 486 KB My Computer III object(s) 486 KB III object(s) My Computer III object(s) My Computer <td></td> <td>See also: Python Source Cantera-1.3 ck2ctml.exe</td> <td>License.txt</td>		See also: Python Source Cantera-1.3 ck2ctml.exe	License.txt
12 object(s) 486 KB My Computer I2 object(s) Microsoft Excel Image: Settings Microsoft Excel Image: Settings Microsoft Visual C++ 6.0 Image: Settings Microsoft Visual C++ 6.0 Image: Settings Image: Settings Image: Settings Image: Set		My Network Places My Computer mixmaster.py README.txt	
Image: Section of the section of th		I 12 object(s) 486 KB 💭 My Comp	uter //
S D still Shut Down	Vinicip Programs Image: Programs Image: Documents Image: Documents </th <th>Excel PowerPoint Word Visual C++ 6.0 Strator Visual Studio 6.0 MATLAB examples MixMaster Python Examples MATLAB tutorials</th> <th>Start meni</th>	Excel PowerPoint Word Visual C++ 6.0 Strator Visual Studio 6.0 MATLAB examples MixMaster Python Examples MATLAB tutorials	Start meni

The Thermodynamic Properties Window

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

74 MixMaster			
File Windows Help			
Mechanisms			
Set State	✓ Temperature	300.0	к
Equilibrate	Pressure	1.0	atm
	🗖 Density	0.0818936095742	kg/m3
	🔲 Internal Energy	-1210.80742097	kJ / kg
	🔲 Enthalpy	26.4686073631	kJ / kg
	Entropy	64.9103159567	kJ / kg_K

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)

ged			//	
7% MixMaster				
File Windows Help		/	/ /	
Mechanisms		/		
Set State	🗖 Temperature	574.070222287	K	
Equilibrate	Pressure	1.0	atm	
	🗖 Density	0.0427963024705	kg/m3	
	🔲 Internal Energy	1632.38891795	kJ / kg	
	🔽 Enthalpy	4000. d	kJ / kg	
	🗖 Entropy	74.3135304698	kJ / kg_K	
Species	Moles	Moles		specify the composition
H2	1.0	C Mass		
	0.0			
02	0.0	 O Concentration 		
ОН	0.0	Hide Missing		
H20	0.0	- Species	1	
HO2	0.0	Clear		
H202	0.0	Normalize		
AR	10.0			

Units

Double-click on a unit string to change units

74 MixMaster			_ I ×	Units 🗵	
File Windows Help				O Pa	
Mechanisms				O atm	
Set State	🛛 🗖 Temperature 🛛	574.070222287	к	O bar	
Equilibrate	Pressure	1013.25	mbar	• mbar	
	🗖 Density 🛛	0.0427963024705	kg/m3	C torr	
	🔲 Internal Energy 🛛	1632.38891795	kJ / kg	ОК	double-click here
	🔽 Enthalpy	4000.0	kJ / kg		
	Entropy	74.3135304698	kJ / kg_K		
Species H2 H O 02 OH	Moles 1.0 0.0 0.0 0.0 0.0 0.0	 Moles Mass Concentration Hide Missing Species 			
H20 H02 H202 AR	0.0 0.0 0.0 0.0	Clear Normalize			

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

7% MixMaster			
File Windows Help			
Mechanisms			
Set State	🔲 Temperatur	e 574.070222287	к
► Equilibrate	Pressure	1.0	atm
	🗖 Density	0.0427963024705	kg / m3
	🔲 Internal Ene	ergy 1632.38891795	kJ / kg
	🔽 Enthalpy	4000. C	kJ / kg
	Entropy	74.3135304698	kJ / kg_K
Species	Moles		
H2	1.0	• Moles	
Н	0.0	O Mass	
0	0.0	C Concentration	
02	0.0	Hide Missing	
UH	0.0	Species	
HD2	0.0	Clear	
H202	0.0		-
AR	0.0]

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 '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

7% Convert CK File	<u>- 0 ×</u>
Input File	Browse
Thermodynamic Database	Browse
Transport Database	Browse
OK Cancel	

- 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

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



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 includedadditional 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

/****	iAriostei	
File	Windows Help	
Mecl	✓ Thermodynamic State	
	Composition	
	Kinetics	ipera
	Reactions	sure
—	Reaction Paths	situ
		iony

- 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

OH + H₂ -> H + H₂O is responsible for 97% of the flux of elemental H from OH to H₂O, and OH + H + M -> H₂O + M is only responsible for 1%