### The Cantera 1.5 Python Demos

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# The Cantera Python demos are located in the demos/python folder

Double-click to launch, or right-click and choose 'Edit with Idle"



### Using IDLE

run it

reactor1.pv - D:\dog\castera-1.5\demos\Pythop\reactor1.pv		
e Edit Format Run Ontions Windows Help	D:\dgg\cantera-1.5\demos\Python	
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Constant-pressure, adiabatic kinetics simulatio		
	Address C D:\dgg\cantera-1.5\demos\Python	
""		
rom Cantera import *		
rom Cantera.Reactor import *	catcomb.py diamond.py flame1.py flame2.py	
rom Cantera import rxnpath	Python	
	seastariau 🦓 🦓 🦓	
ri3 = GRI30()	Python File	
	function1.py isentropic.py mix1.py mix2.py	
r13.setState_TPX(1001.0, OneAtm, 'H2:2,02:1,N2:4	) Modined: 9/10/2003 8/11 PM	
- Reactor(gr13)	Size: 843 bytes 🦓 🦓 🦓	
nv = Reservoir(Air())	Attributes: (normal)	
\ \/ /	npflame1.py reactor1.py reactor2.py rxnpath2.py	
Define a wall between the reactor and the envir	nment,	
make it flexible, so that the pressure in the r	pator 6 m mm -	
at the environment pressure.	7/ Python Shen	
= Wall(r, env)	File Edit Debug Options Windows Help	
$(\lambda = 1.00)$ # Set expansion parameter. $dv$	101325.0	
· · · ·	0.2002-004 2000.935 101325.000 9.0400092+004	
ime = 0.0	8.300e-004 2661.283 101325.000 9.031426e+004	
or n in range(100):	101325.0	
time += 1.e-5	8.400e-004 2661.596 101325.000 9.023193e+004	
r.advance(time)	101325.0	
print '%10.3e %10.3f %10.3f %14.6e' % (r.time	8.500e-004 2661.878 101325.000 9.015821e+004	
r.pres	1 8 600e-004 2662 130 101325 000 9 009229e+004	
<pre>print env.pressure()</pre>	101325.0	
	8.700e-004 2662.356 101325.000 9.003344e+004	
	101325.0	
1	8.800e-004 2662.559 101325.000 8.998100e+004	
odit tho	101325.0	
	101325 0 2002.740 101325.000 8.993436e+004	
	9.000e-004 2662.902 101325.000 8.989298e+004 VIEW TF	IE OUTE
corint	101325.0	
SCHDL	9.100e-004 2663.046 101325.000 8.985637e+004	
	101325.0	
	9.200e-004 2663.174 101325.000 8.982407e+004	
	101325.0	

### Plots

Python does not have built-in graphics like MATLAB does, but it is easy to generate CSV files that can be read by Excel, MATLAB, or other plotting programs.

A Python interface to GNU-Plot is also available in the SciPy package.

The Cantera demos mostly write CSV files.

### **stflame1.py:** Stagnation-point $H_2/O_2/Ar$ flame for a range of mass flow rates



### Grid can not only be refined, but also "pruned" of unnecessary points



0.05

As the flame front moves as the mass flow rate increases, the region where small grid spacing is needed changes. Here the solution in blue began from the one in orange, and as the flame front moved to the right, points were removed from the vicinity of the previous flame front.

## **diamond.py:** Diamond chemical vapor deposition

- Simplified form of a growth mechanism for diamond (100) [Harris and Goodwin, J. Phys. Chem. 97:23-28 (1993)]
- Surface phase with 8 species, 19 reversible reactions, 1 irreversible reaction
- Two bulk phases (gas, solid diamond)



## For some problems, both Python and MATLAB demo scripts are provided

- Catalytic combustion (catcomb.py/catcomb.m)
- Non-premixed counterflow flame (npflame1.py/diffflame.m)
- Isentropic expansion (isentropic.py/istentropic.m)
- Burner-stabilized flame (flame1.py/flame1.m)
- Zero-D kinetics (reactor1.py/reactor1.m)
- See the MATLAB demos presentation for more information about these.