MECH 447 Project 4

Detonations

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Introduction

For this project, we intend to analyze the detonation and deflagration cases of a stoichiometric carbon monoxide/oxygen system. This system thus has the initial conditions of 1 atm, 298 K, and a ratio of 2:1 between CO and O_2. To analyze the detonation, two methods will be used to graph the cases, a perfect gas solution, and an equilibrium solution. For these, we will be heavily using the NASA CEA program to analyze the system through various points of the shock.

Throughout all of this however, it is important that the detonations are assumed to be properly described by the ZND model. This model imposes that a detonation is split between the shock wave and the reaction, with the non-reacting shock wave first passing through the mixture, and then the reaction following behind it. Of this model, several points are important to note. The first is the von Neuman point, where the inert shock begins, meaning that the system acts much like a fluids problem with no change in chemical composition. As the shock travels, it approaches the Chapman-Jouguet Point, where the flow velocity in the reference frame becomes sonic. Following this, the weak detonation curve follows the isentropic line to the constant volume solution, where any point beyond in the detonation is considered not physical.

Following the non-physical region, the deflagration zone can be observed with another Chapman-Jouguet Point that shows the point of fastest possible deflagration with a sonic outflow. Overall, the line that follows form the von Neuman, through the strong and weak detonation, and finally through the deflagration zone is called the Hugoniot curves on a (p,v) diagram.

Thus, for both the perfect gas and equilibrium approach, we will plot the Hugoniot curves to study the differences in assumptions and approaches.

Part 1: Perfect Gas Assumption – Constant γ

To begin, the assumption that a gas is perfect requires us to determine a proper value for γ, or the specific heat ratio:

$$\gamma = \frac{c_p}{c_v}$$

Along with this, we must solve for the heat release of the reaction q by solving for the difference in enthalpy of formation of reactants and products:

$$q = \frac{\sum_R n_i \bar{h}_{f_i}^\circ - \sum_P n_i \bar{h}_{f_i}^\circ}{\sum_R n_i (MW)_i}$$

Using NASA's CEA program to solve for the Chapman Jouguet Point, we can easily solve for the heat release by using output of mole fractions and known enthalpy of formations for the species. As for the specific heat ratio, the reaction and change of gas composition affects the ratio and thus is realistically not constant. To make the perfect gas assumption, the initial γ and final γ were simply averaged to a value of 1.2615. Though a more thorough method could be used, the range of γ is so small that the variations themselves would not meaningfully affect the final product.

Following this, the heat of reaction was non-dimensionalized by the heat capacity and temperature of the initial composition as such:

$$Q = \frac{\Delta q}{c_p T_1} = 13.1785$$

Knowing γ and Q, we can thus plot the Hugoniot curves for both the reacting shock and the non-reacting shock through the following equation:

$$\frac{p_2}{p_1} = \frac{\frac{2\gamma}{\gamma-1}Q - \frac{v_2}{v_1} + \frac{\gamma+1}{\gamma-1}}{\frac{\gamma+1}{\gamma-1}\frac{v_2}{v_1} - 1}$$

From this, the pressure ratio (P_2/P_1) is the independent variable, while we vary the volume ratio (v_2/v_1) throughout the curve.

Along with the curves, the Rayleigh lines are also included for the appropriate detonation and deflagration solutions according to the following equation:

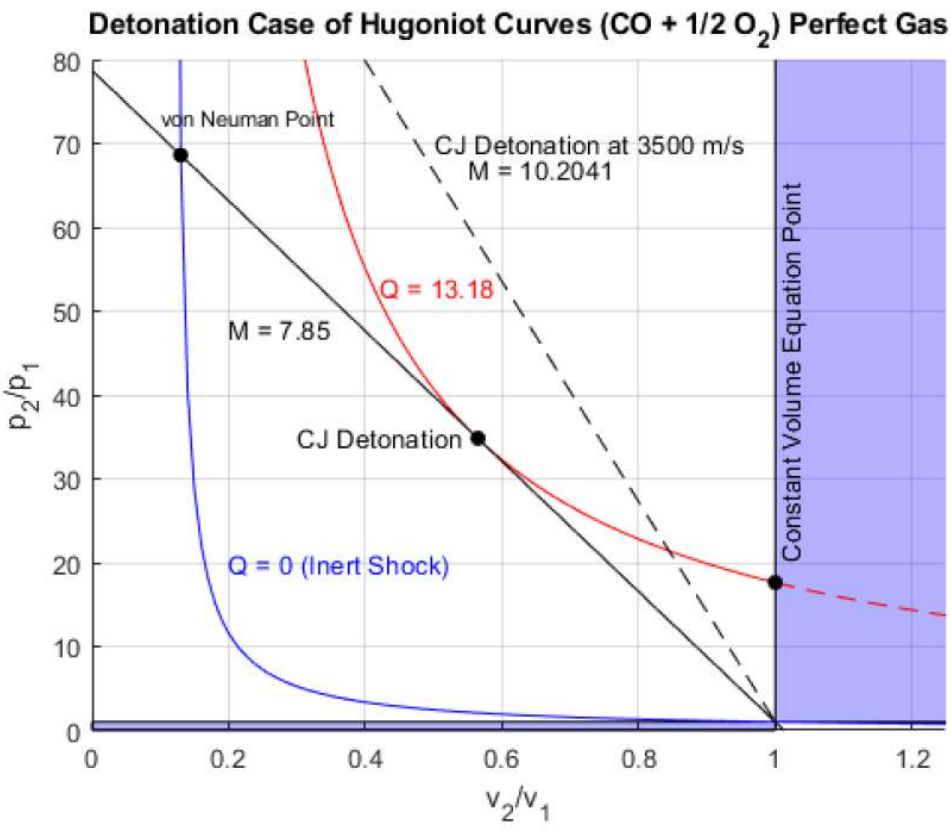
$$\frac{p_2}{p_1} = \gamma {M_{CJ}}^2 \left(1 - \frac{v_2}{v_1}\right) + 1$$

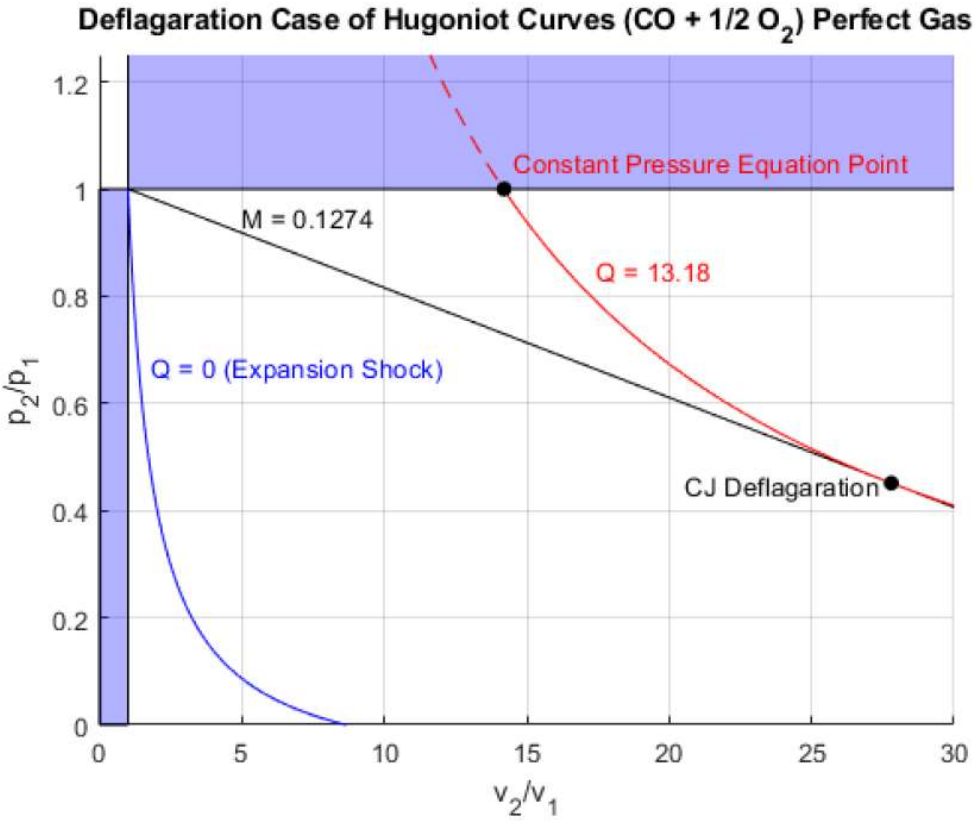
Along with this, the Rayleigh line for the overdriven detonation propagating at 3500 m/s is plotted with its Mach number of 10.2041 being found by dividing the propagation speed by the speed of sound in the original chemical composition of 343 m/s.

Finally, the von Neuman Point is found by finding the intersection of the Rayleigh line with the non-reaction Hugoniot curve, and further checked through the following equations:

$$\frac{p_{vN}}{p_1} = \frac{2\gamma M_1^2 - (\gamma - 1)}{\gamma + 1}$$

$$\frac{\rho_{vN}}{\rho_1} = \frac{v_1}{v_{vN}} = \frac{u_1}{u_{vN}} = \frac{(\gamma + 1) M_1^2}{2 + (\gamma - 1) M_1^2}$$


Detonation Case of Hugoniot Curves (CO + 1/2 O2) Perfect Gas
von Neuman Point
CJ Detonation at 3500 m/s
M = 10.2041
Q = 13.18
M = 7.85
CJ Detonation
Q = 0 (Inert Shock)
Constant Volume Equation Point
p2/p1
v2/v1
0
10
20
30
40
50
60
70
80
0.2
0.4
0.6
0.8
1
1.2


Deflagaration Case of Hugoniot Curves (CO + 1/2 O2) Perfect Gas
Constant Pressure Equation Point
M = 0.1274
Q = 13.18
Q = 0 (Expansion Shock)
CJ Deflagaration
p2/p1
v2/v1
0
0.2
0.4
0.6
0.8
1
1.2
5
10
15
20
25
30

Part 2: Equilibrium Solution

As opposed to the previous part where the Hugoniot curves were solved through equations relating to γ and Q, we will now plot the curves through a full chemical equilibrium approach.

Once again, we can use CEA to plot both the non-reacting curves and the reacting curves, along with Rayleigh lines and Chapman-Jouguet solution points. As CEA already gives the pressure ratio, it is simply a matter of determining the volume ratio in order to plot the curves. This is done by using the fact that mass is conserved, meaning that the density ratio is simply reduced to the inverse of the volume ratio.

With this in mind, we can now plot the strong detonation and inert shock. Due to limitations in the CEA program, only the strong detonation branch is output, meaning that a separate method is required to plot the weak detonation branch.

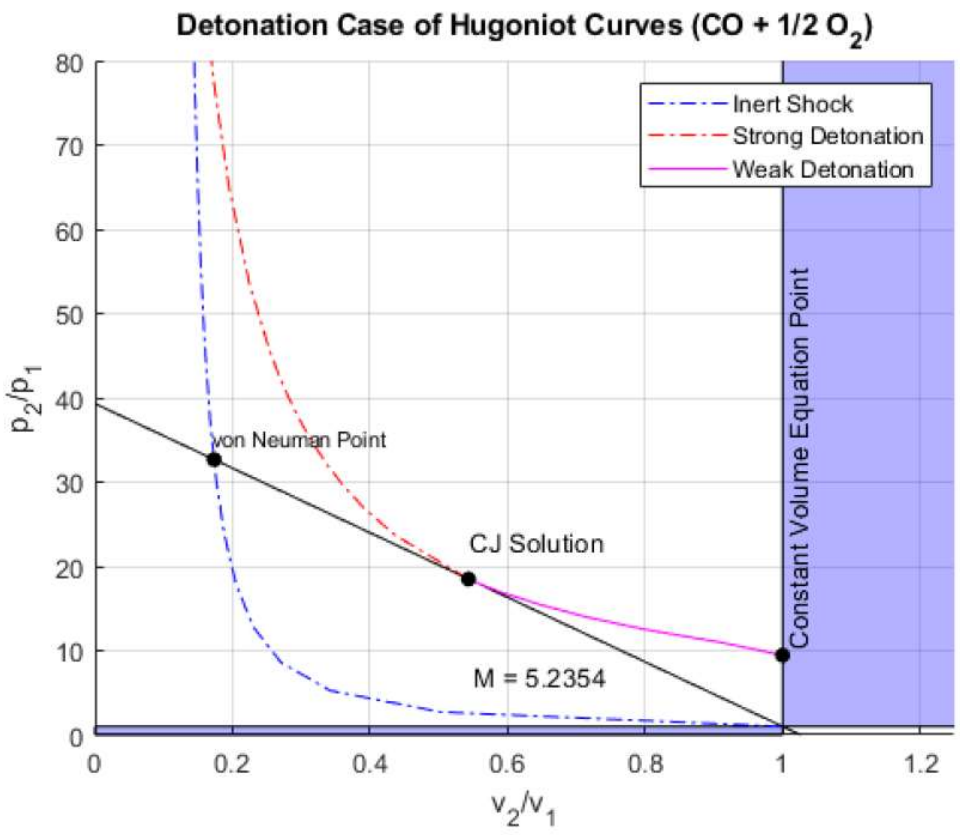
This was done through the use of the CEA's assigned enthalpy and pressure solution (h,p) and keeping the solution in a frozen state. Knowing that the start of the weak detonation branch was at the CJ solution, and that the end was at the constant volume point, we can ensure that the CEA output is correct.

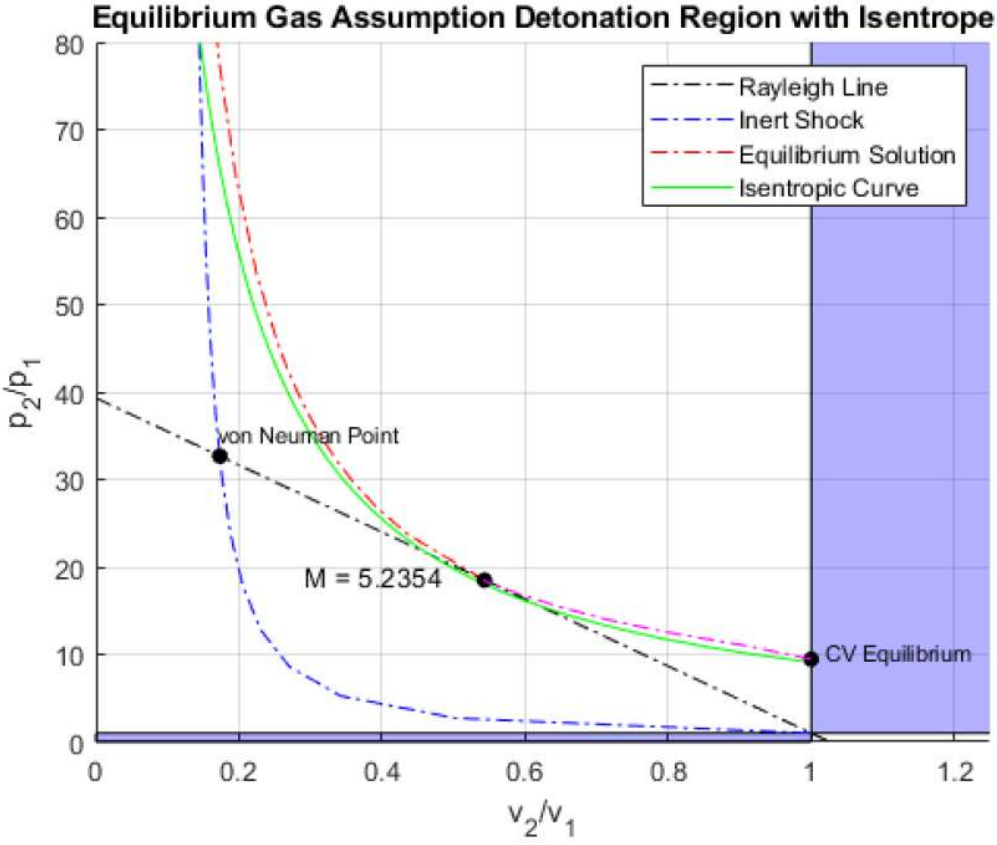
Furthermore, the isentropic curve can be plotted through the use of the (s,p) or (s,v) CEA problems. By solving for the entropy from the specific entropy at the CJ point like so:

$$s = \frac{S}{\rho}\frac{1}{\frac{v_2}{v_1}} = 1.001809\ g - mol/g$$

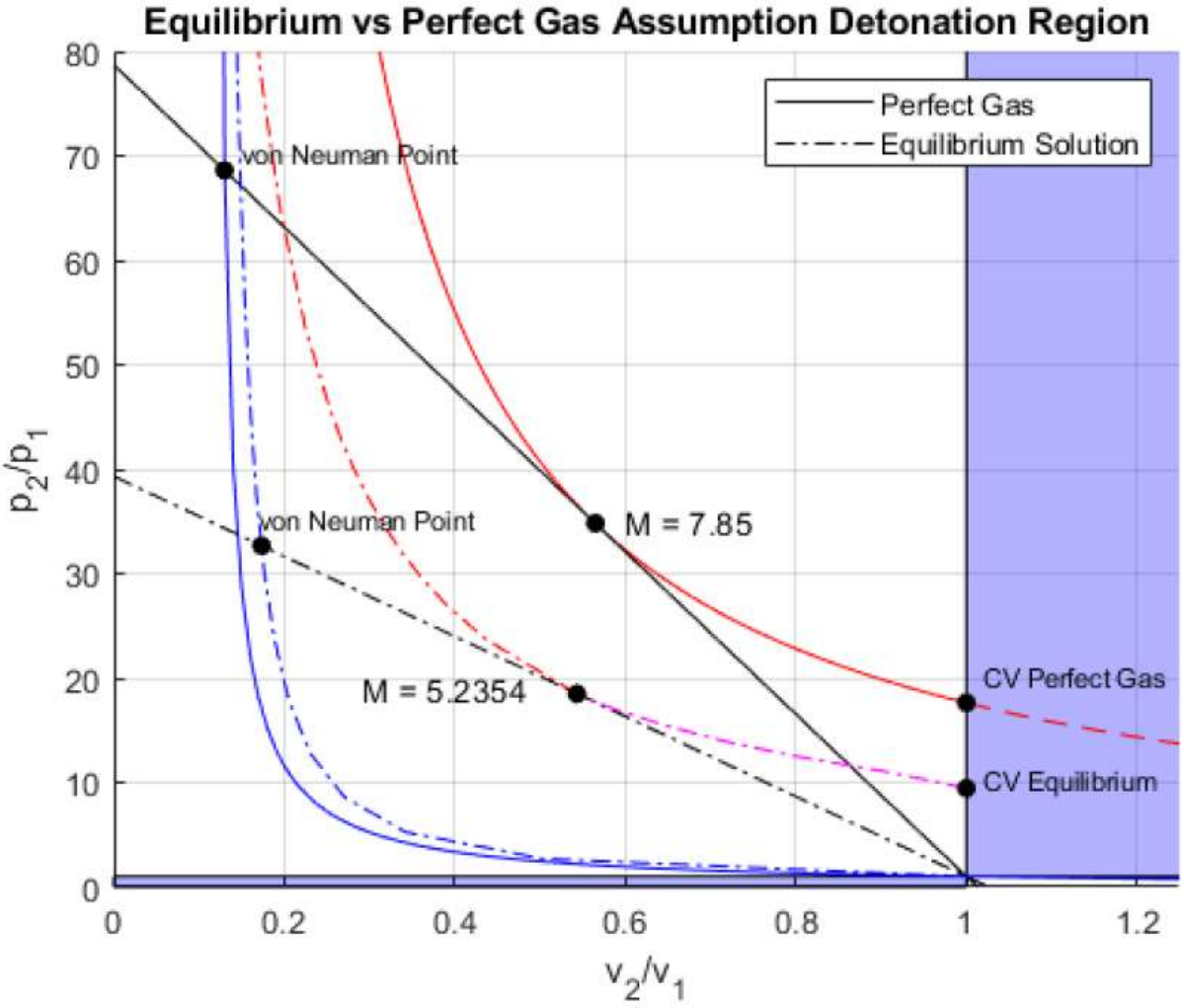
The isentropic line is plotted through the (*p,v*) diagrams. This is important as we know that the weak detonation branch follows the isentropic curve, and thus we expect the solved weak detonation and the plotted isentropic curve to be one and the same.

From the graphs, we can clearly see that the weak detonation and isentropic line do indeed match and converge on the Constant Volume point. Furthermore, the strong detonation curve seems to move away from the isentropic curve and toward the inert shock the farther away from the CJ solution and closer to the von Neuman point it gets.


Detonation Case of Hugoniot Curves (CO + 1/2 O2)
Inert Shock
Strong Detonation
Weak Detonation
Constant Volume Equation Point
von Neuman Point
CJ Solution
M = 5.2354
p2/p1
v2/v1
0
10
20
30
40
50
60
70
80
0.2
0.4
0.6
0.8
1
1.2


Equilibrium Gas Assumption Detonation Region with Isentrope
Rayleigh Line
Inert Shock
Equilibrium Solution
Isentropic Curve
von Neuman Point
M = 5.2354
CV Equilibrium
p2/p1
v2/v1
0
10
20
30
40
50
60
70
80
0.2
0.4
0.6
0.8
1
1.2

With both the perfect gas and equilibrium solutions plotted, we can thus overlay and compare the two:



From this, we can clearly see that the perfect gas assumption has a much higher shock speed at the Chapman-Jouguet Solution point. Following this, this means that the Perfect Gas curve has a much higher pressure ratio at the von Neuman point and constant Volume solution point than the equilibrium solution. Interestingly however, the Equilibrium Solution's inert shock curve is at a higher volume ratio along with its von Neuman Point. This might be due to the assumption that a perfect gas has no intermolecular forces, which would affect the mixture much more in small volumes. This would explain why the error between the two assumptions is much larger at smaller volume ratios. This can be seen also at the constant pressure point in the deflagration region where a bigger volume is needed for the perfect gas to reach the constant pressure point than the equilibrium gas.

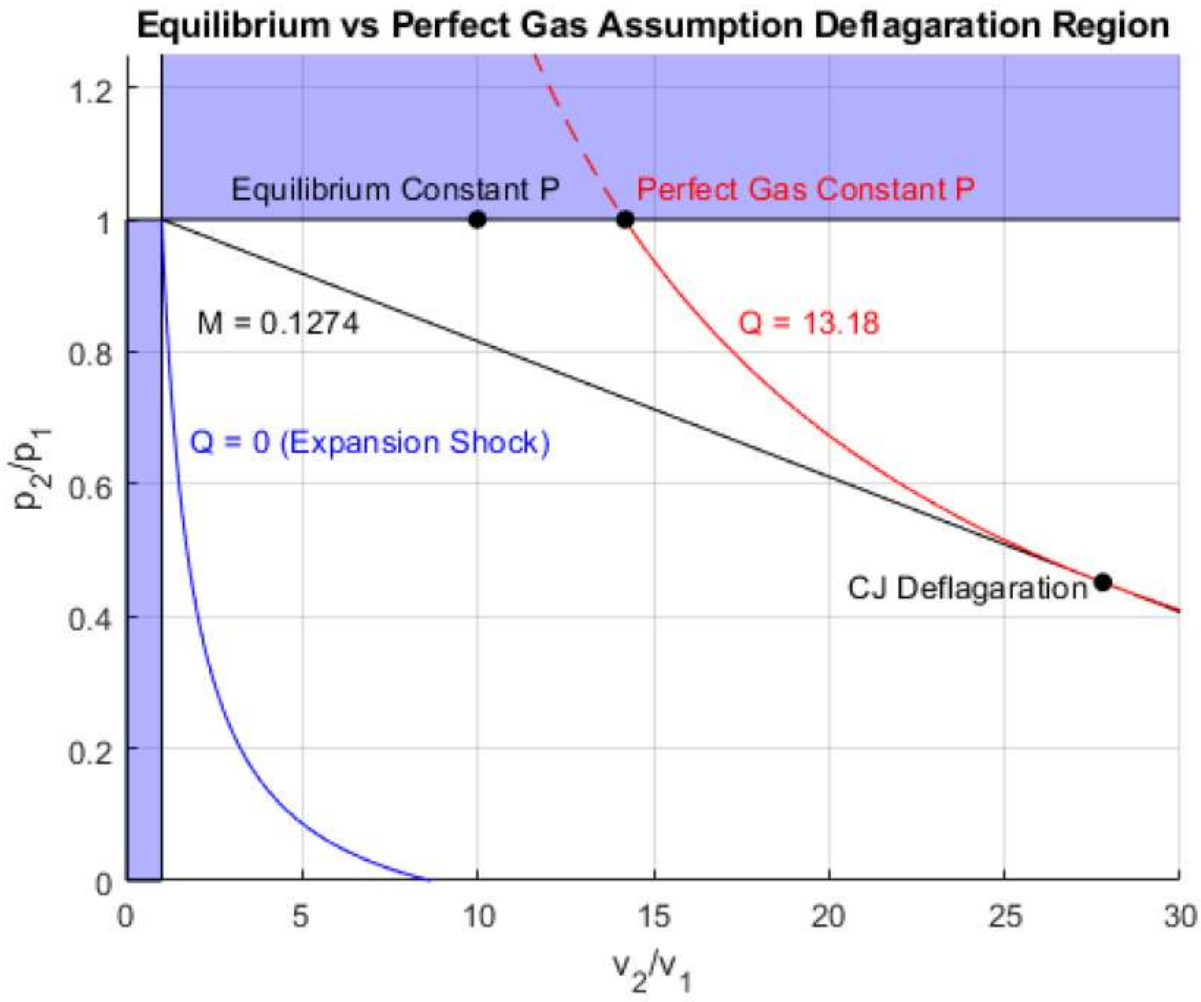


Table 1: Comparison of CJ Solution Points

	Velocity (m/s)	Pressure Ratio	Density Ratio	Temperature Ratio
Perfect Gas	2691.8	34.819	1.7699	11.826
Equilibrium	1795.7	18.497	1.8406	5.657

If we wanted to improve the perfect gas Hugoniot curve, the first step would be to properly determine the specific heat ratio of the reaction. As the relationship between the von Neuman point and CJ point is non-linear, the initial assumption that γ is simply the average of the pre-reaction and post-reaction values is faulty to begin with. Since the reaction has most of its heat and combustion near the CJ point at the point of highest heat, then γ should be closer to the initial value of the mixture. This lower value would result in lower pressures and a closer fit to the equilibrium function as it is directly related to the pressure ratio as seen in the equations for Part 1.

Part 3: Structure of CO/O_2 Detonations

Finally, the final part of the project is to evaluate the full ZND structure of the CO/O_2 Detonation using the SDT toolbox in Cantera. As seen in Project 2, multiple mechanisms can be used to setup the gas structure in Cantera and we had gone through multiple such as the gri30, Galway, and San Diego mechanisms. For this detonation however, we begin with the Davis2005 mechanism that involves a multi-step mechanism to solve the mechanisms of the detonation. However, this mechanism proved to be too complicated for any immediate use and thus required optimization for our specific case. First, all reactions other than the three detailed in Project 2 were removed, leaving the mechanism to only evaluate:

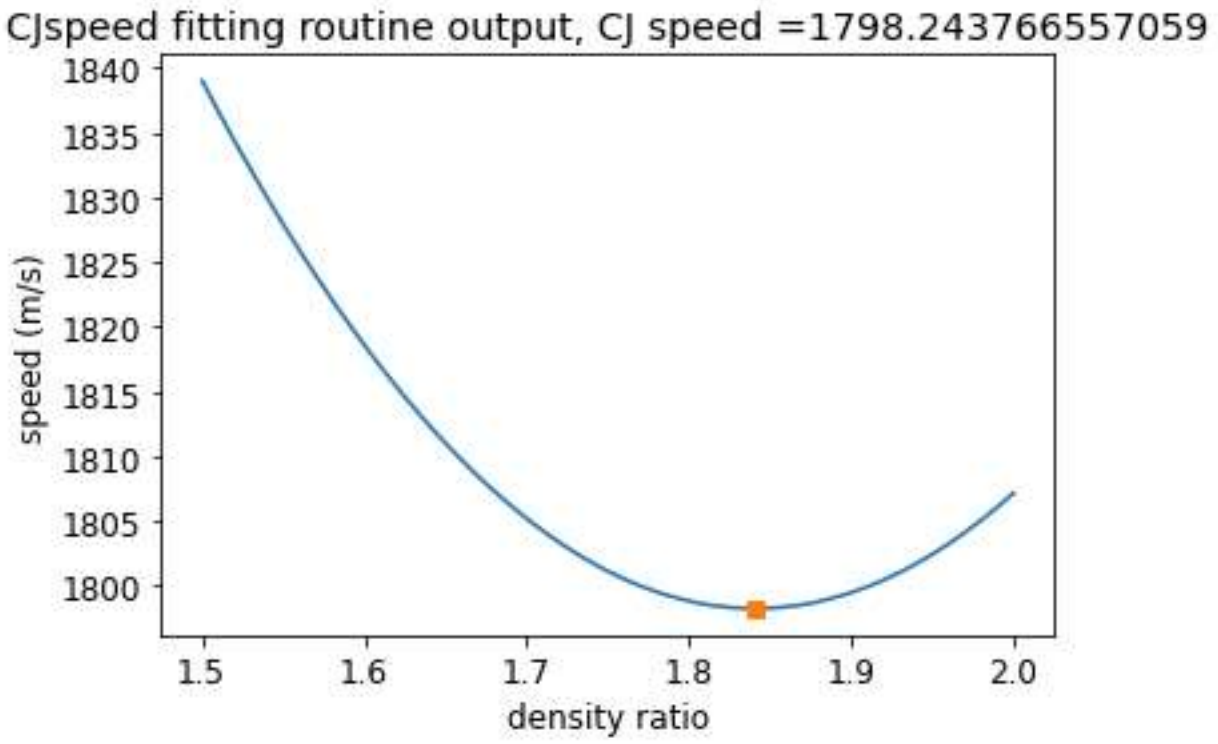
Reaction	A	n	E_a (kJ/kmol)
$CO + O + M \rightleftharpoons CO_2 + M$	1.8×10^{4a}	0.00	9,970
$CO + O_2 \rightleftharpoons CO_2 + O$	2.5×10^{9b}	0.00	200,000
$O + O + M \rightleftharpoons O_2 + M$	1.2×10^{11a}	−1.00	0

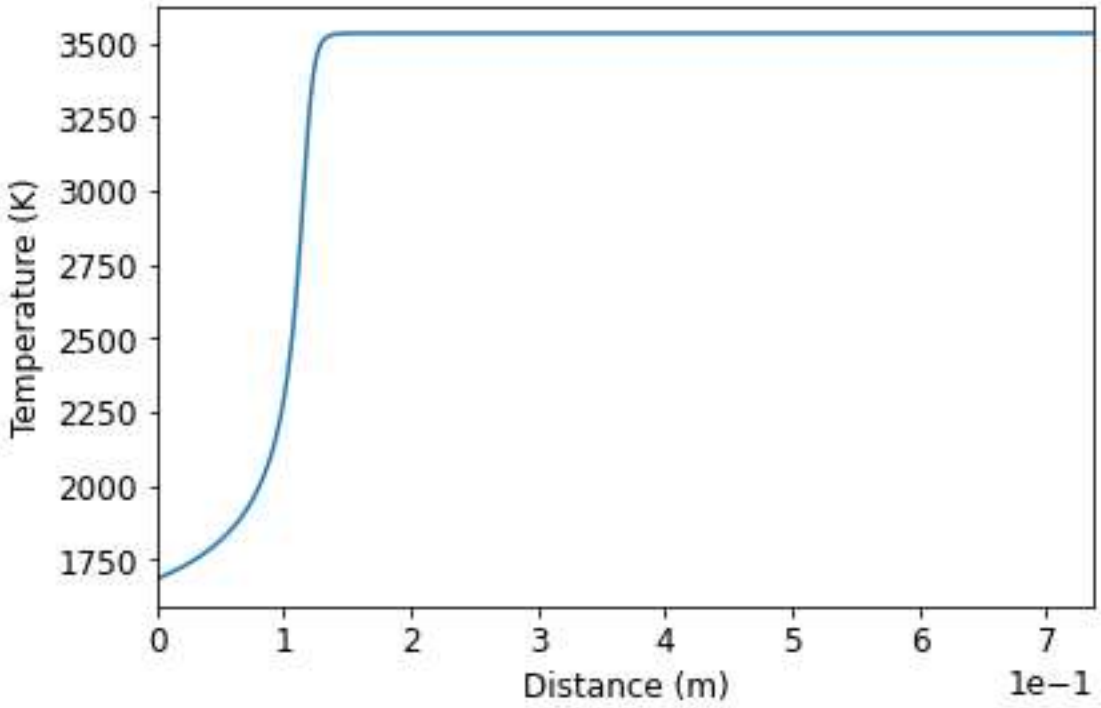
[a] $m^6 kmol^{-2} s^{-1}$

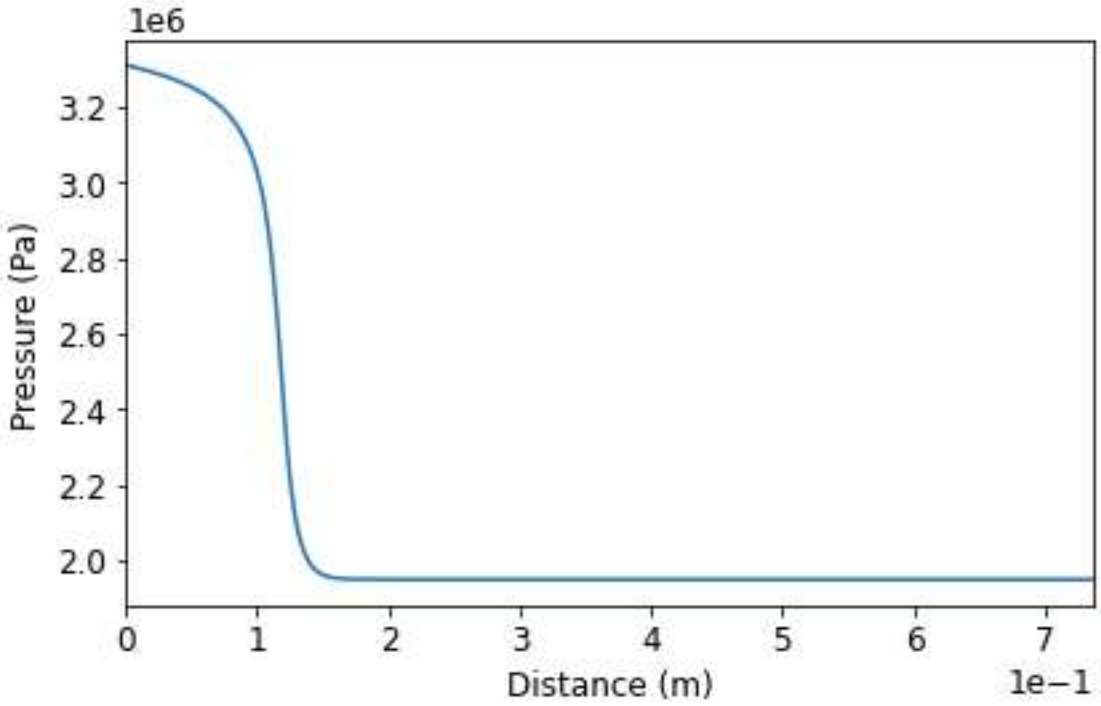
[b] $m^3 kmol^{-1} s^{-1}$

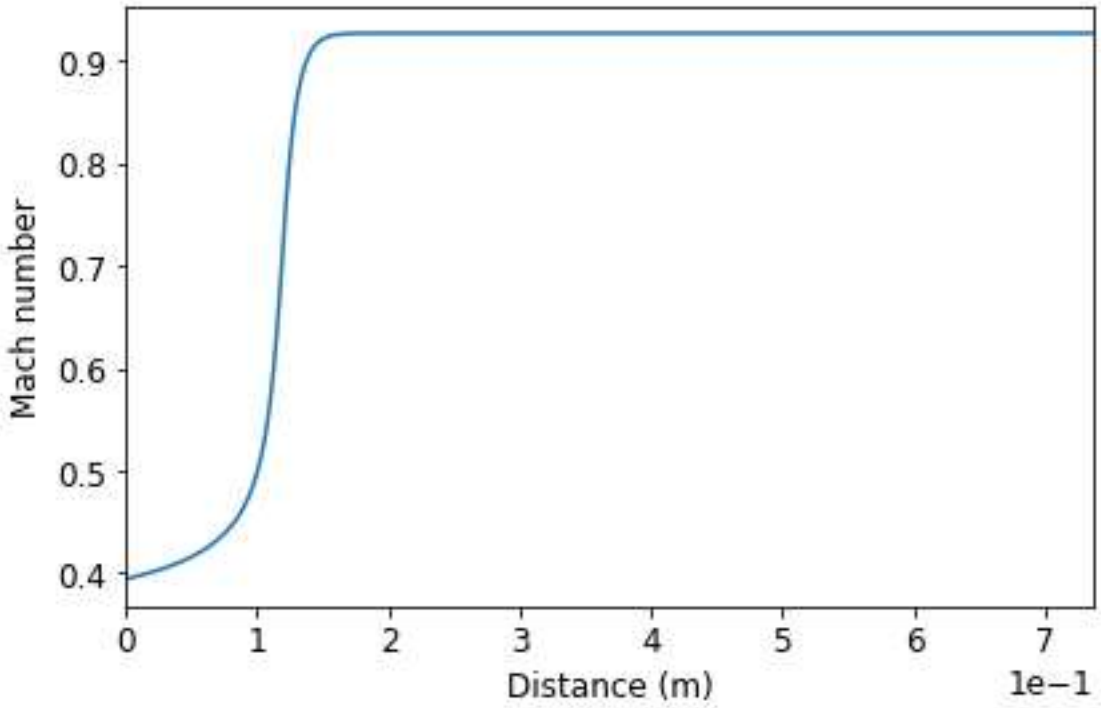
In this case, the M term represents any possible species present in the reactions. As Davis2005 uses an ideal air comprised of numerous trace elements for the three-body reactions involving M, the idea air also had to be modified to only include C, CO, O, and O2.

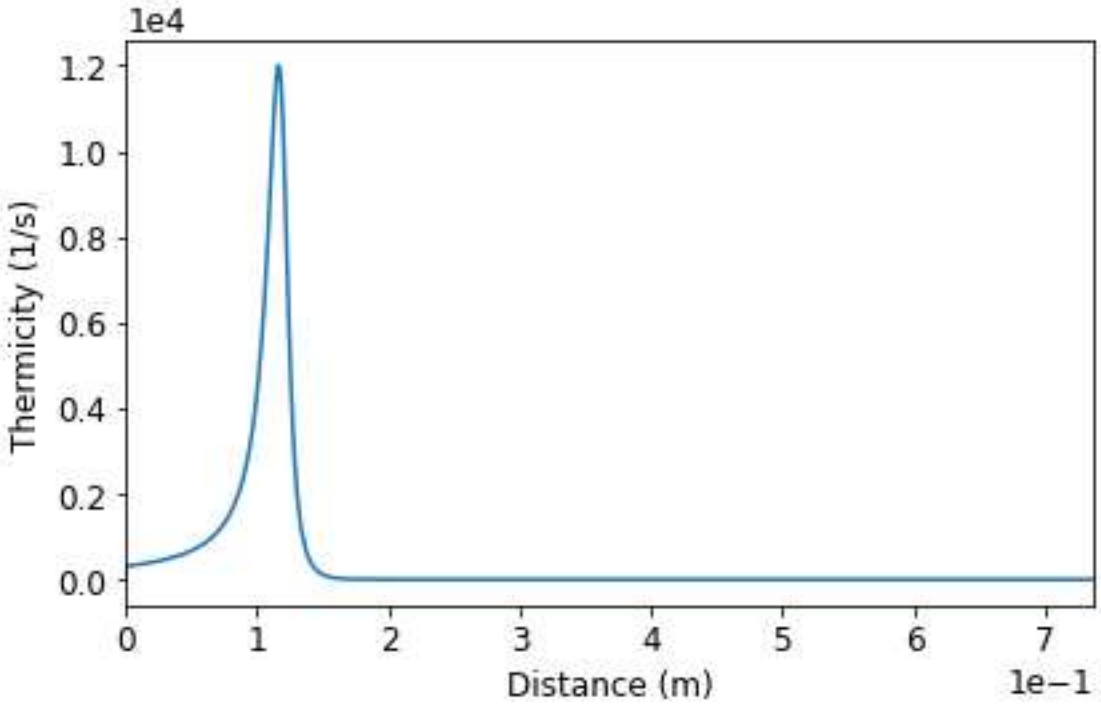
Thus, using the initial temperature and pressure, along with this newly modified 3 step mechanism derived from Davis2005, the CJ solution and ZND structure can be solved and plotted.

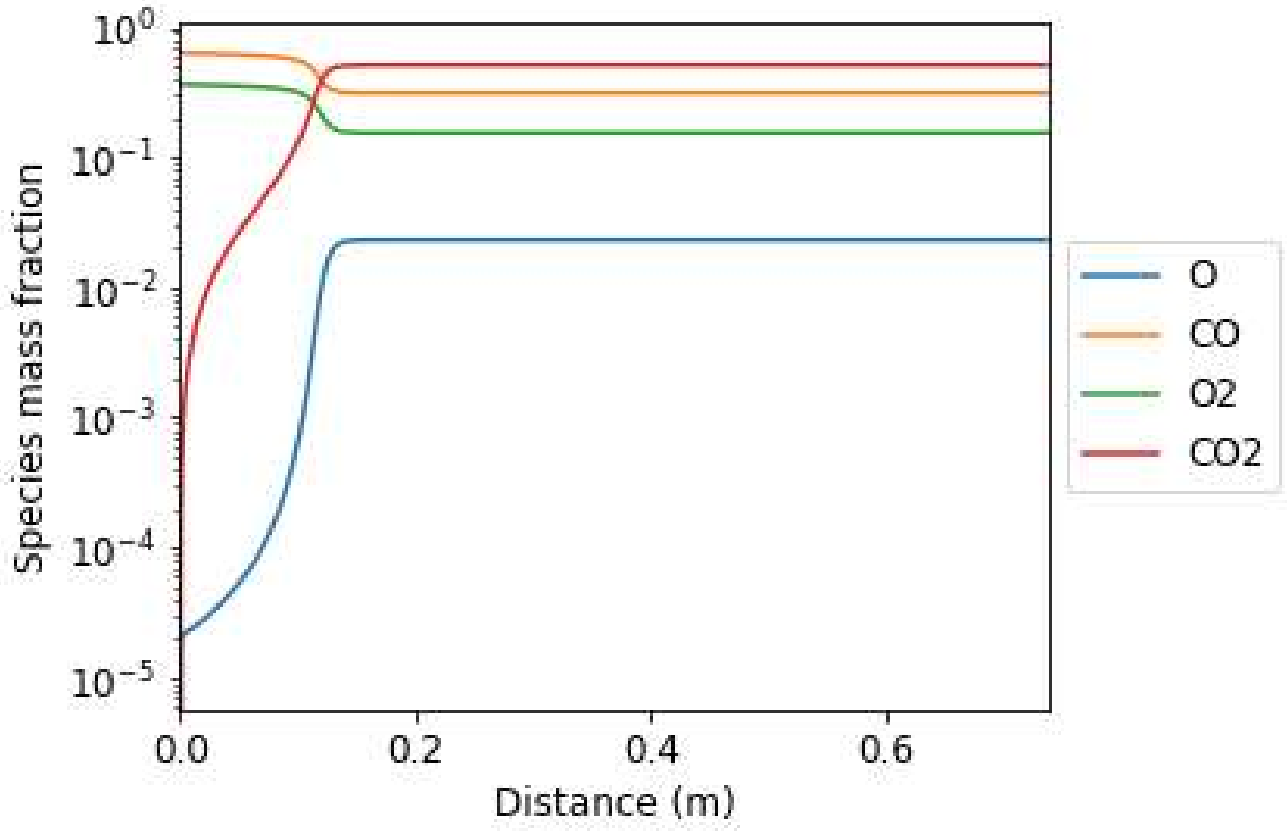



Temperature (K)
3500
3250
3000
2750
2500
2250
2000
1750
0
1
2
3
4
5
6
7
Distance (m)
1e−1


1e6
Pressure (Pa)
3.2
3.0
2.8
2.6
2.4
2.2
2.0
0
1
2
3
4
5
6
7
Distance (m)
1e−1


Mach number
0.9
0.8
0.7
0.6
0.5
0.4
0
1
2
3
4
5
6
7
Distance (m)
1e−1


1e4
Thermicity (1/s)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
3
4
5
6
7
Distance (m)
1e−1



Most important of these graphs is the thermicity spike at about 0.1 m. Thermicity represents the influence of the chemical reaction on the flow velocity. This spike shows when the system experiences the most change along with when thermicity drops to zero. When at zero, thermicity represents when the system's flow velocity is equal to the frozen sound speed found at the von Neuman point, thus meeting the sonic condition. Knowing from the ZND structure, the maximum change in the chemical reaction is right before sonic conditions are met as energy flows into the mixture during a subsonic Rayleigh flow. This is clearly shown in all other plots, most notably the Mach number and the species mass fractions. For the flow velocity, the subsonic flow accelerates towards sonic as heat is input, with sonic being reached at the saddle point of thermicity at around .15 m. For species mass fraction, the initial conditions are mostly maintained with the largest change in mass fractions coming at the saddle point where the system fully reacts in all its sub-mechanisms and reaches equilibrium at around 0.15 m.

These relationships can also be shown for temperature and pressure where the subsonic Rayleigh flow resulting from the original inert shock at the von Neuman point proceeds to have heat input and reacts to reach the sonic Chapman-Jouguet Point.

Conclusion

Overall, this project has shown the difference in Hugoniot curves for a perfect gas solution compared to a chemical equilibrium solution. It is clearly shown that a perfect gas results in a much faster flow resulting in higher pressures at the CJ and von Neuman points, while also having smaller volume ratios for its inert shock response. To properly correct this, it is recommended to properly evaluate a better specific heat ratio value for the perfect gas solution. This is due to the reaction not happening evenly throughout the strong detonation branch, meaning that the specific heat ratio only truly changes near the end. This leads to the true average guess to be lower. This would result in a more realistic solution with pressure ratios much closer to the ones seen in the chemical equilibrium curves.

Furthermore, the weak detonation curves were able to be plotted through the use of frozen compositions past the Chapman-Jouguet point. This supports the idea of the ZND structure where the reaction follows the inert shock wave and adds heat until sonic conditions are met. After these sonic conditions, the weak detonation wave is shown to follow the isentropic curve until the constant volume point where the wave no longer becomes feasible. For further studies, it would be interesting to do similar plots but for the deflagration regions with an isentropic curve to see if the weak deflagration curve follows it. This would mean that the reaction would either resume or change equilibrium at the weak Chapman-Jouguet point as it once again no longer meets sonic conditions and adjusts.

Finally, the final part of the project solved for the ZND structure and clearly shows numerically what the ZND theory is. The ZND structure is comprised of a planar inert shock that changes a supersonic flow to subsonic, quickly being followed by a reaction which adds heat to the flow. Following the idea of Rayleigh flow, this heat decreases pressure, increases temperature, and increases flow speed in the direction making the flow sonic. At that point, the CJ solution, the reaction fully completes, and the products can be seen to have reached equilibrium.

Python Script

```
# -*- coding: utf-8 -*-
"""
Created on Fri Dec 18 22:00:59 2020

@author: Louis Bourque
Adapted from SDT toolbox demo ZNDshk
"""

from sdtoolbox.postshock import CJspeed, PostShock_fr
from sdtoolbox.znd import zndsolve
from sdtoolbox.utilities import CJspeed_plot, znd_plot
import cantera as ct


P1 = 101325
T1 = 298
U1 = 1798.244 #From CEA and SDT toolbox
q = 'CO:2 O2:1'
mech = 'My3step.cti'

# Set up gas object
gas1 = ct.Solution(mech)
gas1.TPX = T1,P1,q

# Find CJ speed and related data, make CJ diagnostic plots
cj_speed,R2,plot_data = CJspeed(P1,T1,q,mech,fullOutput=True)
CJspeed_plot(plot_data,cj_speed)


# Find post shock state for given speed
gas = PostShock_fr(cj_speed, P1, T1, q, mech)

# Solve ZND ODEs, make ZND plots
znd_out = zndsolve(gas,gas1,U1,t_end=1e-3,advanced_output=True)
znd_plot(znd_out,major_species = 'All')


print('Reaction zone pulse width (exothermic length) = %.4g m' % znd_out['exo_len_ZND'])
print('Reaction zone induction length = %.4g m' % znd_out['ind_len_ZND'])
print('Reaction zone pulse time (exothermic time) = %.4g s' % znd_out['exo_time_ZND'])
print('Reaction zone induction time = %.4g s' % znd_out['ind_time_ZND'])
```

```
units(length='cm', time='s', quantity='mol', act_energy='cal/mol')

ideal_gas(name='gas',
          elements="O H C N Ar He",
          species="""O  CO    O2   CO2""",
          reactions='all',
          transport='Mix',
          initial_state=state(temperature=300.0, pressure=OneAtm))

#-------------------------------------------------------------------------------
# Species data
#-------------------------------------------------------------------------------


species(name='H2',
        atoms='H:2',
        thermo=(NASA([200.00, 1000.00],
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                       2.01572094E-08, -7.37611761E-12, -9.17935173E+02,
                       6.83010238E-01]),
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                     [ 3.33727920E+00, -4.94024731E-05,  4.99456778E-07,
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        transport=gas_transport(geom='linear',
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                                polar=0.79,
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                     [ 2.50000000E+00,  7.05332819E-13, -1.99591964E-15,
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                      -4.46682853E-01]),
                NASA([1000.00, 3500.00],
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                      -4.46682914E-01])),
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                                diam=2.05,
                                well_depth=145.0),
        note='L7/88')

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        atoms='Ar:1',
        thermo=(NASA([300.00, 1000.00],
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                      4.36600000E+00]),
             NASA([1000.00, 5000.00],
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                      0.00000000E+00,  0.00000000E+00, -7.45375000E+02,
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        thermo=(NASA([300.00, 1000.00],
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                NASA([1000.00, 5000.00],
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                    2.05193346E+00]),
                NASA([1000.00, 3500.00],
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                      4.78433864E+00])),
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                                diam=2.75,
                                well_depth=80.0),
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        atoms='H:1 O:1',
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        note='S9/01')

species(name='HCO',
        atoms='H:1 C:1 O:1',
        thermo=(NASA([200.00, 1000.00],
                    [ 4.22118584E+00, -3.24392532E-03,  1.37799446E-05,
                     -1.33144093E-08,  4.33768865E-12,  3.83956496E+03,
                      3.39437243E+00]),
                NASA([1000.00, 3500.00],
                    [ 2.77217438E+00,  4.95695526E-03, -2.48445613E-06,
                      5.89161778E-10, -5.33508711E-14,  4.01191815E+03,
                      9.79834492E+00])),
        transport=gas_transport(geom='nonlinear',
                                diam=3.59,
                                well_depth=498.0),
        note='L12/89')

species(name='HO2',
        atoms='H:1 O:2',
        thermo=(NASA([200.00, 1000.00],
                    [ 4.30179801E+00, -4.74912051E-03,  2.11582891E-05,
                     -2.42763894E-08,  9.29225124E-12,  2.94808040E+02,
                      3.71666245E+00]),
                NASA([1000.00, 3500.00],
                    [ 4.01721090E+00,  2.23982013E-03, -6.33658150E-07,
                      1.14246370E-10, -1.07908535E-14,  1.11856713E+02,
                      3.78510215E+00])),
        transport=gas_transport(geom='nonlinear',
                                diam=3.458,
```

```
                               well_depth=107.4,
                               rot_relax=1.0),
        note='L5/89')

species(name='H2O',
        atoms='H:2 O:1',
        thermo=(NASA([200.00, 1000.00],
                     [ 4.19864056E+00, -2.03643410E-03,  6.52040211E-06,
                      -5.48797062E-09,  1.77197817E-12, -3.02937267E+04,
                      -8.49032208E-01]),
                NASA([1000.00, 3500.00],
                     [ 3.03399249E+00,  2.17691804E-03, -1.64072518E-07,
                      -9.70419870E-11,  1.68200992E-14, -3.00042971E+04,
                       4.96677010E+00])),
        transport=gas_transport(geom='nonlinear',
                               diam=2.605,
                               well_depth=572.4,
                               dipole=1.844,
                               rot_relax=4.0),
        note='L8/89')

species(name='CO',
        atoms='C:1 O:1',
        thermo=(NASA([200.00, 1000.00],
                     [ 3.57953347E+00, -6.10353680E-04,  1.01681433E-06,
                       9.07005884E-10, -9.04424499E-13, -1.43440860E+04,
                       3.50840928E+00]),
                NASA([1000.00, 3500.00],
                     [ 2.71518561E+00,  2.06252743E-03, -9.98825771E-07,
                       2.30053008E-10, -2.03647716E-14, -1.41518724E+04,
                       7.81868772E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.65,
                               well_depth=98.1,
                               polar=1.95,
                               rot_relax=1.8),
        note='TPIS79')

species(name='O2',
        atoms='O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 3.78245636E+00, -2.99673416E-03,  9.84730201E-06,
                      -9.68129509E-09,  3.24372837E-12, -1.06394356E+03,
                       3.65767573E+00]),
                NASA([1000.00, 3500.00],
                     [ 3.28253784E+00,  1.48308754E-03, -7.57966669E-07,
                       2.09470555E-10, -2.16717794E-14, -1.08845772E+03,
                       5.45323129E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.458,
```

```
                               well_depth=107.4,
                               polar=1.6,
                               rot_relax=3.8),
        note='TPIS89')

species(name='H2O2',
        atoms='H:2 O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 4.27611269E+00, -5.42822417E-04,  1.67335701E-05,
                      -2.15770813E-08,  8.62454363E-12, -1.77025821E+04,
                       3.43505074E+00]),
                NASA([1000.00, 3500.00],
                     [ 4.16500285E+00,  4.90831694E-03, -1.90139225E-06,
                       3.71185986E-10, -2.87908305E-14, -1.78617877E+04,
                       2.91615662E+00])),
        transport=gas_transport(geom='nonlinear',
                               diam=3.458,
                               well_depth=107.4,
                               rot_relax=3.8),
        note='L7/88')

species(name='CO2',
        atoms='C:1 O:2',
        thermo=(NASA([200.00, 1000.00],
                     [ 2.35677352E+00,  8.98459677E-03, -7.12356269E-06,
                       2.45919022E-09, -1.43699548E-13, -4.83719697E+04,
                       9.90105222E+00]),
                NASA([1000.00, 3500.00],
                     [ 3.85746029E+00,  4.41437026E-03, -2.21481404E-06,
                       5.23490188E-10, -4.72084164E-14, -4.87591660E+04,
                       2.27163806E+00])),
        transport=gas_transport(geom='linear',
                               diam=3.763,
                               well_depth=244.0,
                               polar=2.65,
                               rot_relax=2.1),
        note='L7/88')


#-----------------------------------------------------------------------------
# Reaction data
#-----------------------------------------------------------------------------

falloff_reaction('CO + O (+ M) <=> CO2 (+ M)',
                 kf=[1.362000e+10, 0.0, 2384.0],
                 kf0=[1.173000e+24, -2.79, 4191.0],
                 efficiencies='CO2:3.6 CO:1.75')
# 99MUE/KIM * 0.76

reaction('CO + O2 <=> CO2 + O', [1.119000e+12, 0.0, 47700.0])
```

```
# 86TSA/HAM * 0.44

three_body_reaction('O + O + M <=> O2 + M', [1.200000e+17, -1.0, 0.0],
                    efficiencies='CO2:3.6 CO:1.75')
```

Table of Contents

Project 4 - Detonation

Louis Bourque - 260714602

```
clc
clear

[Vweak,Pweak] = weak(); %weak detonation from CEA


% Enthalpy of Formation (kJ/kmol)
hfCO = -110530;
hfCO2 = -393520;
hfO = 249190;
hfO2 = 0;
```

Part 1

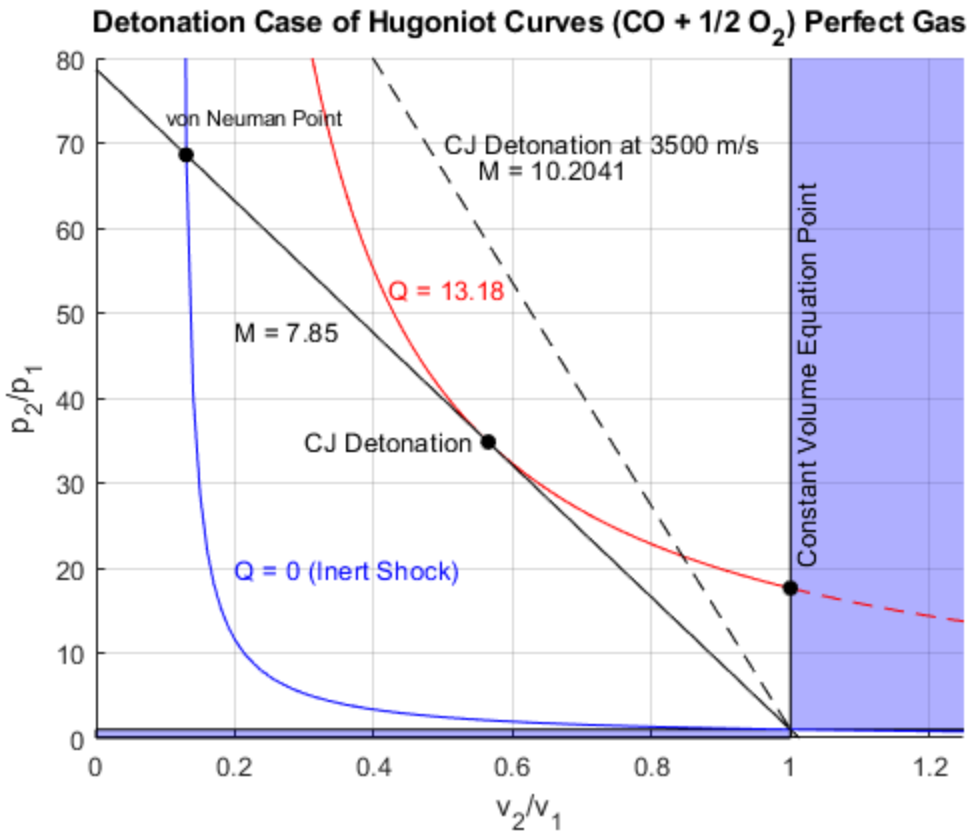
```
cp_ini = 0.9959; %kJ/(kg K)
T_ini = 298; %(K)

%CEA Results
nCO = 0.38166;
nCO2 = 0.40287;
nO = 0.04929;
nO2 = 0.16618;

y_react = 1.3977;
y_burn = 1.1253;

% Reactants
COini = 0.66667;
O2ini = 0.33333;

% Molecular Weight of Reactancts (kg/kmol) or (g/mol)
COw = 28.011;
O2w = 31.999;

% Estimate q
nhf_react = (COini*hfCO + O2ini*hfO2);
nhf_prod = (nCO*hfCO + nCO2*hfCO2 + nO*hfO + nO2*hfO2);
```

```
nMW = (COw*COini + O2w*O2ini);

q_estimate = (nhf_react - nhf_prod)/nMW;
y = (y_react + y_burn)/2;

Q = q_estimate/(cp_ini*T_ini);
```

Detonation Zone

```
V_det = (0:.01:1.25);
P_det0 = zeros(1,length(V_det));
P_det = zeros(1,length(V_det));
Pcj_det = zeros(1,length(V_det));
P_ray = zeros(1,length(V_det));

% Chapman Jouguet Detonation Case Rayleigh Line
Mcj_det = sqrt(Q*(y+1) + 1 + sqrt(((y+1)*Q + 1)^2 - 1));

% Rayleigh Line for specified speed of propagation
speed = 3500; %m/s
C = 343; %m/s
M = speed/C;

for i = 1:length(V_det)
    P_det0(i) = (-V_det(i) + (y+1)/(y-1))/(((y+1)/(y-1))*V_det(i) -
 1);
    P_det(i) = ((2*y*Q)/(y-1) - V_det(i) + (y+1)/(y-1))/((y
+1)*V_det(i)/(y-1) - 1);
    Pcj_det(i) = y*Mcj_det^2*(1 - V_det(i)) + 1;
    P_ray(i) = y*M^2*(1 - V_det(i)) + 1;
end

% Finding CJ Point for Detonation
CJ_det = find(abs(P_det-Pcj_det) < 0.1);
CJ_dety = sum(P_det(CJ_det))/length(CJ_det);
CJ_detx = V_det(round(mean(CJ_det)))-.005; % .005 is adjusting factor
 to fit marker on plot due to rounding

% Finding von Neumann point
vN = find(abs(P_det0-Pcj_det) < 0.1);
vNy = mean(Pcj_det(vN((vN < 100))));
vNx = V_det(round(mean(vN((vN < 100)))));

% Finding Constant Volume point
ConV = P_det(V_det() == 1);

% Plot Detonation
figure(1)
grid on
hold on

ylim([0 80]);
xlim([0 1.25]);
```

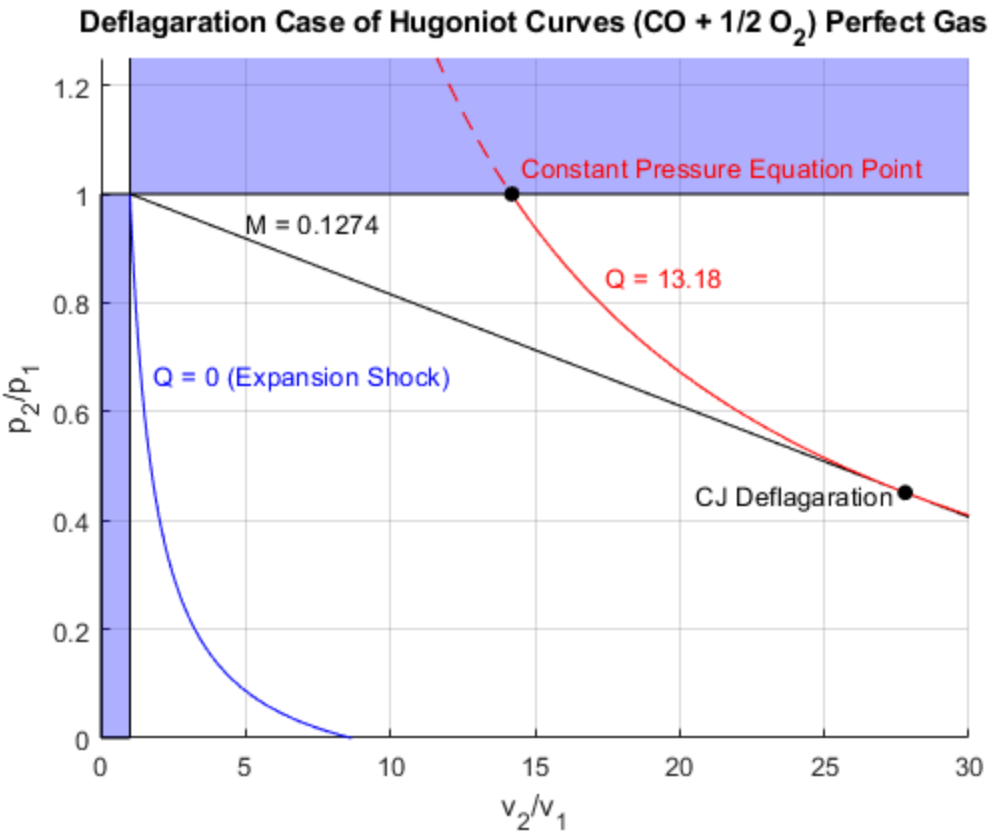
```
% Plot Forbidden Zones
patch([1 1 50 50],[1 200 200 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')

plot(V_det(13:126),P_det0(13:126),'b') % Plot for Q = 0
plot(V_det(13:100),P_det(13:100),'r',V_det(101:end),P_det(101:end),'r--') %
 Plot for solved Q with forbidden zone dashed
plot(V_det,Pcj_det,'k') % Plot M slope for solved
plot(V_det,P_ray,'k--') % Plot M slope for 3400 m/s wave

plot(CJ_detx,CJ_dety,'.','MarkerSize',20,'Color','black'); % Marker
 for CJ Solution
plot(vNx,vNy,'.','MarkerSize',20,'Color','black'); % Marker for von
 Neuman Point
plot(1,ConV,'.','MarkerSize',20,'Color','black'); % Marker for
 Constant Volume

alpha(0.3)

% Add Text
text(.2,20,'Q = 0 (Inert Shock)','Color','blue')
text(.42,53,'Q = 13.18','Color','red','FontSize',10)
text(.2,48,'M = 7.85','Color','black')
text(.3,35,'CJ Detonation','Color','black')
text(.5,70,'CJ Detonation at 3500 m/s','Color','black')
text(.55,67,'M = 10.2041','Color','black')
text(.1,73,'von Neuman Point','Color','black','FontSize',8)
set(text(1.02,20,'Constant Volume Equation
 Point','Color','black'),'Rotation',90)

% Labels
xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Detonation Case of Hugoniot Curves (CO + 1/2 O_2) Perfect Gas')

hold off
```



Deflagaration Zone

```
V_flag = (1:.1:30);
P_flagO = zeros(1,length(V_flag));
P_flag = zeros(1,length(V_flag));
Pcj_flag = zeros(1,length(V_flag));

Mcj_flag = sqrt(Q*(y+1) + 1 - sqrt(((y+1)*Q + 1)^2 - 1));

for i = 1:length(V_flag)
    P_flagO(i) = (-V_flag(i) + (y+1)/(y-1))/(((y+1)/(y-1))*V_flag(i) -
 1);
    P_flag(i) = ((2*y*Q)/(y-1) - V_flag(i) + (y+1)/(y-1))/((y
+1)*V_flag(i)/(y-1) - 1);
    Pcj_flag(i) = y*Mcj_flag^2*(1 - V_flag(i)) + 1;
end

% Finding CJ Point for Deflagaration
CJ_flag = find(abs(P_flag-Pcj_flag) < 0.00001);
CJ_flagy = sum(P_flag(CJ_flag))/length(CJ_flag);
CJ_flagx = V_flag(round(mean(CJ_flag)))-.005; % .005 is adjusting
 factor to fit marker on plot due to rounding


% Split Q line into forbidden and not forbidden for clarity
```

```
Forb_flag = (P_flag >= 1);

top_flag = P_flag;
bot_flag = P_flag;

bot_flag(Forb_flag) = NaN;
top_flag(~Forb_flag) = NaN;

figure(2)
grid on
hold on
ylim([0 1.25]);
xlim([0 30])

% Shade forbidden regions
patch([1 1 50 50],[1 50 50 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')


plot(V_flag,P_flagO,'b') % Plot Q = 0
plot(V_flag,Pcj_flag,'k') % Plot M Slope
plot(V_flag,bot_flag,'r',V_flag,top_flag,'r--') %Plot Solved Q, dashed
 for forbidden zone
plot(V_flag(133),1,'.','MarkerSize',20,'Color','black'); % Marker for
 constant point
plot(CJ_flagx,CJ_flagy,'.','MarkerSize',20,'Color','black'); % Marker
 for CJ Solution

alpha(0.3)

% Add Text
text(1.8,.67,'Q = 0 (Expansion Shock)','Color','blue')
text(5,.95,'M = 0.1274','Color','black')
text(17.4,.85,'Q = 13.18','Color','red')
text(14.5,1.05,'Constant Pressure Equation Point','Color','red')
text(20.5,.45,'CJ Deflagaration','Color','black')

xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Deflagaration Case of Hugoniot Curves (CO + 1/2 O_2) Perfect
 Gas')

hold off
```



Part 2

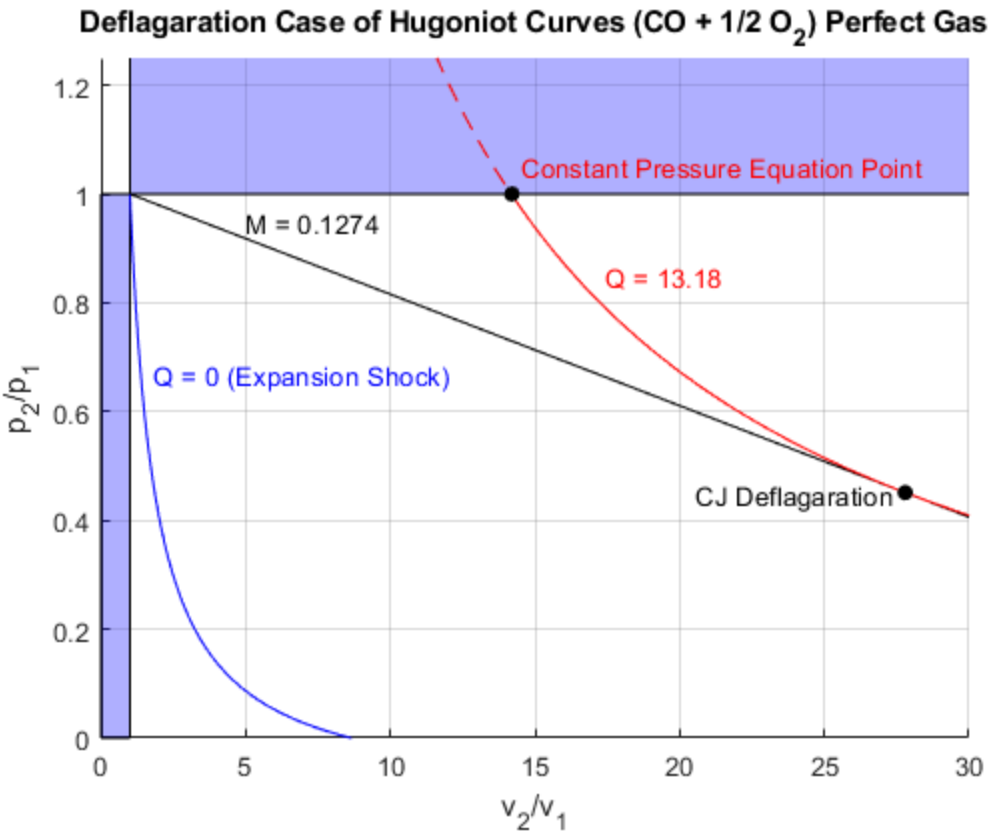
```
% CEA Results
Pcea = 18.497;
Mcj = 5.2354;
Pcj = zeros(1,length(V_det));

y_cea = 1.3977;

for i = 1:length(V_det)
    Pcj(i) = y_cea*Mcj^2*(1 - V_det(i)) + 1;
end
```

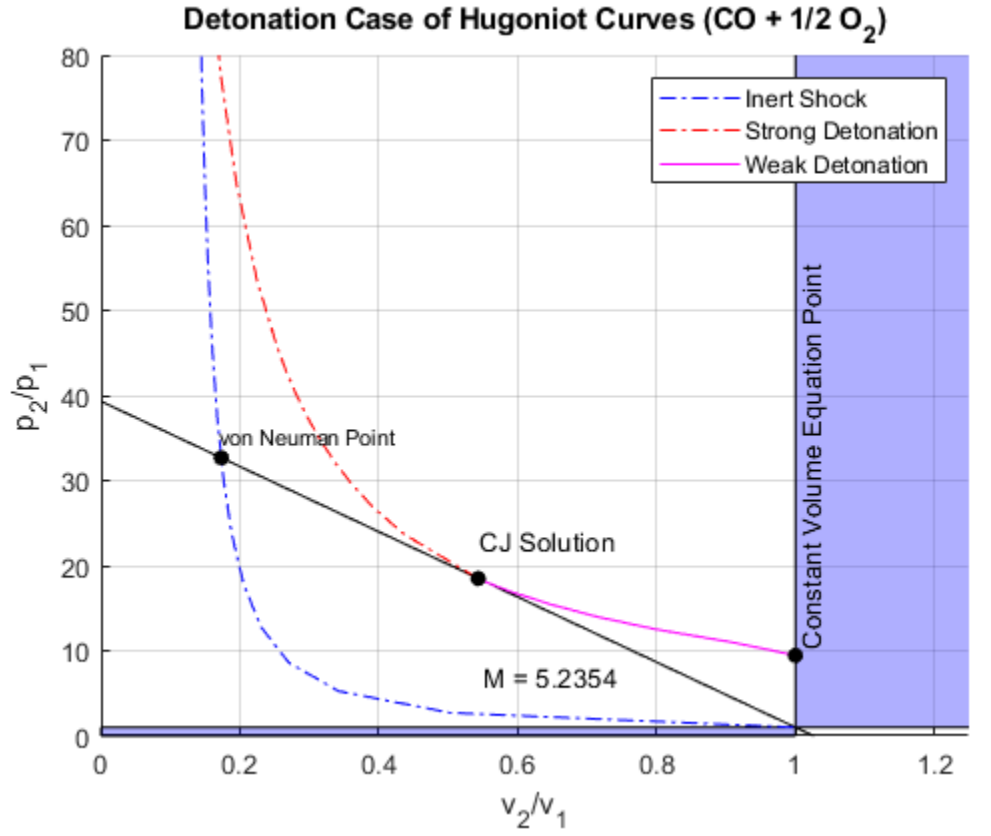
```
% From CEA Inert Shock
M_frozen = [0.9981 1.5686 2.1496 2.7305 3.3115 3.8924 4.4734 5.0253
 5.6063 6.1872 6.7682 7.3491 7.9301 8.5111 9.0920 9.6730 10.2539
 10.8349 11.4159 11.6192];
P_frozen = [1.011 2.707 5.246 8.602 12.792 17.824 23.699 30.061 37.58
 45.942 55.147 65.197 76.093 87.834 100.422 113.857 128.14 143.272
 159.256 165.053];
V_frozen = 1./[1.0028 1.9861 2.9196 3.6988 4.3391 4.8686 5.3104 5.6639
 5.9804 6.251 6.4850 6.6896 6.8703 7.0313 7.1758 7.3066 7.4256 7.5350
 7.6367 7.671];
```

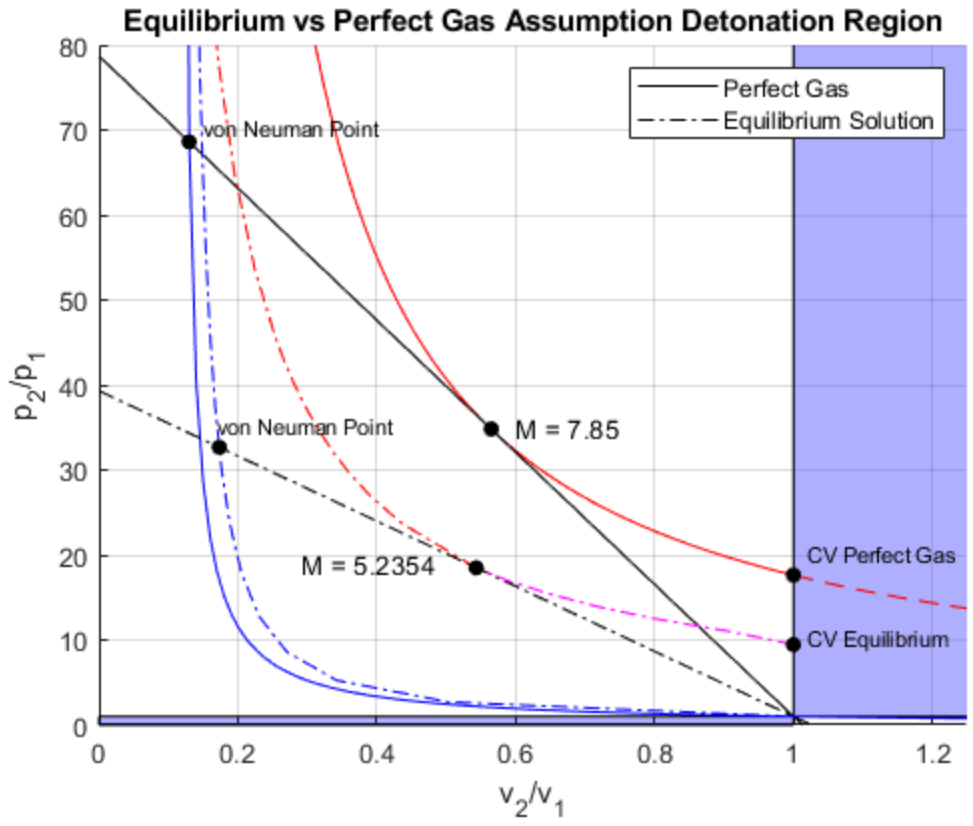
```
% Equilibrium Calculation CEA
M_eq = [5.2354 5.3739 5.5191 5.6644 5.8096 5.9548 6.1001 6.2453 6.3906
 6.5358 6.9715 7.5525 8.1334 8.7144];
P_eq = [18.497 23.726 26.85 29.652 32.33 34.959 37.571 40.189 42.825
 45.487 53.677 65.188 77.453 90.514];
V_eq = 1./[1.8406 2.2944 2.5507 2.7745 2.9826 3.1815 3.3744 3.5627
 3.7476 3.9296 4.4609 5.1407 5.7875 6.398];

Vcea = V_eq(1);

% Plot
figure(3)
grid on
hold on

h = zeros(1,3);

ylim([0 80]);
xlim([0 1.25]);

% Plot Forbidden Zones
patch([1 1 50 50],[1 200 200 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')

plot(V_det,Pcj,'k')
h(1) = plot(V_frozen, P_frozen, 'b-.','DisplayName','Inert Shock');
h(2) = plot(V_eq, P_eq, 'r-.','DisplayName','Strong Detonation');

h(3) = plot(Vweak,Pweak,'m','DisplayName','Weak Detonation');

plot(Vcea,Pcea,'.','MarkerSize',20,'Color','black'); % Marker for CJ
 Solution
plot(1,9.45531,'.','MarkerSize',20,'Color','black'); % Marker for
 Constant Volume Solution from CEA

alpha(0.3)

% Add Text
text(Vcea,23,'CJ Solution','Color','black')
text(.55,7,'M = 5.2354','Color','black')
set(text(1.02,10,'Constant Volume Equation
 Point','Color','black'),'Rotation',90)
text(.17,35,'von Neuman Point','Color','black','FontSize',8)

plot(.1733,32.67,'.','MarkerSize',20,'Color','black'); % Marker for
 von Neuman Point Equilibrium From Graph

% Labels
xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Detonation Case of Hugoniot Curves (CO + 1/2 O_2)')
legend(h);
```

```
hold off

% Overlay/Compare Graphs
figure(4)
grid on
hold on

h1 = zeros(1,2);

ylim([0 80]);
xlim([0 1.25]);

% Plot Forbidden Zones
patch([1 1 50 50],[1 200 200 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')

% Perfect Gas
plot(V_det(13:100),P_det(13:100),'r',V_det(101:end),P_det(101:end),'r--') %
 Plot for solved Q with forbidden zone dashed
h1(1) = plot(V_det,Pcj_det,'k','DisplayName','Perfect Gas'); % Plot M
 slope for solved
plot(V_det(13:126),P_det0(13:126),'b')

% Equilibrium
h1(2) = plot(V_det,Pcj,'k-.','DisplayName','Equilibrium Solution');
plot(V_frozen, P_frozen, 'b-.')
plot(V_eq, P_eq, 'r-.')
plot(Vweak,Pweak,'m-.');

%Constant Volume Solutions
plot(1,9.45531,'.','MarkerSize',20,'Color','black'); % Equilibrium
plot(1,ConV,'.','MarkerSize',20,'Color','black'); % Perfect

plot(Vcea,Pcea,'.','MarkerSize',20,'Color','black');
plot(CJ_detx,CJ_dety,'.','MarkerSize',20,'Color','black');

plot(vNx,vNy,'.','MarkerSize',20,'Color','black'); % Marker for von
 Neuman Point Perfect
plot(.1733,32.67,'.','MarkerSize',20,'Color','black'); % Marker for
 von Neuman Point Equilibrium From Graph

alpha(0.3)

% Add Text
legend(h1(1:2));
text(1.02,10,'CV Equilibrium','Color','black','FontSize',8)
text(1.02,20,'CV Perfect Gas','Color','black','FontSize',8)

text(.29,19,'M = 5.2354','Color','black')
text(.6,35,'M = 7.85','Color','black')

text(.15,70,'von Neuman Point','Color','black','FontSize',8)
text(.17,35,'von Neuman Point','Color','black','FontSize',8)
```

```
% Labels
xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Equilibrium vs Perfect Gas Assumption Detonation Region')

hold off

% Compare Deflagaration
figure(5)
grid on
hold on
ylim([0 1.25]);
xlim([0 30])

% Shade forbidden regions
patch([1 1 50 50],[1 50 50 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')


plot(V_flag,P_flag0,'b') % Plot Q = 0
plot(V_flag,Pcj_flag,'k') % Plot M Slope
plot(V_flag,bot_flag,'r',V_flag,top_flag,'r--') %Plot Solved Q, dashed
 for forbidden zone
plot(V_flag(133),1,'.','MarkerSize',20,'Color','black'); % Marker for
 constant point
plot(CJ_flagx,CJ_flagy,'.','MarkerSize',20,'Color','black'); % Marker
 for CJ Solution
plot(9.9892,1,'.','MarkerSize',20,'Color','black'); % Constant Volume
 Equilibrium (T_2/T_1) from CEA

alpha(0.3)

% Add Text
text(1.8,.67,'Q = 0 (Expansion Shock)','Color','blue')
text(2,.85,'M = 0.1274','Color','black')
text(17.4,.85,'Q = 13.18','Color','red')
text(14.5,1.05,'Perfect Gas Constant P','Color','red')
text(20.5,.45,'CJ Deflagaration','Color','black')
text(3,1.05,'Equilibrium Constant P','Color','black')


xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Equilibrium vs Perfect Gas Assumption Deflagaration Region')

hold off
```


Deflagaration Case of Hugoniot Curves (CO + 1/2 O2) Perfect Gas
Constant Pressure Equation Point
M = 0.1274
Q = 13.18
Q = 0 (Expansion Shock)
CJ Deflagaration
p2/p1
v2/v1
0
0.2
0.4
0.6
0.8
1
1.2
0
5
10
15
20
25
30


Detonation Case of Hugoniot Curves (CO + 1/2 O2)
Inert Shock
Strong Detonation
Weak Detonation
von Neuman Point
CJ Solution
M = 5.2354
Constant Volume Equation Point
p2/p1
v2/v1
0
10
20
30
40
50
60
70
80
0
0.2
0.4
0.6
0.8
1
1.2


Equilibrium vs Perfect Gas Assumption Detonation Region
Perfect Gas
Equilibrium Solution
von Neuman Point
von Neuman Point
M = 7.85
M = 5.2354
CV Perfect Gas
CV Equilibrium
p2/p1
v2/v1
0
10
20
30
40
50
60
70
80
0
0.2
0.4
0.6
0.8
1
1.2

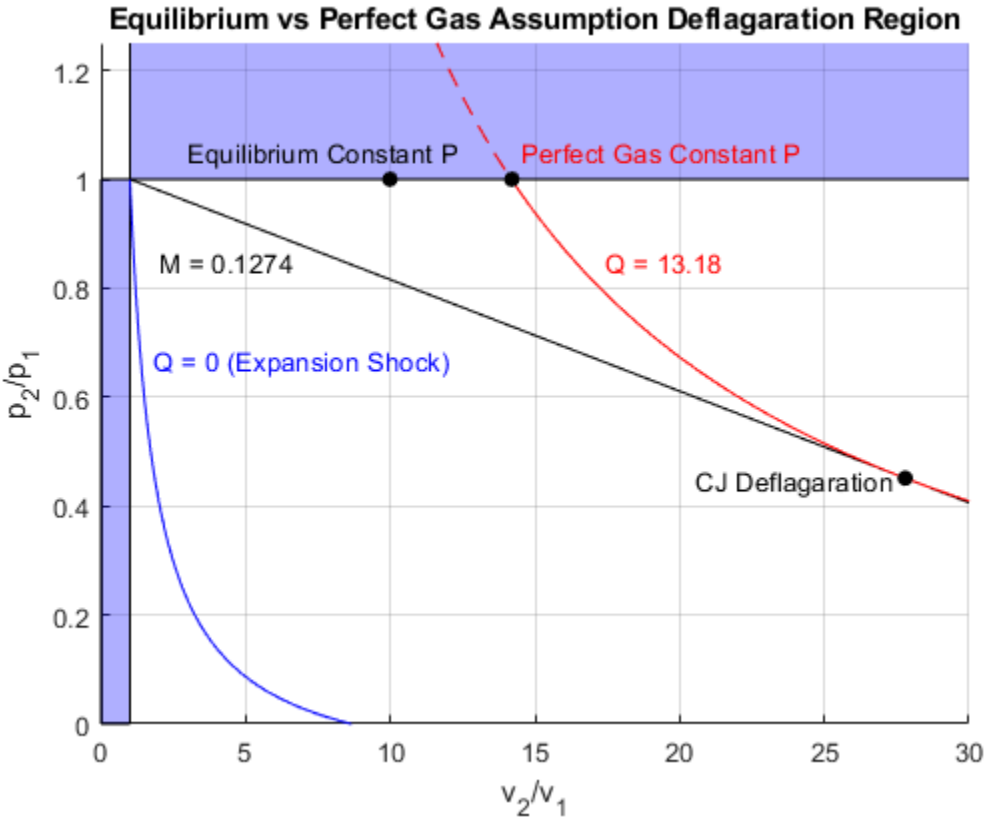

Equilibrium vs Perfect Gas Assumption Deflagaration Region
Equilibrium Constant P
Perfect Gas Constant P
M = 0.1274
Q = 13.18
Q = 0 (Expansion Shock)
CJ Deflagaration
p2/p1
v2/v1
0
0.2
0.4
0.6
0.8
1
1.2
0
5
10
15
20
25
30

Table Of CJ Properties

```
MT = [Mcj_det*C;Mcj*C];
PT = [CJ_dety;Pcea];
DT = [1.8406;5.7778];
TT = [11.826;5.657];

varRow = {'Perfect Gas','Equilibrium'};
varName = {'Velocity (m/s)','Pressure Ratio','Density
 Ratio','Temperature Ratio'};

Table1 = table(MT,PT,DT,TT,'VariableNames',varName,'RowNames',varRow)
```

Table1 =

2×4 table

	Velocity (m/s)	*Pressure Ratio*	*Density Ratio*	*Temperature Ratio*
Perfect Gas	*2691.8*	*34.819*	*1.8406*	*11.826*
Equilibrium	*1795.7*	*18.497*	*5.7778*	*5.657*

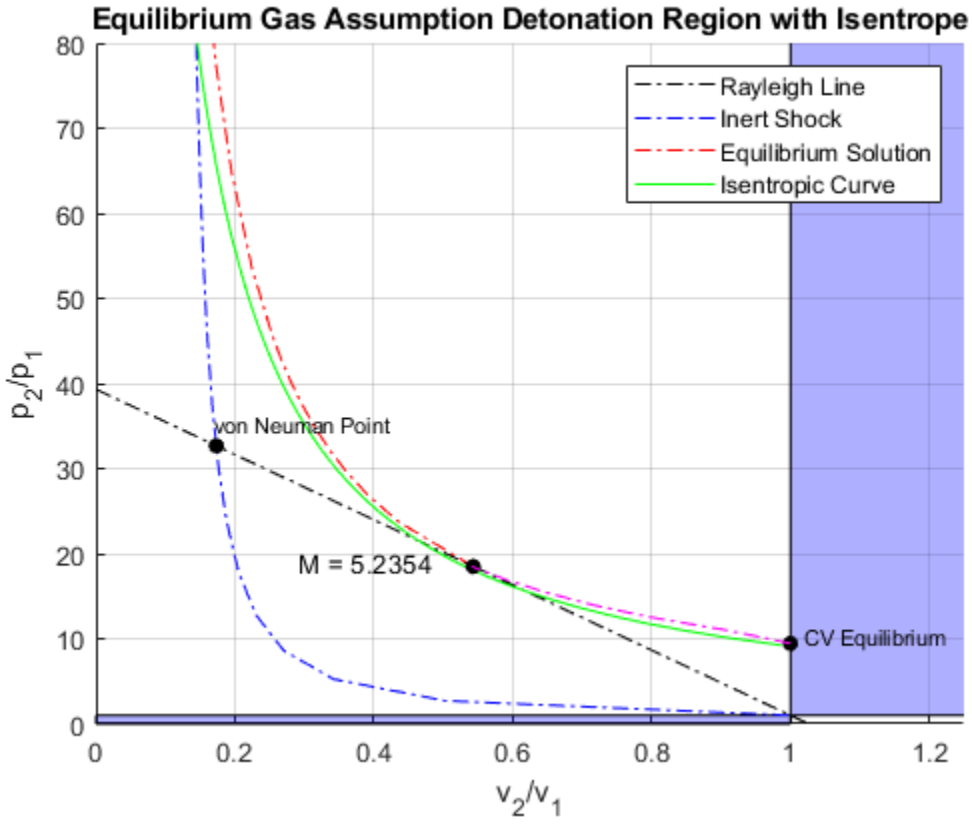
Plotting Isentrope

```
P1 = 1; %atm
T1 = 298; %K
M1 = 29.34; %1/n

s =[
   9.2409E+00  3.2977E+03  3.5605E+01;
   1.0106E+01  3.3207E+03  3.5517E+01;
   1.0980E+01  3.3423E+03  3.5434E+01;
   1.1861E+01  3.3627E+03  3.5358E+01;
   1.2750E+01  3.3820E+03  3.5286E+01;
   1.3647E+01  3.4003E+03  3.5218E+01;
   1.4550E+01  3.4177E+03  3.5154E+01;
   1.5460E+01  3.4344E+03  3.5094E+01;
   1.6376E+01  3.4504E+03  3.5036E+01;
   1.7299E+01  3.4657E+03  3.4982E+01;
   1.8227E+01  3.4805E+03  3.4929E+01;
   1.9161E+01  3.4947E+03  3.4879E+01;
   2.0100E+01  3.5084E+03  3.4831E+01;
   2.1044E+01  3.5217E+03  3.4785E+01;
   2.1994E+01  3.5345E+03  3.4741E+01;
   2.2948E+01  3.5470E+03  3.4698E+01;
   2.3908E+01  3.5591E+03  3.4657E+01;
```

```
2.4872E+01  3.5708E+03  3.4617E+01;
2.5840E+01  3.5822E+03  3.4579E+01;
2.6813E+01  3.5933E+03  3.4542E+01;
2.7791E+01  3.6042E+03  3.4506E+01;
2.8772E+01  3.6147E+03  3.4471E+01;
2.9758E+01  3.6250E+03  3.4437E+01;
3.0748E+01  3.6351E+03  3.4404E+01;
3.1741E+01  3.6449E+03  3.4372E+01;
3.2739E+01  3.6546E+03  3.4341E+01;
3.3740E+01  3.6640E+03  3.4310E+01;
3.4745E+01  3.6732E+03  3.4281E+01;
3.5754E+01  3.6822E+03  3.4252E+01;
3.6766E+01  3.6911E+03  3.4224E+01;
3.7782E+01  3.6998E+03  3.4196E+01;
3.8801E+01  3.7083E+03  3.4169E+01;
3.9824E+01  3.7167E+03  3.4143E+01;
4.0850E+01  3.7249E+03  3.4117E+01;
4.1879E+01  3.7329E+03  3.4092E+01;
4.2911E+01  3.7409E+03  3.4067E+01;
4.3946E+01  3.7487E+03  3.4043E+01;
4.4985E+01  3.7563E+03  3.4020E+01;
4.6027E+01  3.7639E+03  3.3996E+01;
4.7071E+01  3.7713E+03  3.3974E+01;
4.8119E+01  3.7786E+03  3.3951E+01;
4.9169E+01  3.7858E+03  3.3930E+01;
5.0223E+01  3.7929E+03  3.3908E+01;
5.1279E+01  3.7999E+03  3.3887E+01;
5.2338E+01  3.8068E+03  3.3866E+01;
5.6602E+01  3.8335E+03  3.3787E+01;
5.7674E+01  3.8399E+03  3.3768E+01;
5.8749E+01  3.8463E+03  3.3749E+01;
5.9827E+01  3.8525E+03  3.3731E+01;
6.0907E+01  3.8587E+03  3.3713E+01;
6.1990E+01  3.8649E+03  3.3695E+01;
6.3075E+01  3.8709E+03  3.3677E+01;
6.4163E+01  3.8769E+03  3.3660E+01;
6.5253E+01  3.8828E+03  3.3643E+01;
6.6345E+01  3.8886E+03  3.3626E+01;
6.7440E+01  3.8944E+03  3.3609E+01;
6.8537E+01  3.9001E+03  3.3593E+01;
6.9636E+01  3.9058E+03  3.3577E+01;
7.0738E+01  3.9114E+03  3.3561E+01;
7.1842E+01  3.9169E+03  3.3545E+01;
7.2948E+01  3.9224E+03  3.3530E+01;
7.4057E+01  3.9278E+03  3.3514E+01;
7.5167E+01  3.9331E+03  3.3499E+01;
8.1876E+01  3.9642E+03  3.3413E+01;
8.3002E+01  3.9692E+03  3.3399E+01;
8.4129E+01  3.9741E+03  3.3385E+01;
8.5259E+01  3.9791E+03  3.3371E+01;
8.6390E+01  3.9839E+03  3.3358E+01;
8.7524E+01  3.9887E+03  3.3345E+01;
8.8660E+01  3.9935E+03  3.3332E+01;
8.9797E+01  3.9983E+03  3.3319E+01;
```

```
   9.0936E+01  4.0030E+03  3.3306E+01;
   9.2078E+01  4.0076E+03  3.3293E+01;
   9.3221E+01  4.0122E+03  3.3281E+01;
   9.4366E+01  4.0168E+03  3.3268E+01;
   9.5513E+01  4.0214E+03  3.3256E+01;
   9.6662E+01  4.0259E+03  3.3244E+01;
   9.7813E+01  4.0304E+03  3.3232E+01;
   9.8965E+01  4.0348E+03  3.3220E+01;
   1.0012E+02  4.0392E+03  3.3208E+01;
   1.0128E+02  4.0436E+03  3.3197E+01;
   1.0243E+02  4.0479E+03  3.3185E+01;
   1.0359E+02  4.0522E+03  3.3174E+01;
   1.0476E+02  4.0565E+03  3.3162E+01]; %P2 T2 M2

Vs = zeros(1,length(s));
Ps = zeros(1,length(s));

for i = 1:length(s)
   Vs(i) = (P1*s(i,2)*M1)/(s(i,1)*T1*s(i,3));
   Ps(i) = s(i,1)/P1;
end

% Overlay/Compare Graphs
figure(6)
grid on
hold on

h2 = zeros(1,4);

ylim([0 80]);
xlim([0 1.25]);

% Plot Forbidden Zones
patch([1 1 50 50],[1 200 200 1], 'b')
patch([0 0 1 1],[0 1 1 0], 'b')


% Equilibrium
h2(1) = plot(V_det,Pcj,'k-.','DisplayName','Rayleigh Line');
h2(2) = plot(V_frozen, P_frozen, 'b-.','DisplayName','Inert Shock');
h2(3) = plot(V_eq, P_eq, 'r-.','DisplayName','Equilibrium Solution');
h2(4) = plot(Vs,Ps,'g','DisplayName','Isentropic Curve');

%Constant Volume Solutions
plot(1,9.45531,'.','MarkerSize',20,'Color','black'); % Equilibrium
plot(Vcea,Pcea,'.','MarkerSize',20,'Color','black');
plot(.1733,32.67,'.','MarkerSize',20,'Color','black'); % Marker for
 von Neuman Point Equilibrium From Graph

plot(Vweak,Pweak,'m-.');

alpha(0.3)

% Add Text
```

```
text(1.02,10,'CV Equilibrium','Color','black','FontSize',8)
text(.29,19,'M = 5.2354','Color','black')
text(.17,35,'von Neuman Point','Color','black','FontSize',8)

legend(h2)

% Labels
xlabel('v_2/v_1')
ylabel('p_2/p_1')
title('Equilibrium Gas Assumption Detonation Region with Isentrope')

hold off
```



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```
function [Vweak,Pweak] = weak()
    CEAweak = [
   1.1146E+01  1.3198;
   1.2666E+01  1.4998;
   1.4185E+01  1.6798;
   1.5705E+01  1.8597;
   1.7225E+01  2.0397;
   1.8745E+01  2.2197]; % P rho



    P1 = 1; %atm
    T1 = 298; %K
    M1 = 29.34; %1/n
    D1 = 1.199826;

    Vweak = zeros(1,length(CEAweak)+1);
    Pweak = zeros(1,length(CEAweak)+1);

    Vweak(1) = 1;
    Vweak(2:end) = D1./CEAweak(:,2);

    Pweak(1) = 9.45531;

    for i = 1:length(CEAweak)
       Pweak(i+1) = CEAweak(i,1)*(0.986923)/P1;
    end

end


ans =

    1.0000    0.9091    0.8000    0.7143    0.6452    0.5882    0.5405
```

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