MaxPlomer

For Prof: T. Lu

Combustion Project – HCCI engine simulation

Derivation of Equations:

$$f = ?$$
$$R = ?$$
$$\omega = 2\pi f$$

Solve for alpha from R

$$R = \frac{V_{\max}}{V_{\min}} = \frac{1+\alpha}{1-\alpha}$$
$$R - R\alpha = 1 + \alpha$$
$$R - 1 = [R+1]\alpha$$
$$\alpha = \frac{R-1}{R+1}$$

*There are 53 chemkin species

*53 Mass fractions then pressure and temperature, 55 variables total (NV)

*For initial conditions setup a vector NV long, all zeros

Mixture is Methane & air with phi=0.3

$$CH_4 + 2O_2 = 2H_2O + CO_2$$
$$\frac{n_{fuel}}{n_{ox}} = \phi\left[\frac{n_{fuel}}{n_{ox}}\right]_{st}$$

Phi/2 CH4, 1 O2, 3.76 N2

Initial Mass Fraction Values, are therefore:

$$Y_{CH4,0} = \frac{\phi * .5 * WT_{CH4}}{total}$$

$$Y_{O2,0} = \frac{WT_{O2}}{total}$$

$$Y_{N2,0} = \frac{3.76 * WT_{N2}}{total}$$

Initial Pressure = 1 atm

Initial Temperature = 300K – 500K

Initial average molecular weight

$$\overline{MW}_0 = \frac{1}{\sum_{i=1}^{K} Y_{i,0} / MW_i}$$

Time span for simulation: 1 cycle

$$f = \frac{cycles}{t} \qquad \text{use:} \qquad t = \frac{1}{f}$$

Use the initial conditions array y0 in the ode15s() function

Now for the functions inside the ignfun() function

Average molecular weight:

$$\overline{MW} = \frac{1}{\sum_{i=1}^{K} Y_i / MW_i}$$

Average Density

$$\rho = \frac{p\,\overline{MW}}{R_u T}$$

c_v

Function ckcvml(T,chem)./W gives c_v per mass of a chemical at a specific T. (W is vector of molecular weights)

Create a vector c_v, make equal to function ckcvml(P,chem)./W,

Average Cv per mass of mixture

$$\overline{c}_{v,mass} = \sum_{i=1}^{k} Y_i c_{v,i}$$

u

Function ckuml(T,chem)./W gives u per mole of a chemical at a specific T, to convert to u per mass, must divide by molecular weight

Create a vector u, make equal to function ckuml(T,chem)./W

Need: $\frac{dv}{dt}$ (Change in specific volume per time)

From: $V = \overline{V}\left[1 + \alpha \cos(\omega t)\right]$ Where V=Volume,

$$pv = RT$$

$$p_0 v_0 = \frac{R_u}{\overline{MW}_0} * T$$

$$v_0 = \frac{R_u T_0}{p_0 \overline{MW}_0}$$

$$\frac{dv}{dt} = \frac{v_0}{1+\alpha}\left[-\alpha\omega \sin(\omega t)\right]$$

$\dot{\omega}$ (Molar Production Rate)

Function ckwyp(P,T,Y,chem) gives molar production rate of a species at a specific Pressure and Temperature

Create a vector omegadot, make equal to function ckwyp(P,T,Y,chem)

Change in mass fraction per time, Use this equation for $\frac{\mathrm{dy}}{\mathrm{dt}}(1)$ through $\frac{\mathrm{dy}}{\mathrm{dt}}(53)$

$$\frac{dY_i}{dt} = v \dot{\omega}_i MW_i \quad \text{with} \quad v = \frac{1}{\rho}$$

Change in pressure per time, Use this equation for $\frac{\mathrm{dy}}{\mathrm{dt}}(54)$

From ideal gas:

$$pv = R_g T$$

$$v\frac{dp}{dt} + p\frac{dv}{dt} = \frac{d(R_g T)}{dt}$$

$$\frac{dp}{dt} = \frac{\left[\frac{d(R_g T)}{dt} - p\frac{dv}{dt}\right]}{v} = \left[\frac{d(R_g T)}{dt} - p\frac{dv}{dt}\right] * \rho$$

$$\frac{dp}{dt} = \left[\frac{dR_g * T + \frac{R_u}{\overline{MW}} dT}{dt} - p\frac{dv}{dt}\right] * \rho$$

$$R_g = R_u * \sum_{i=1}^{K} Y_i / MW_i$$

$$dR_g = R_u * \sum_{i=1}^{K} dY_i / MW_i$$

$$\frac{dp}{dt} = \left[T * R_u * \sum_{i=1}^{K} \left(\frac{dY_i}{dt}\right) / MW_i + \frac{R_u}{\overline{MW}} \frac{dT}{dt} - p\frac{dv}{dt}\right] * \rho$$

Change in Temperature per time, Use this equation for $\frac{\mathrm{dy}}{\mathrm{dt}}(55)$

$$\bar{c}_v \frac{dT}{dt} + p\frac{dv}{dt} + v\sum_{i=1}^{k} u_k \dot{\omega}_k MW_k = 0$$

$$\frac{dT}{dt} = \frac{-\left[p\frac{dv}{dt} + \frac{1}{\rho} * \sum_{i=1}^{k} u_k \dot{\omega}_k MW_k\right]}{\bar{c}_v}$$

Results:

I formed the equations into a function that calculated temperature, pressure, and the mass fractions of all species, through 1 cycle (the four output vectors: temp, pressure, mass frac , time). Varying initial temperature, compression ratio R, and engine frequency f (the inputs for the function), I determined whether ignition occurred by checking if half the initial mass fraction was greater than the final mass fraction. Due to a slight fluctuation between the initial and final mass fraction of the fuel during compression with no ignition, it did not work to say that if the initial mass fraction equaled the final mass fraction there was no ignition.

I also evaluated the equations for, after determining if ignition occurred, the difference between the ignition time and the time at which maximum temperature occurred. To do this I just found the column of these values in their respective vectors, then found the difference in time by subtracting the values in the time vector at those prescribed column positions.

In addition I evaluated the maximum temperature that is created for the same range of R and F. This turned out to be important for my Dt between ignition and Tmax time graph at T0=500K and f=30-200Hz, because it looked as though a point had ignition, there was a change in mass fraction more than half of the initial value. When I checked the same point on the Tmax graph at T0=500K and f=30-200Hz, you could clearly see that ignition did not occur.

Domain of simulation:

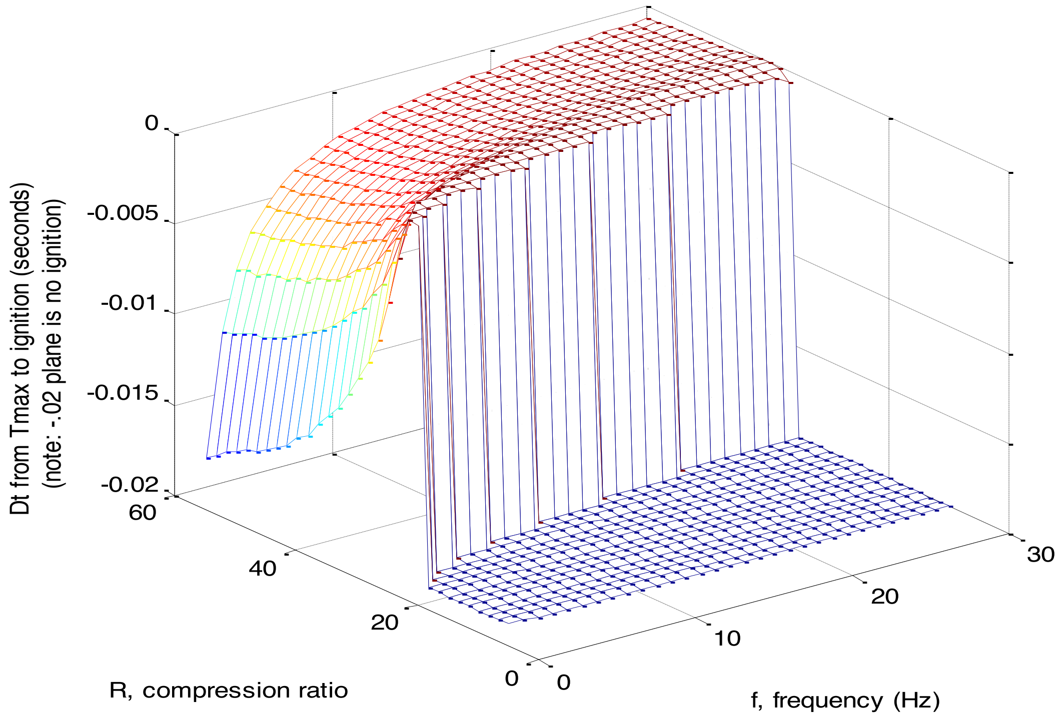
Varying T0 from 300K - 500K (3 increments, therefore @300, 400 & 500 K)

Varying f from 2 to 200 Hz, two separate plots 2-30Hz and 30-200Hz. Reason: to better see the shape of the plots due to the steep cutoff that occurs around very low frequencies. (31 increments)

Varying R from 10-60 for low frequencies and 10-70 for high frequencies. Reason: to best present the border between ignition and no ignition. (31 increments)

Results from Low Frequencies: 2 to 30 Hz

Figure 1: @ T0 = 300K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
2	25	26.67
7.6	30	33.33
15.07	33.33	38.33
30	36.67	43.33

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	No ignition	No ignition
30	3.867	7.6
40	18.8	Not on graph
50	30*	Not on graph

* (could be higher, 30 is maximum for this range)

At this temperature of T0=300K and frequency range of 2 through 30 Hz, high compression ratios, say above 40 need a high frequency, say above 20 Hz to maximize efficiency. You can notice that different compression ratios have different amount of frequency range that allow maximum efficiency. From this chart, an R value of 36.67 has a T_{max} close in time to its ignition for a range of frequency starting at 12 Hz ending at the edge of the graph at 30 Hz.

Figure 2: @ T0 = 300K

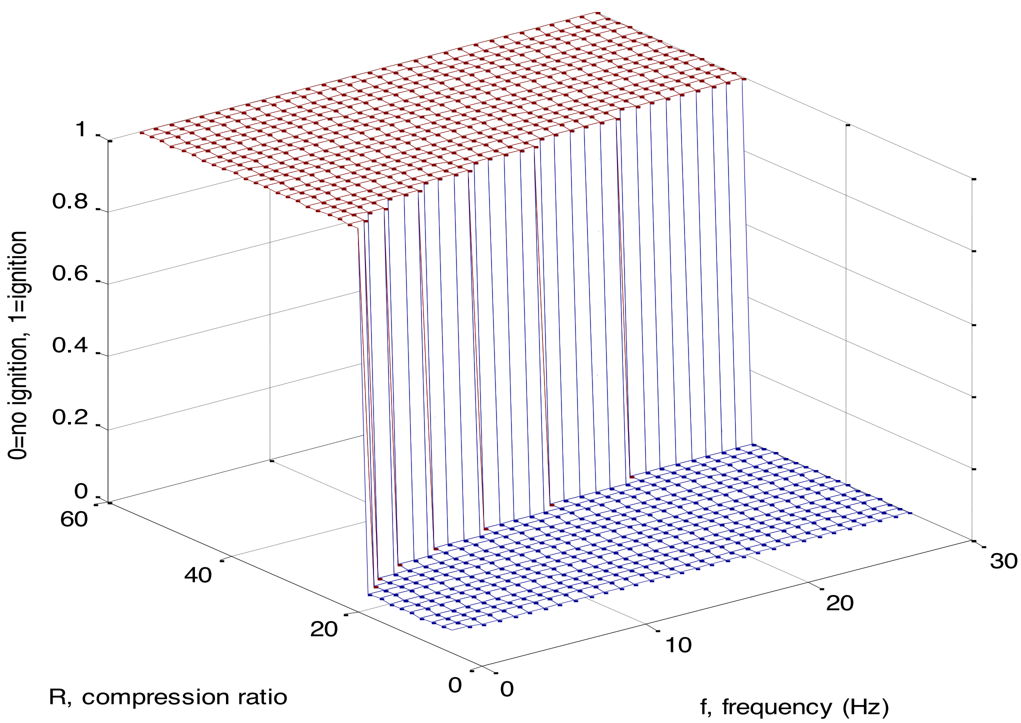


Figure 3: @ T0 = 300K

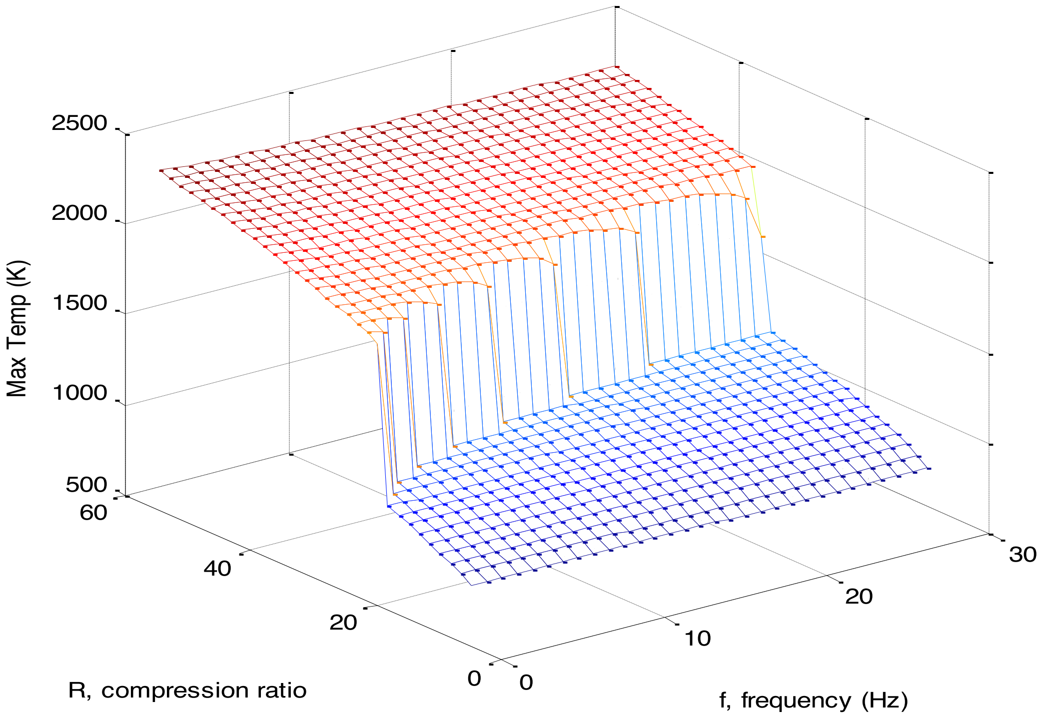
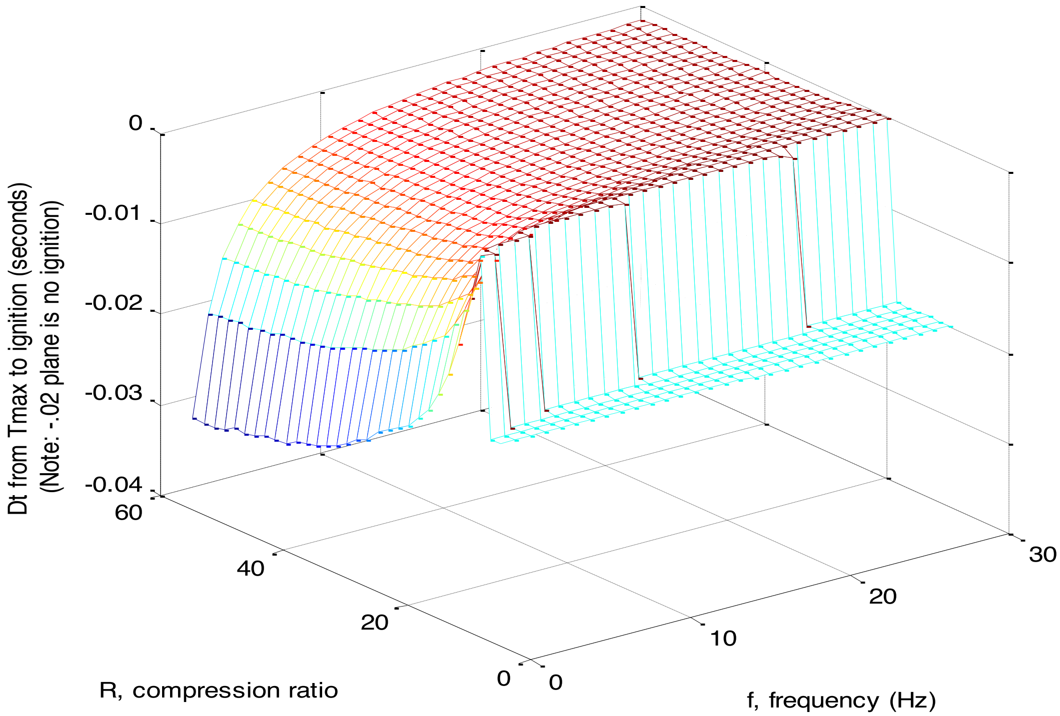


Figure 4: @ T0 = 400K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
2	13.33	15
7.6	16.67	18.33
15.07	18.33	20
30	20	23.33

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	14.13	Not on graph
30	30*	Not on graph
40	30*	Not on graph
50	30*	Not on graph

* (could be higher, 30 is maximum for this range)

At this temperature of T0=400K and frequency range of 2 through 30 Hz, high compression ratios, say above 40 need a high frequency, say above 20 Hz to maximize efficiency. From this chart, an R value of 20 has a T_{max} close in time to its ignition for a range of frequency starting at 12 Hz ending at the edge of the graph at 30 Hz.

Figure 5: @ T0 = 400K

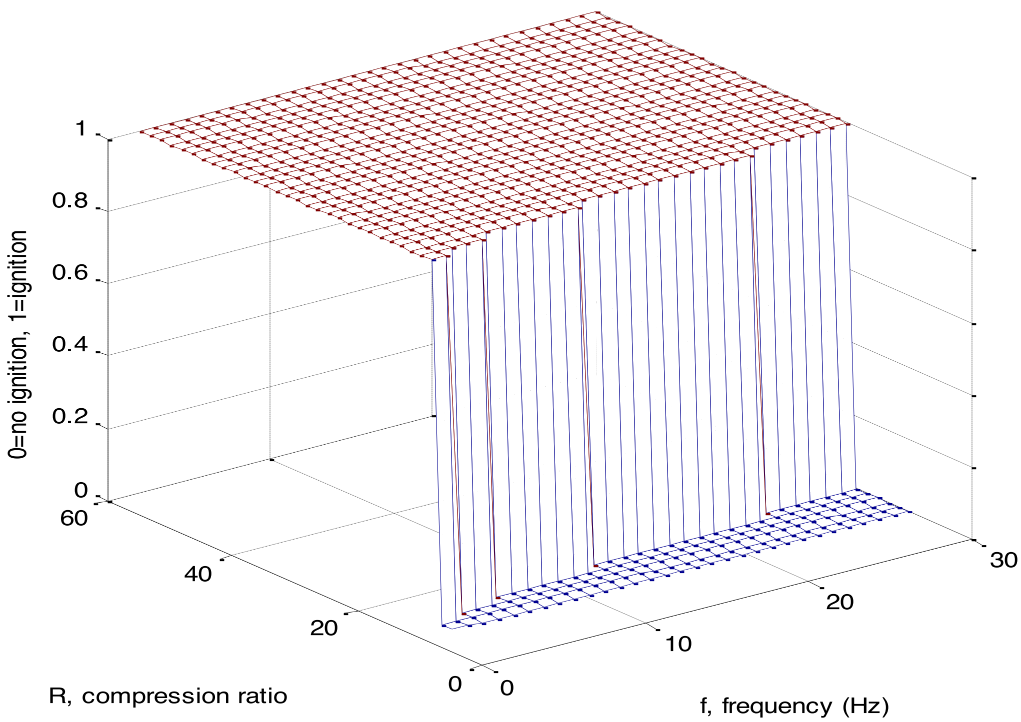


Figure 6: @ T0 = 400K

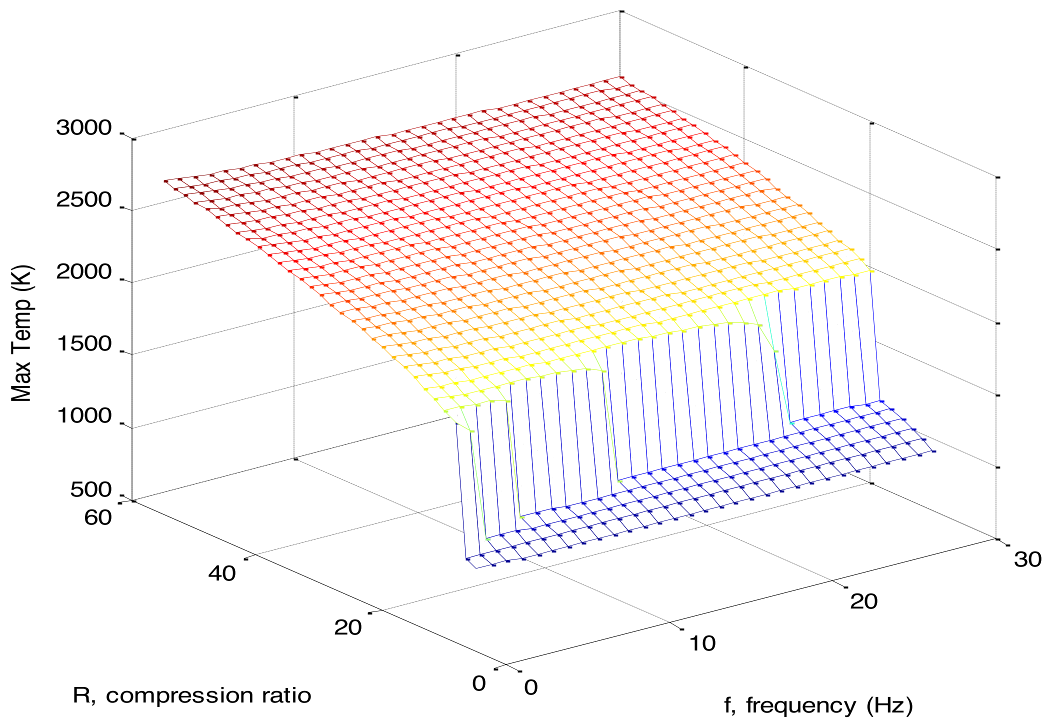
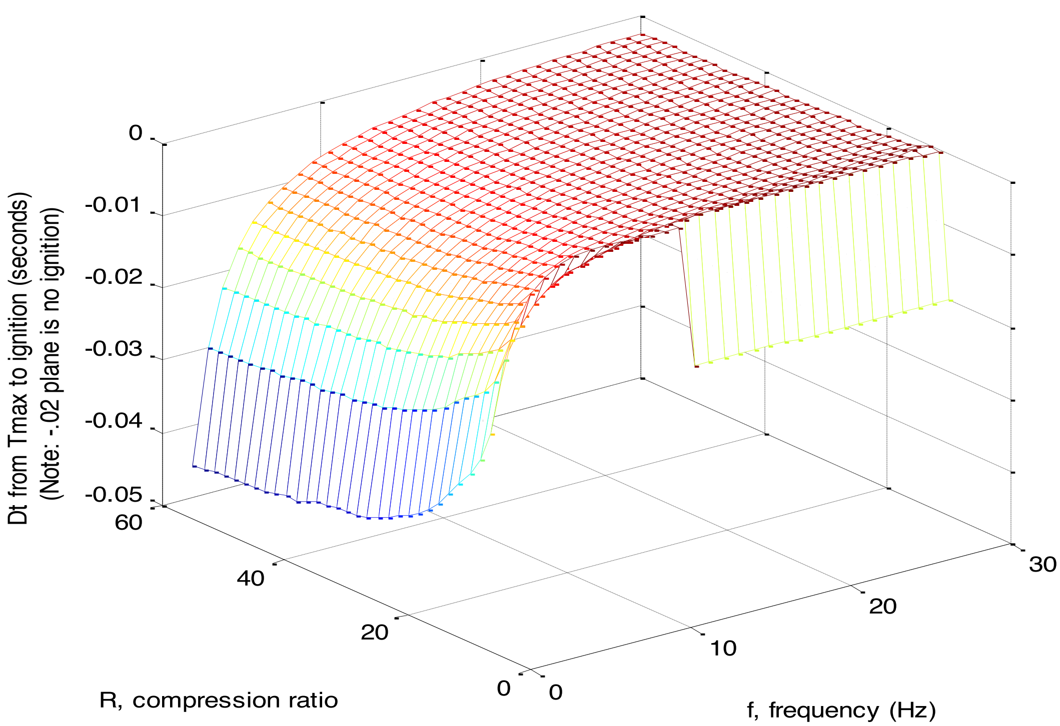


Figure 7: @ T0 = 500K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
2	10**	10**
7.6	10**	10
15.07	11.67	13.33
30	11.67	13.33

**(Could be lower, 10 is minimum for this range)

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	30*	Not on graph
30	30*	Not on graph
40	30*	Not on graph
50	30*	Not on graph

* (could be higher, 30 is maximum for this range)

At this temperature of T0=500K and frequency range of 2 through 30 Hz, high compression ratios, say above 40 need a high frequency, say above 20 Hz to maximize efficiency. From this chart, an R value of 11.67 has a T_{max} close in time to its ignition for a range of frequency starting at 12 Hz ending at the edge of the graph at 30 Hz.

Figure 8: @ T0 = 500K

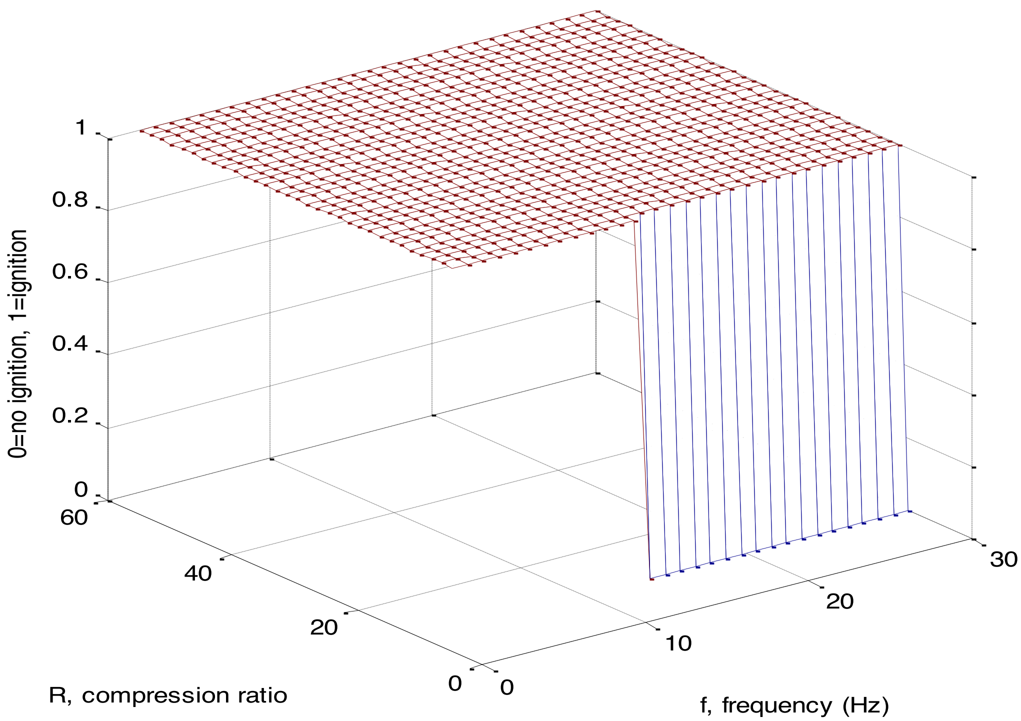
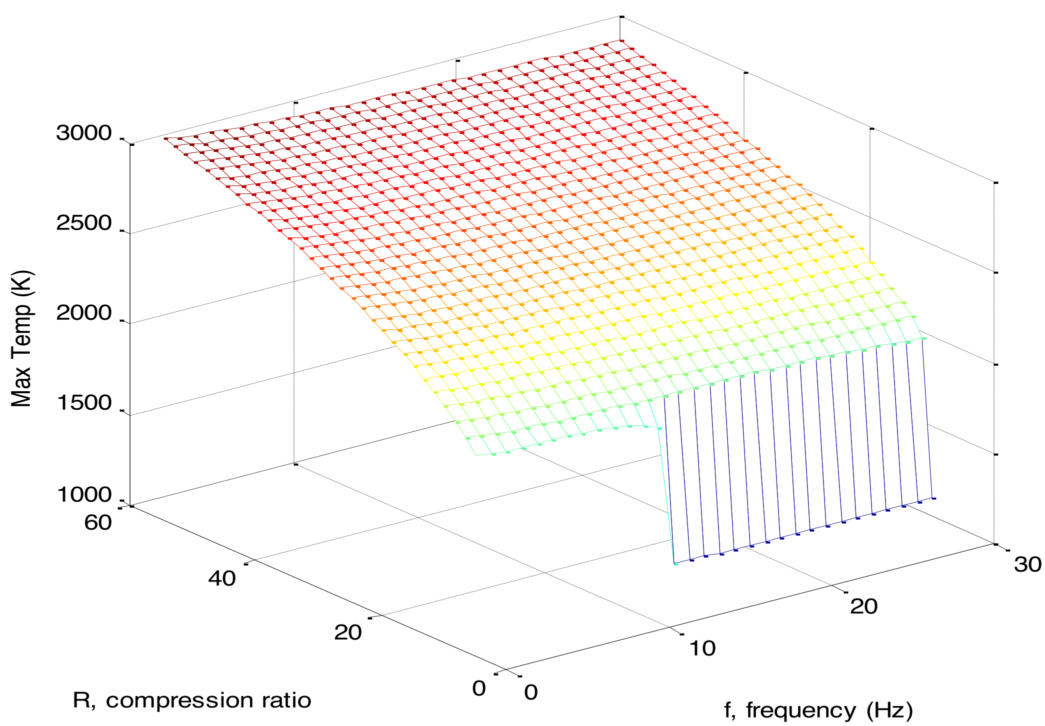
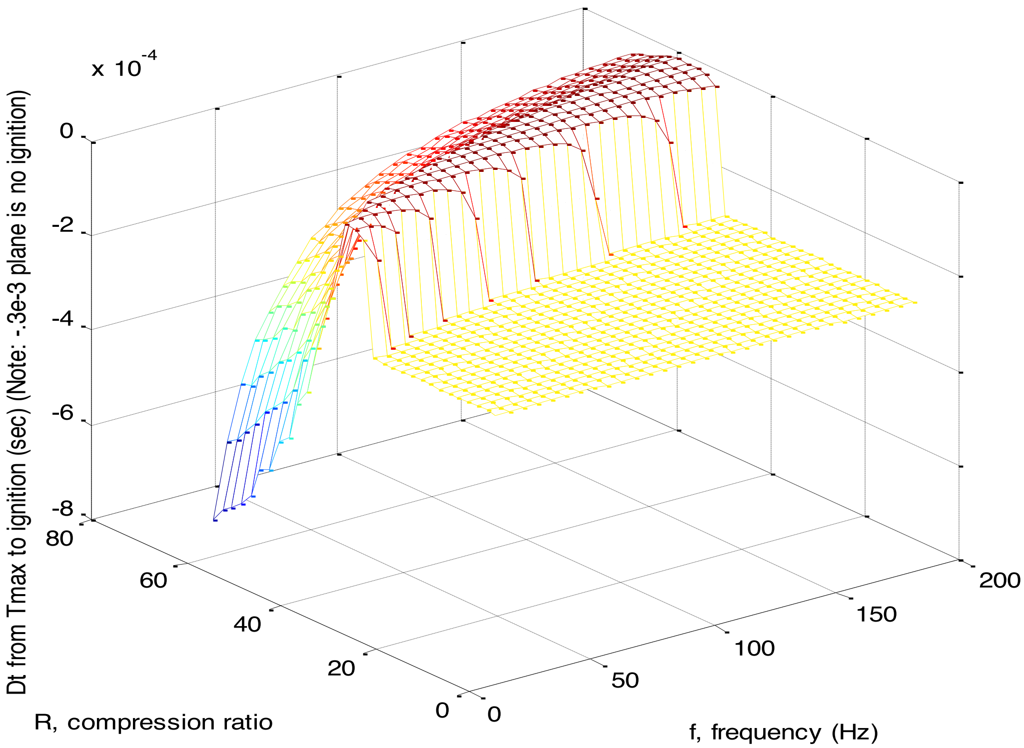


Figure 9: @ T0 = 500K



Results from High Frequencies: 30 to 200 Hz

Figure 1: @ T0 = 300K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
52.67	42	46
103.7	46	54
149	50	58
200	52	62

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	No ignition	No ignition
30	No ignition	No ignition
40	30**	47

50	75.33	177.3

**(Could be lower, 30 is minimum for this range)

At this temperature of T0=300K and frequency range of 30 through 200 Hz, high compression ratios, say above 60 need a high frequency, say above 160 Hz to maximize efficiency. From this chart, an R value of 52 has a T_{max} close in time to its ignition for a range of frequency starting at 85 Hz ending at the edge of the graph at 200 Hz.

Figure 2: @ T0 = 300K

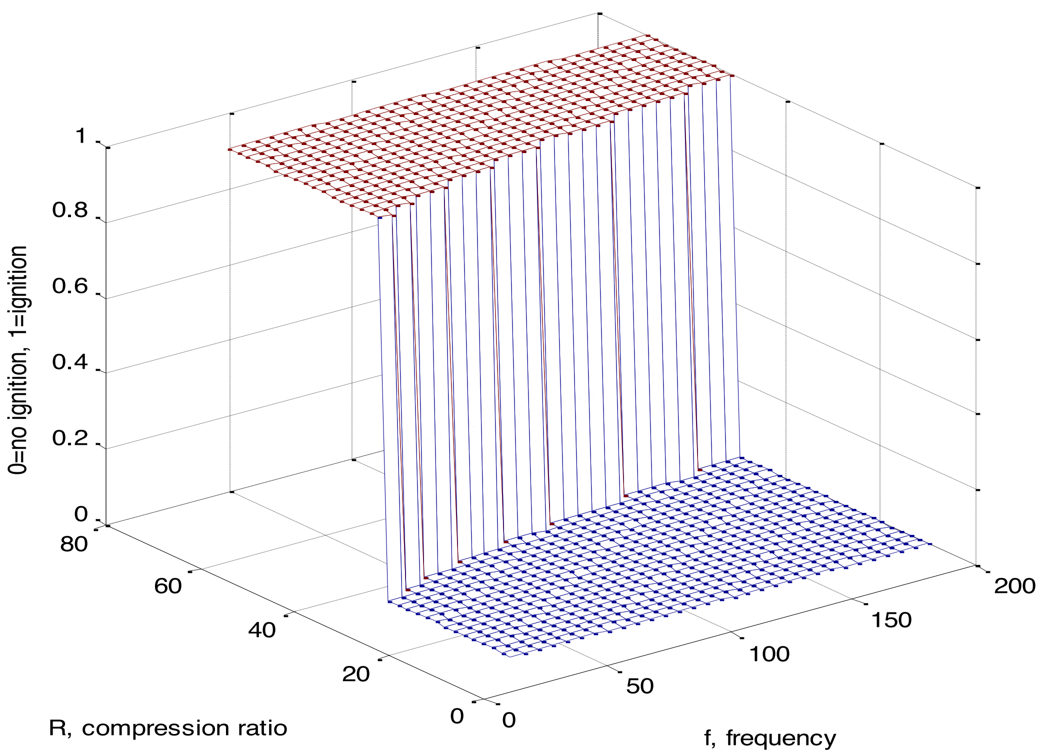


Figure 3: @ T0 = 300K

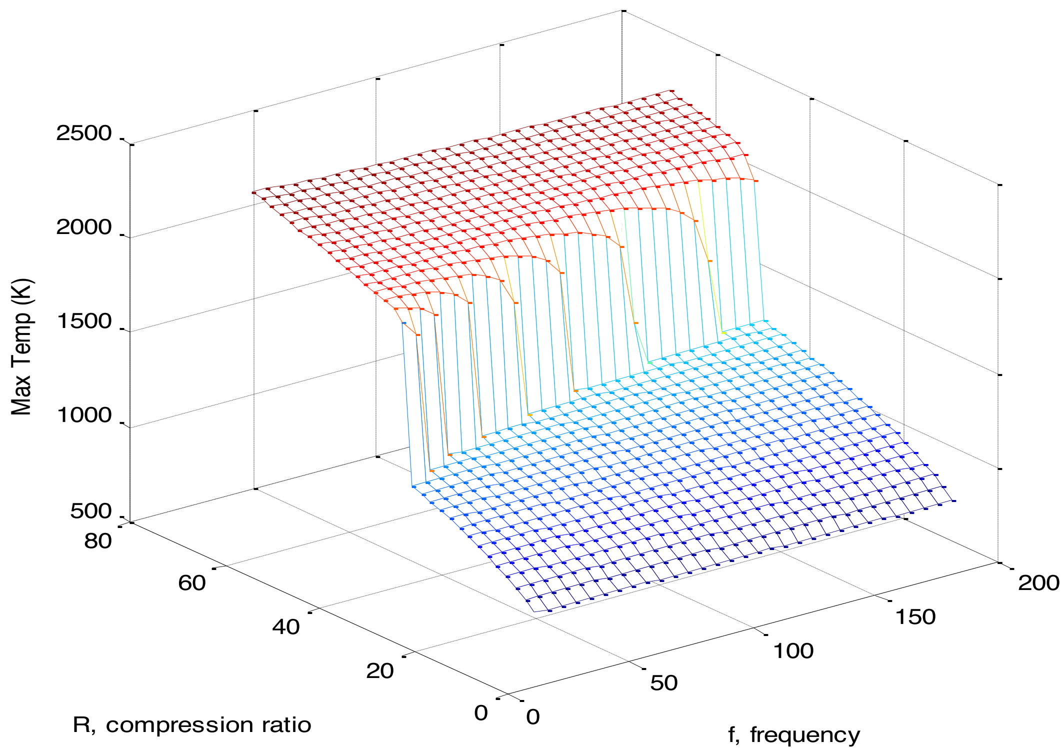
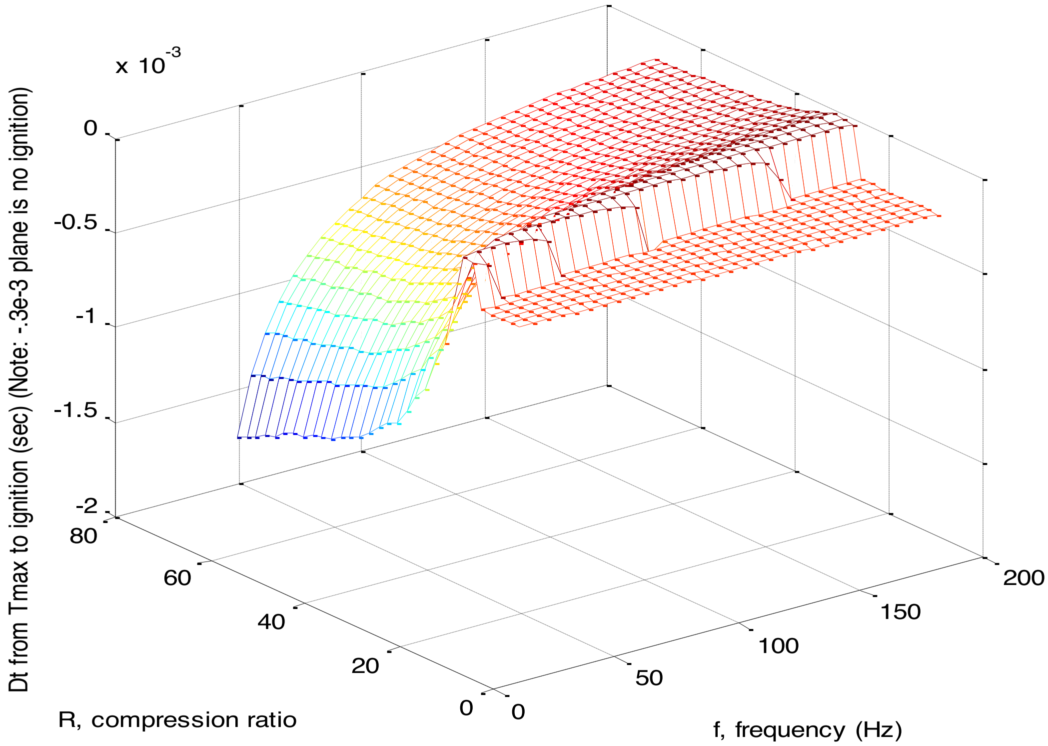


Figure 4: @ T0 = 400K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
52.67	22	24
103.7	24	28
149	26	30
200	28	32

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	30*	35.67
30	120.7	Not on graph
40	200**	Not on graph
50	200**	Not on graph

*(might be lower, 30 is minimum for this graph)

**(might be higher, 200 is maximum for this graph)

At this temperature of T0=400K and frequency range of 30 through 200 Hz, high compression ratios, say above 60 need a high frequency, say above 160 Hz to maximize efficiency. From this chart, an R value of 28 has a T_{max} close in time to its ignition for a range of frequency starting at 85 Hz ending at the edge of the graph at 200 Hz.

Figure 5: @ T0 = 400K

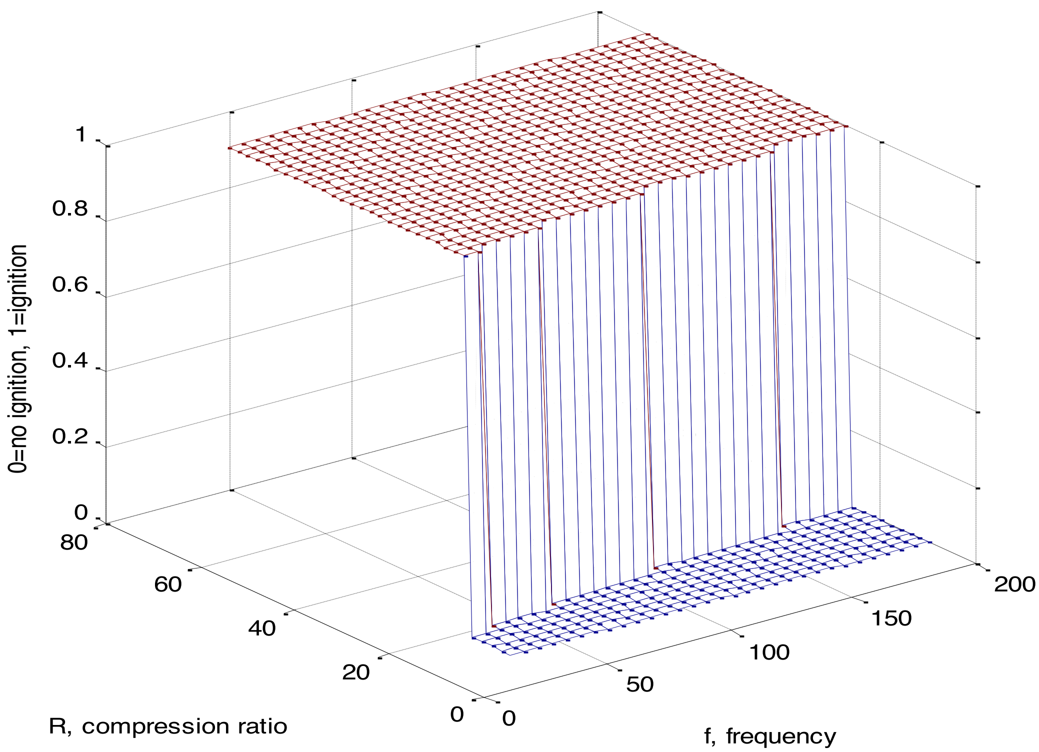


Figure 6: @ T0 = 400K

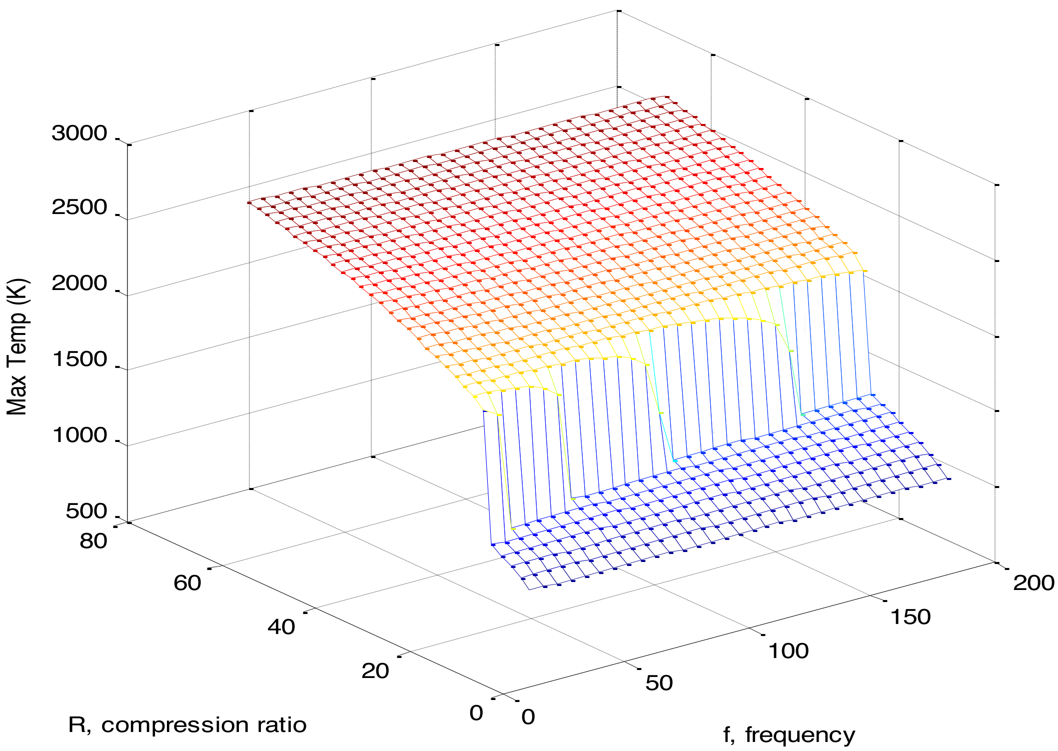
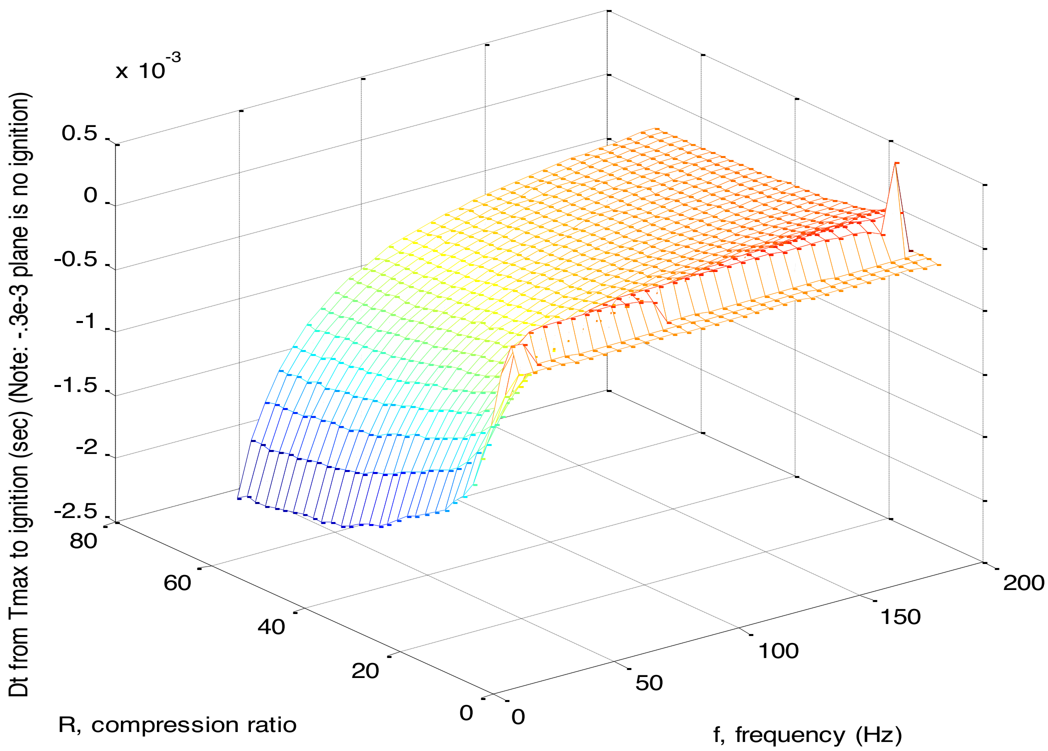


Figure 7: @ T0 = 500K



Frequency, f	Minimum Compression ratio, R, needed for ignition	Maximum Compression ratio, R, until ignition occurs too far before T_{max}
52.67	14	16
103.7	16	18
149	16	20
200	18	20

Compression ratio, R	Minimum Frequency, f, needed for ignition to occur close to T_{max}	Maximum frequency, f, before ignition does not occur
20	160.3	Not on graph
30	200*	Not on graph
40	200*	Not on graph
50	200*	Not on graph

*(might be higher, 200 is maximum for graph)

What was very interesting is that at R=16 and and f=194.3 it reports that ignition occurs and that it occurs after T_{max}. but when checking that point on the maximum temperature chart I found that ignition did not occur at that point, but rather for some weird reason the mass fraction of CH4 just goes down at a time after the peak temperature. From this chart, an R value of 16 has a T_{max} close in time to its ignition for a range of frequency starting at 70 Hz ending at the edge of the graph at 194.3 Hz.

Figure 8: @ T0 = 500K

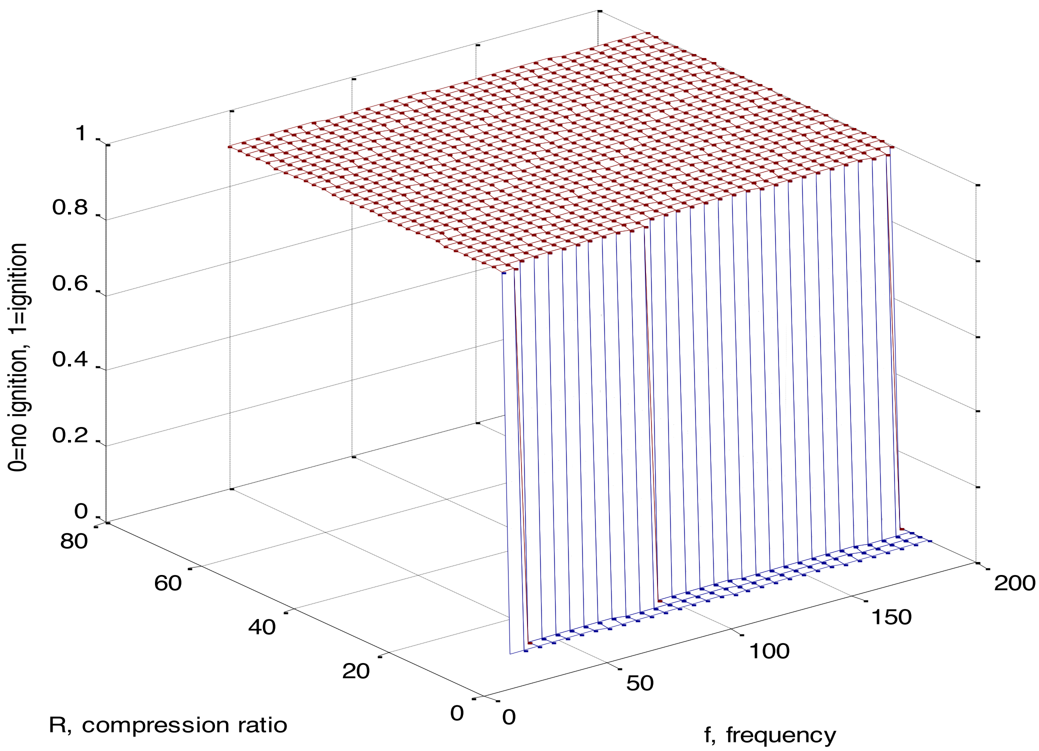
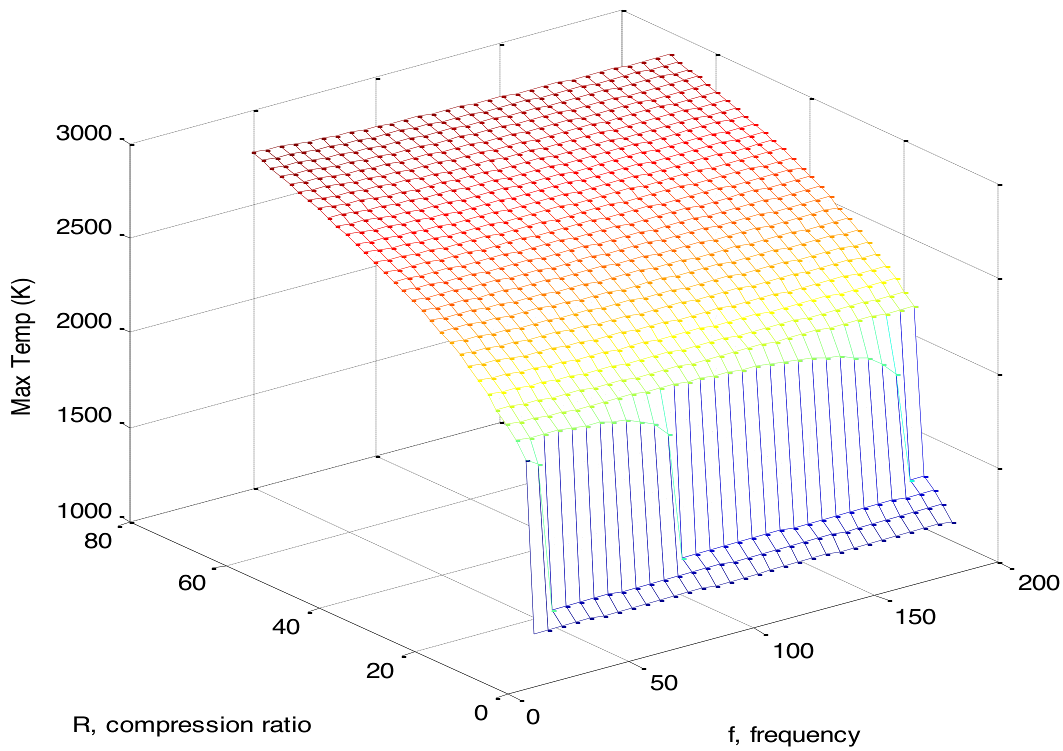


Figure 9: @ T0 = 500K



Overall Conclusions

We noticed that the greatest range of efficient frequencies occurred with the highest T0 temperature. At T0=500 K an R value of 16 can have efficient use from 70-190 Hz. If you have a lower compression engine you can boost the frequency, and range of frequencies, it can ignite at by boosting the initial temperature.

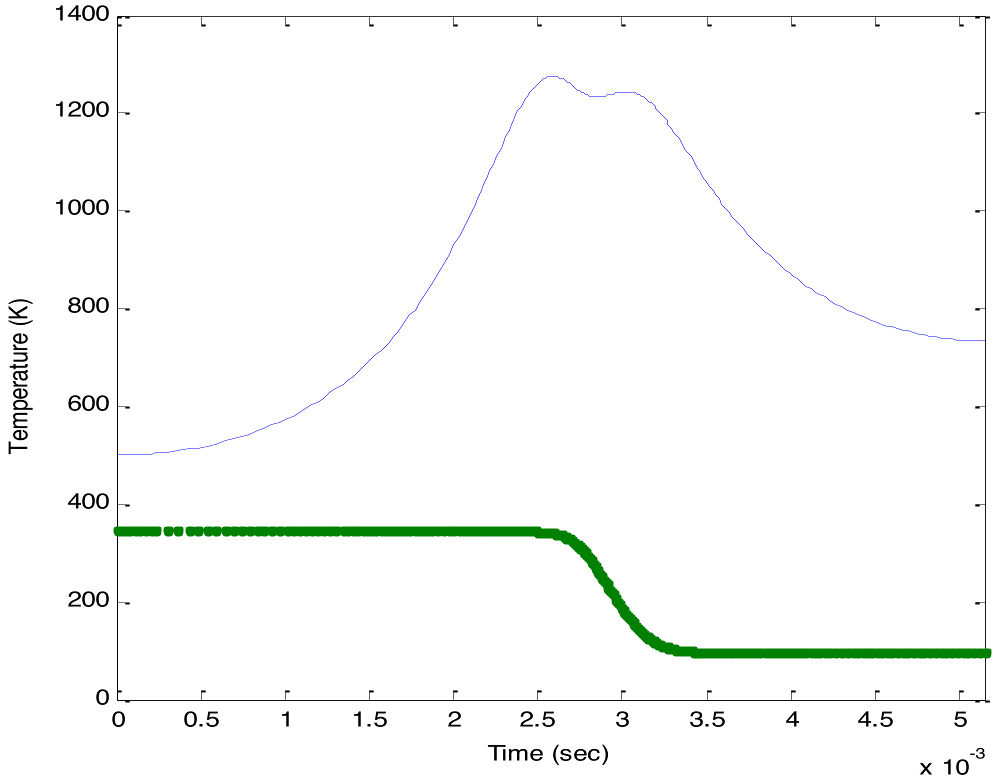
Unusual False ignition Result

Running my original code from part 1 of the assignment, with:

R=16

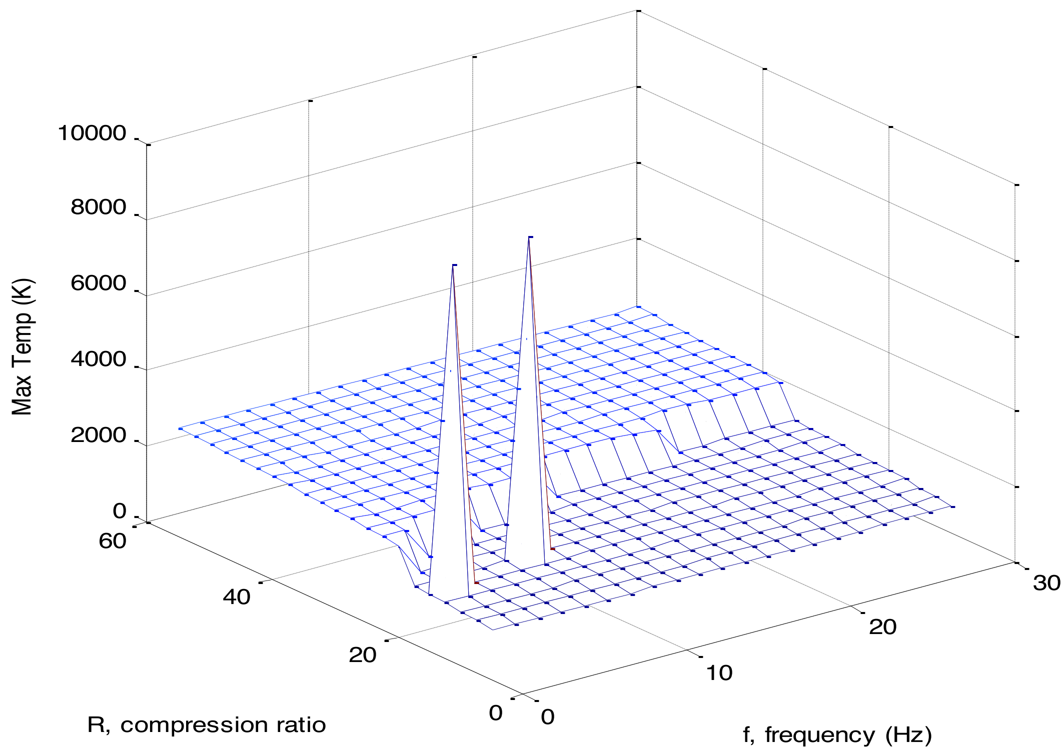
f=194.3 Hz

and a bottom line, which is Y_{CH4}*20000, for some reason this occurs.



Unusual Maximum Temperature Results at low frequencies

When I ran my code I saw something unusual during a low frequency 2-30Hz test with T0=300K, R=10-60 and a 21x21 matrix , I got two twin peaks at R=20 and f=3.4 Hz with T_{max}=9490 K and R=22.5 and f=9 Hz with T_{max}=9374 K that dwarf the surrounding temperatures. When I increased to a 31x31 matrix or decreased to 11x11 matrix, the effect disappeared.

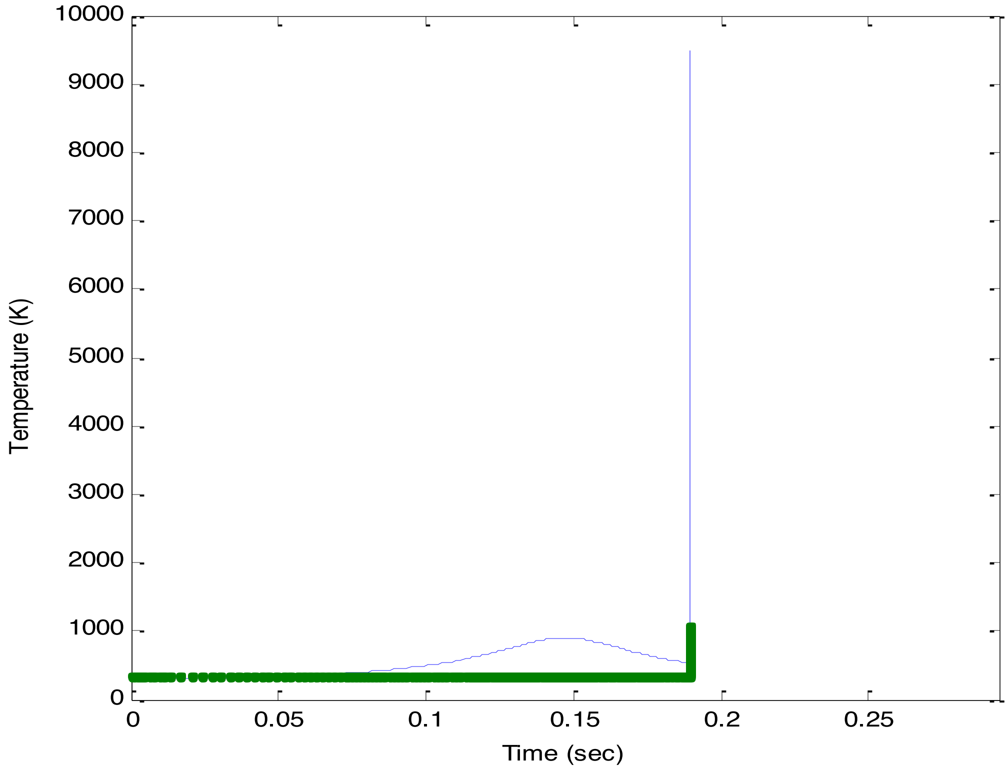


Running my original code from part 1 of the assignment, with:

R=20

f=3.4 Hz

and a bottom line, which is Y_{CH4}*20000, for some reason this occurs, same thing happens at the other point.



Alternate Ideas:

Had brainstormed about making a 2-D plot of the ignition area using a poly plot shape, but found it easier and quicker to just use the 3-D plot, although the 2-D plot might present the information a little more clearly. For my purposes this was not necessary because I can easily view the data in the .fig matlab files.

Example code:

```
pdepoly([-1 0 0 1 1 -1],[0 0 1 1 -1 -1]);
```

Files used and descriptions:

"CBPJ2to30hz.m" - displays max temp, ignition and Dt btw ignition time and max temp time, with f=2-30Hz , T0=300-500K ,and R=10-60

"CBPJ30to200hz.m"- displays max temp, ignition and Dt btw ignition time and max temp time, with f=30-200Hz , T0=300-500K ,and R=10-70

"CBPJ2to30hz_twinpeak_21matrix.m" - same as the CBPJ2to30hz file, except instead of using a 31x31 matrix I used a 21x21 matrix and 2 weird points occur where the temperature peaks towards the end of the cycle mysteriously and throws off the Tmax graph.

"CBPJfun.m" - I turned part 1 of the project into a function that I referenced in the other CBPJ files.

"MaxPlomercombproject.m" - Exact working version of code turned in for part 1 of assignment

"fig3_2to30Hz_21matrix.fig" – Max Temperature figure from T0=300K, f=2-30Hz R=10-60, with 21x21 row matrix, it shows a weird occurance at R=20 and f=3.4 Hz and R=22.5 and f=9 Hz.

"fig7_30to200Hz_31matrix.fig" – Dt between ignition and max temp figure from T0=500K, f=30-200Hz R=10-70, with 21x21 row matrix, it shows a weird occurrence at R=16 and f=194.3 Hz