Investigation of different chemical mechanisms accuracy using GRI-Mech 3.0 as reference mechanism

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1. Introduction

GRI-Mech 3.0 is the most common chemical mechanism designed and optimized to model natural gas combustion. Using Cantera software gas pameters during combustion of stechiometric mixture of air and hydrogen for different chemical mechanisms and different ignition temperatures will be shown. Combustion will take place in a 20 dm^3 sphere where initial pressure is 101325 Pa. Three different initial temperatures and 6 different chemical mechanisms will be used to show differences in results. Temperatures are following: 293 K, 393 K, 493 K. Chemical mechanisms are following: gri30 – as reference, gri30_highT, h2air_highT, h2-n2o_highT, Wang_highT, Konnov. Exept of Cantera I will also use csv, matplotlib and zndMZ_reactionLength.

2. Mathematical model

Solver is a homogeneous zero-dimensional reactor. By default, they are closed (no inlets or outlets), have fixed volume, and have adiabatic, chemically-inert walls. These properties may all be changed by adding appropriate components, e.g. Wall, MassFlowController and Valve. A reservoir is a reactor with a constant state. The temperature, pressure, and chemical composition in a reservoir never change from their initial values. Then a mass flow controller maintains a specified mass flow rate independent of upstream and downstream conditions. The equation used to compute the mass flow rate is.

$$\dot{m} = \max(\dot{m}_0, 0.0),$$

where $\dot{m}_0$ is either a constant value or a function of time. Note that if $\dot{m}_0 < 0$, the mass flow rate will be set to zero, since reversal of the flow direction is not allowed.

3. Results

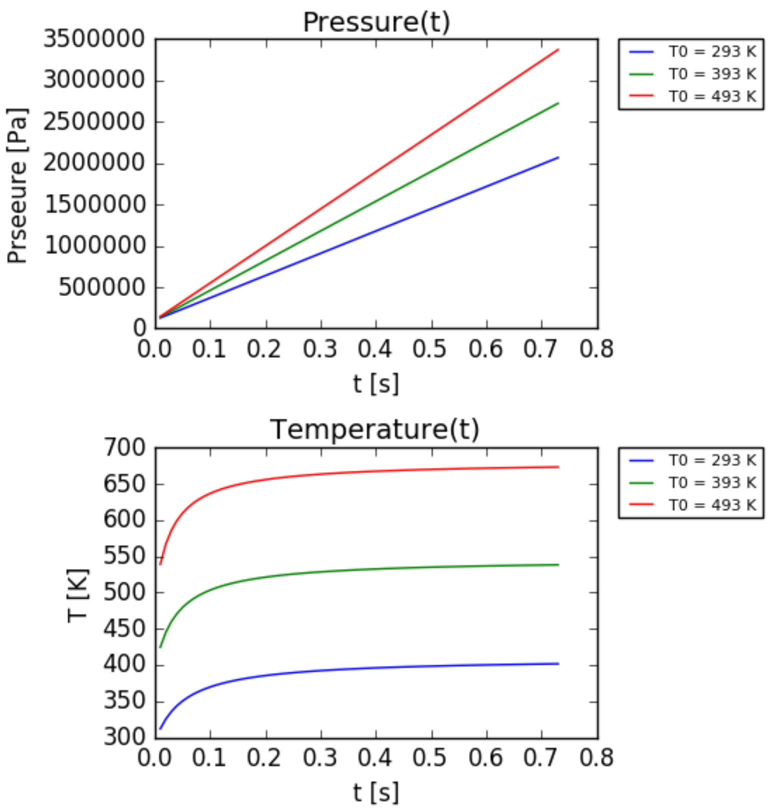

Figure 1: Pressure and temperature during combustion using gri 30 mechanism

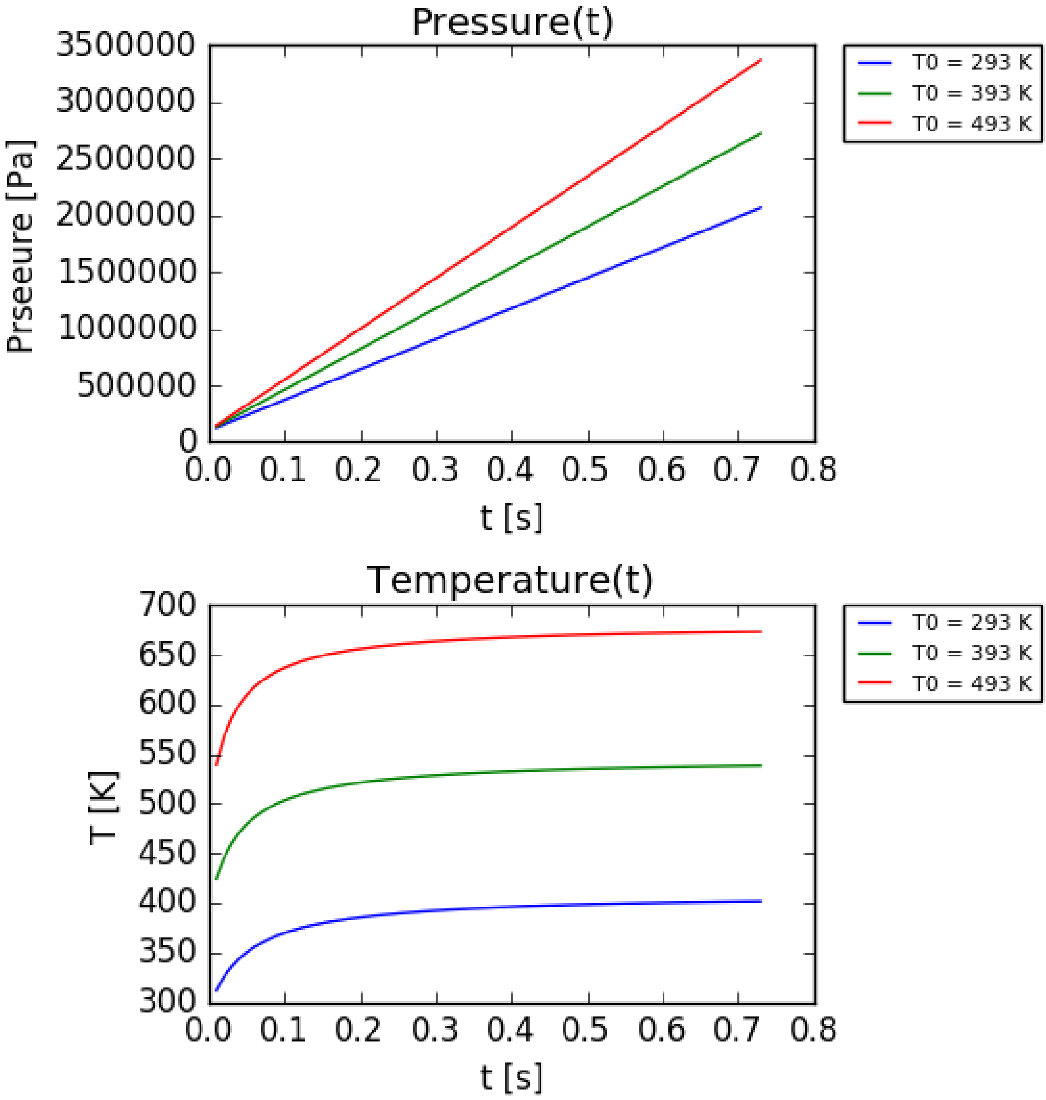

Figure 2: Pressure and temperature during combustion using gri 30_highT mechanism.

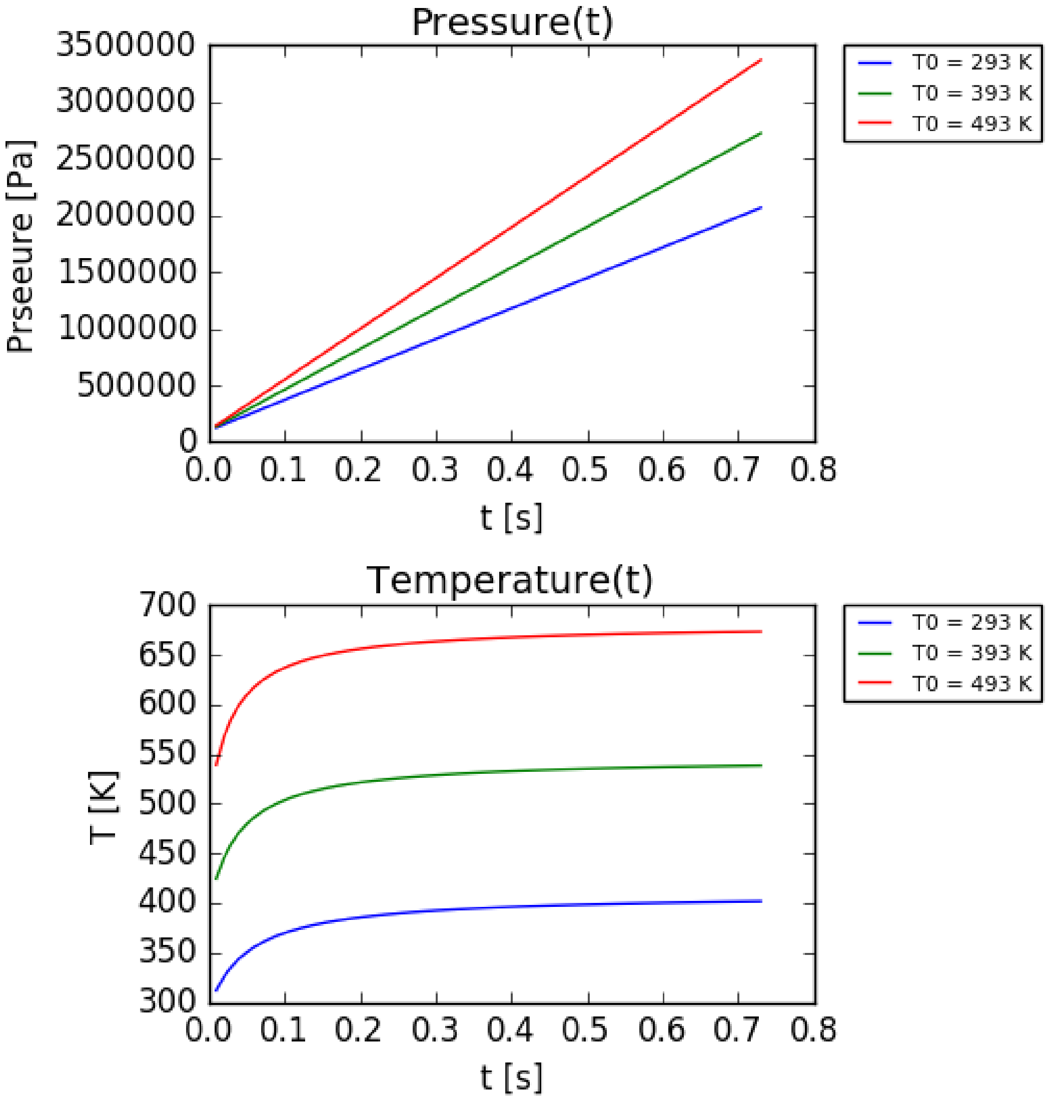

Figure 3: Pressure and temperature during combustion using h2air_highT mechanism.

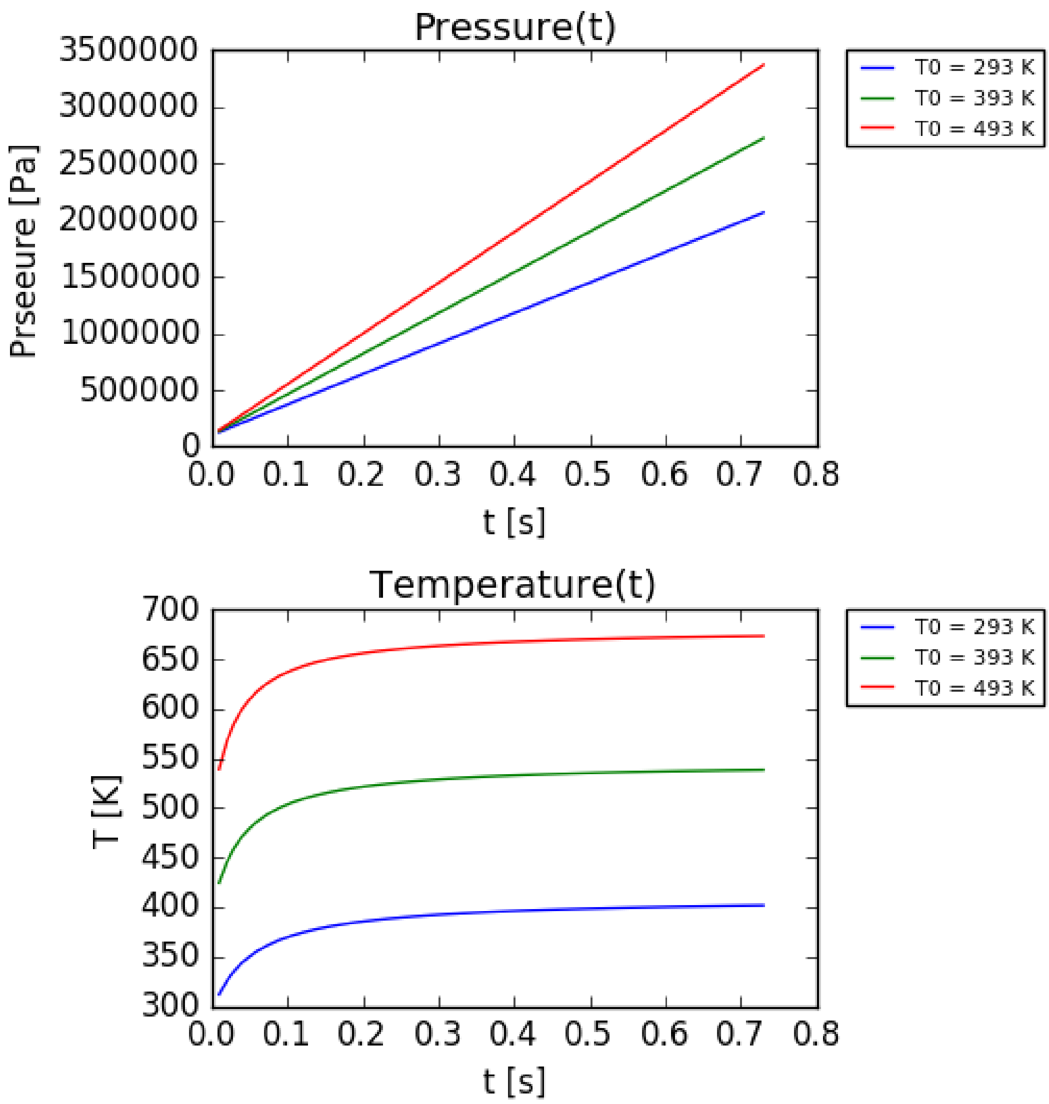

Figure 4: Pressure and temperature during combustion using h2-n2o_highT mechanism.

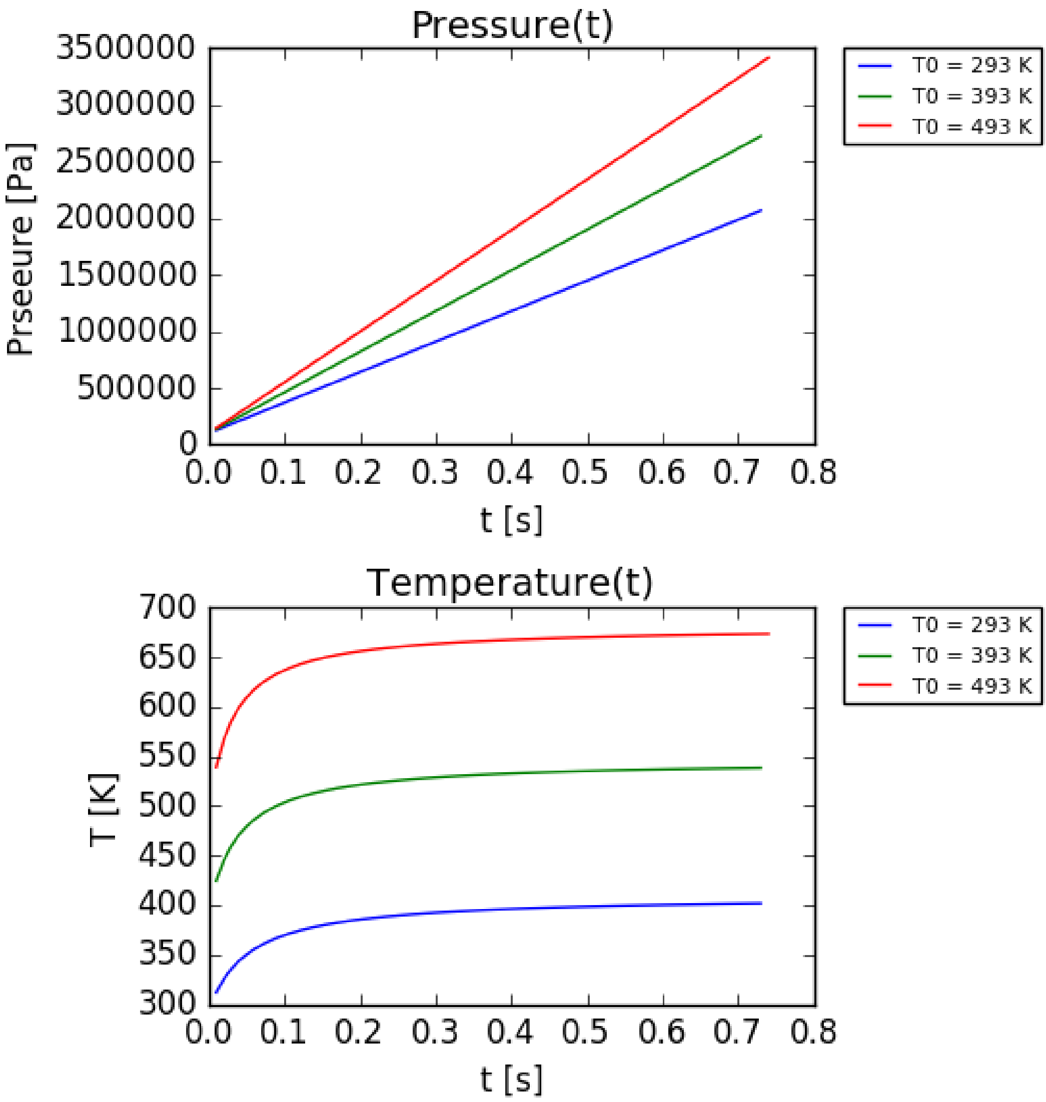

Figure 5: Pressure and temperature during combustion using Konnov mechanism.

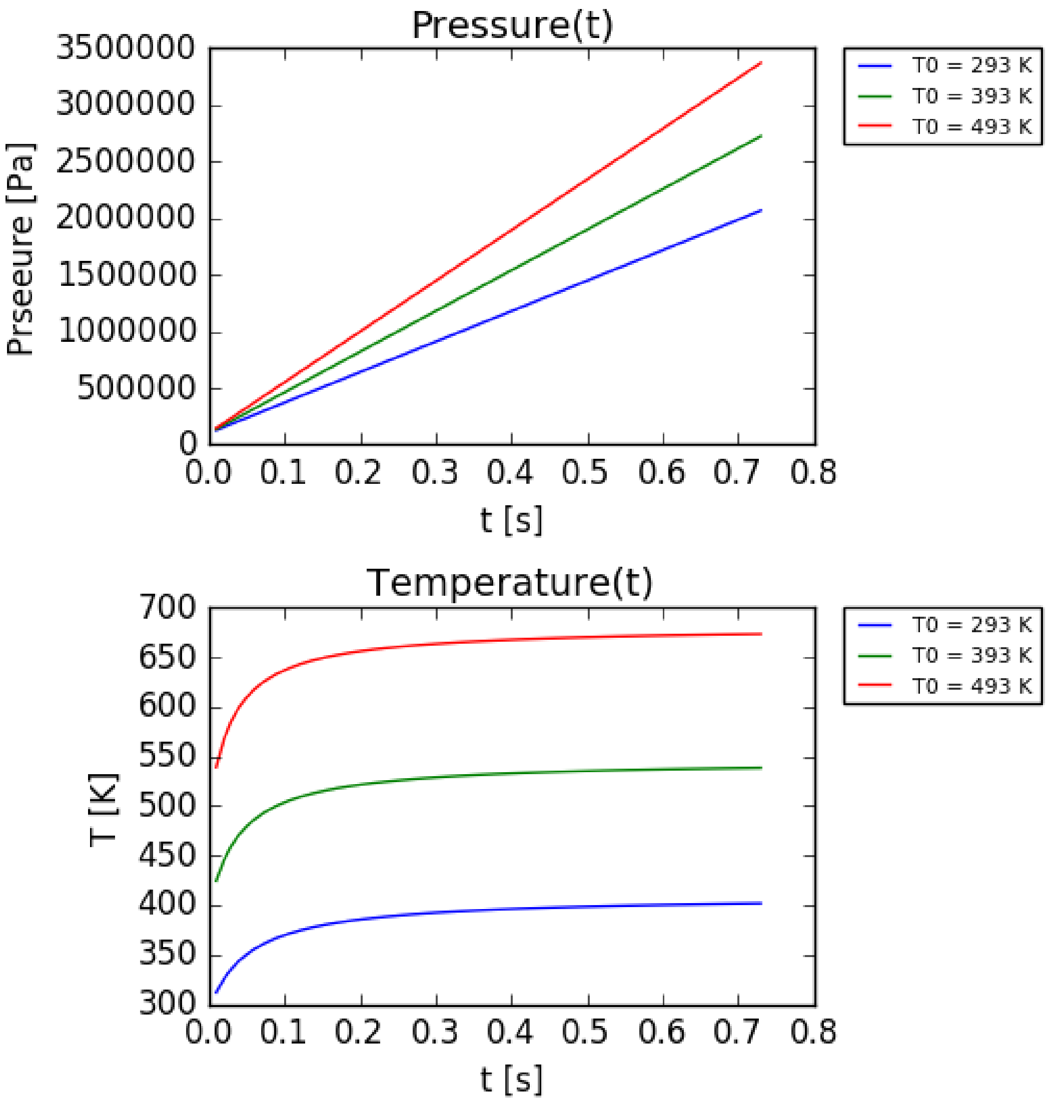

Figure 6: Pressure and temperature during combustion using Wang_highT mechanism.

As we can see those 6 previous graphs are almost identical and show the same results. Pressure in every case increases linearly but the higher initial temperature is the faster pressure increases. Final pressure vary from 2 MPa to 3,5MPa. Temperature increases non linearly but the same conclusion can be obtained as in pressure graphs – the higher initial pressure is the greater temperature gradient is. Final Temperatures vary from 400 K to 680 K.

Human eye can not see the difference in previous graphs so more calculations and graphs are needed. Using simple method

$$y = \frac{T_{gri\,30} - T_{mech}}{T_{gri\,30}} * 100\% \qquad (1)$$

$$z = \frac{P_{gri\,30} - P_{mech}}{P_{gri\,30}} * 100\% \qquad (2),$$

differences will be shown.

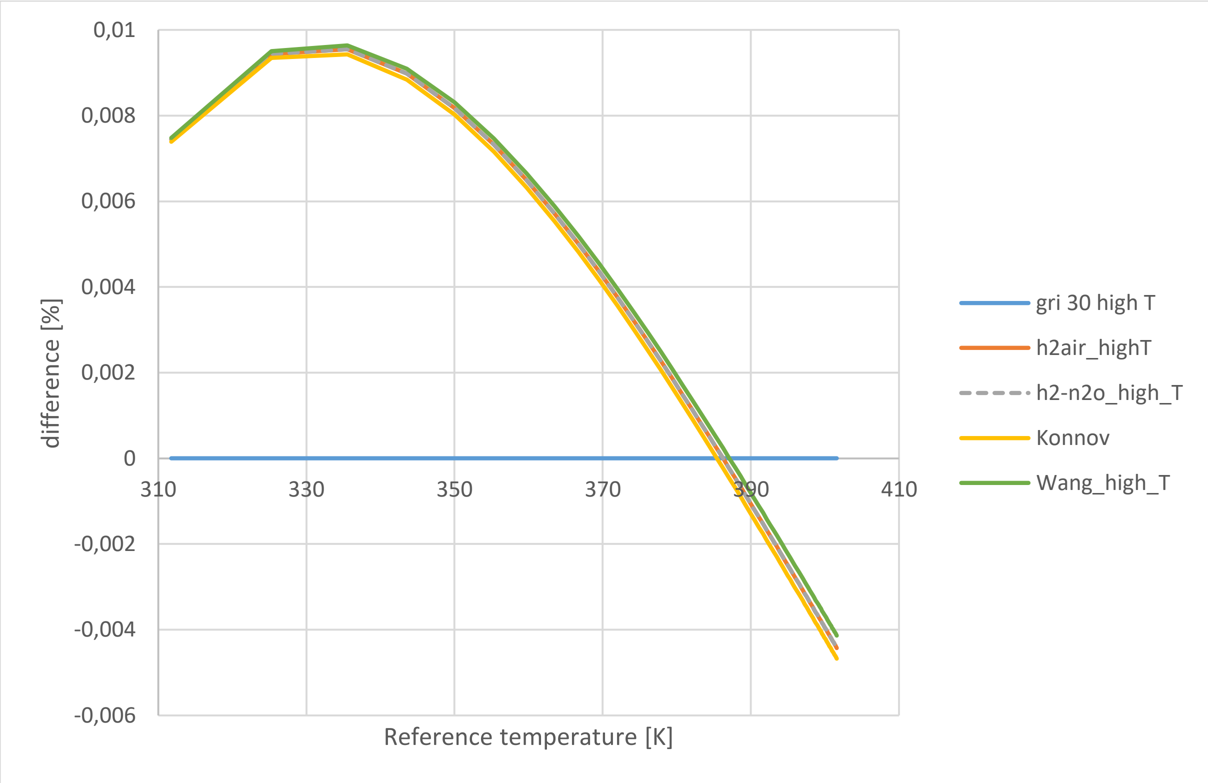

Figure 7: Temperature difference during combustion for initial temperature T0 = 293 [K] using gri 30 temperatures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -004% to 0,01%.

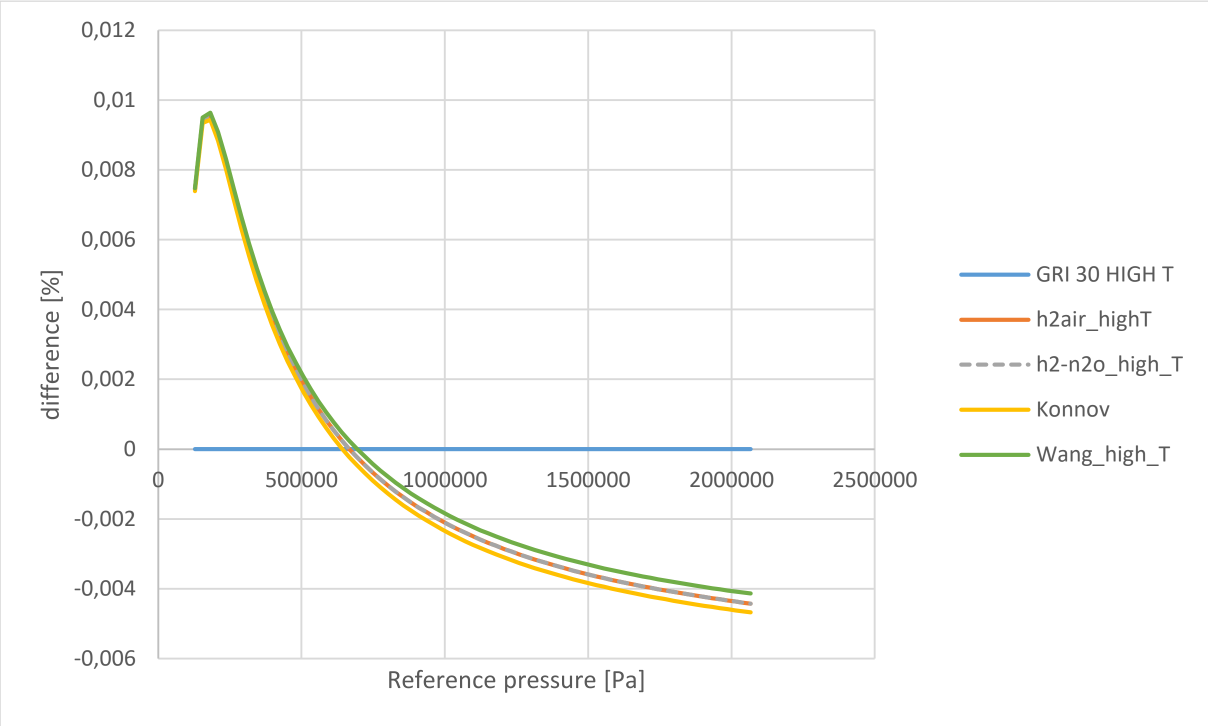

Figure 8: Pressure difference during combustion for initial temperature T0 = 293 [K] using gri 30 pressures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -004% to 0,01%.

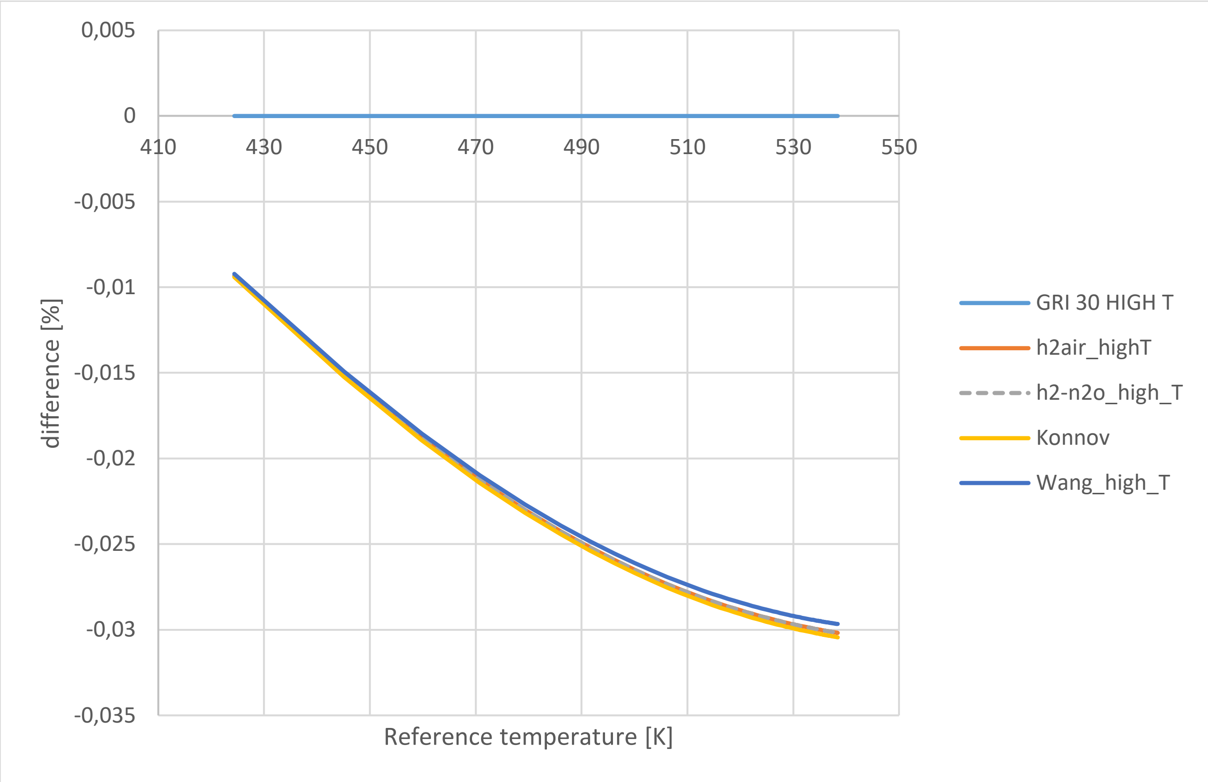

Figure 9: Temperature difference during combustion for initial temperature T0 = 393 [K] using gri 30 temperatures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -0,03% to -0,01%. Except form gri 30 highT all of the mechanisms shown decreased values comparing to the values form gri mech 30. Difference is approximately 3 times greater than in Figure 7.

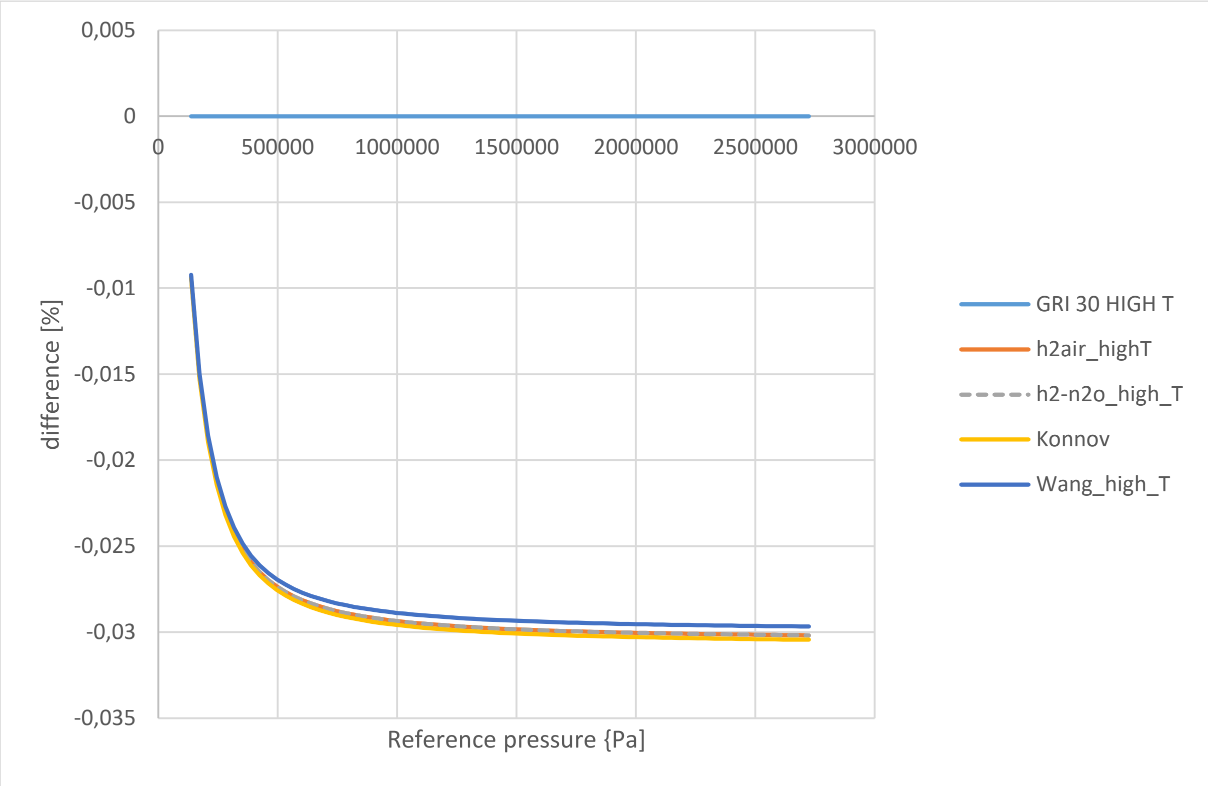

Figure 10: Pressure difference during combustion for initial temperature T0 = 393 [K] using gri 30 pressures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -0,03% to -0,01%. Except form gri 30 highT all of the mechanisms shown decreased values comparing to the values form gri mech 30. From initial pressure to 5 bar difference gradient is much greater than from 5 bar to the end.

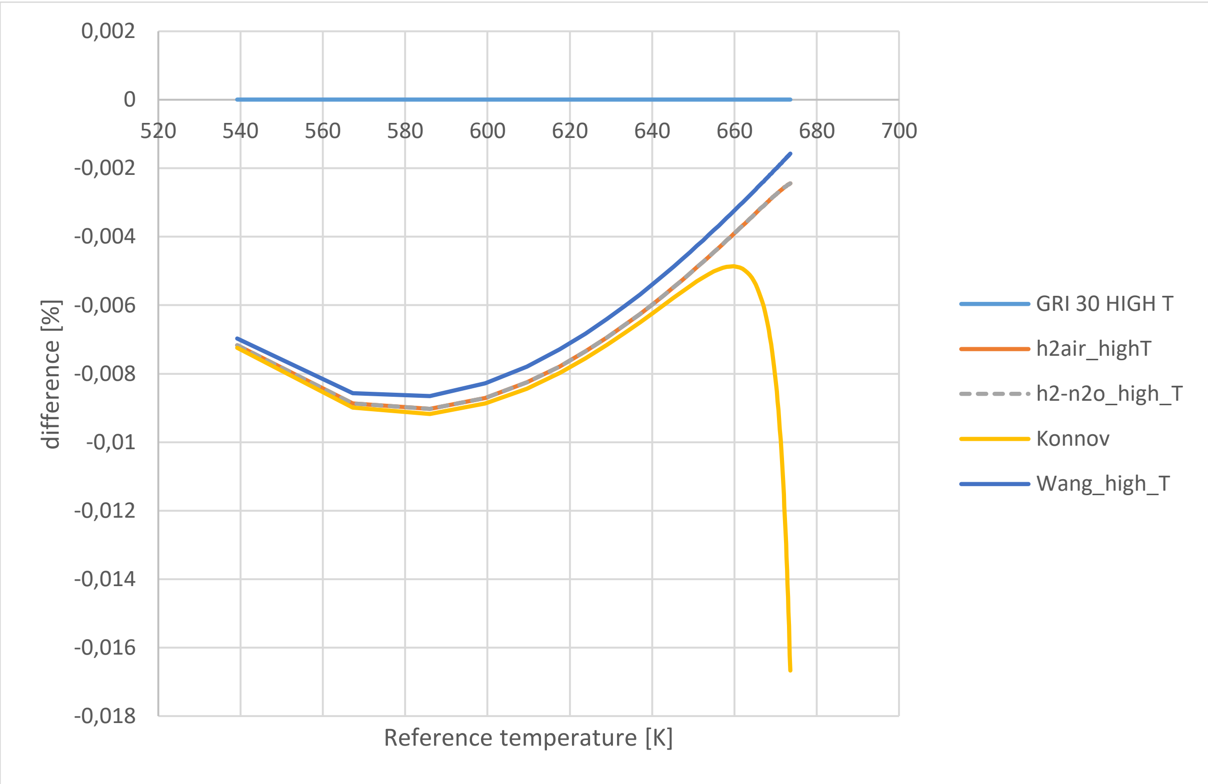

Figure 11: Temperature difference during combustion for initial temperature T0 = 493 [K] using gri 30 temperatures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -0,009% to -0,002%. Except form gri 30 highT all of the mechanisms shown decreased values comparing to the values form gri mech. We can also see anomaly in Konnov mechanism behavior, after 650 K difference stars to increase rapidly up to -0,017%. Difference is approximately 3 times smaller than in Figure 7.

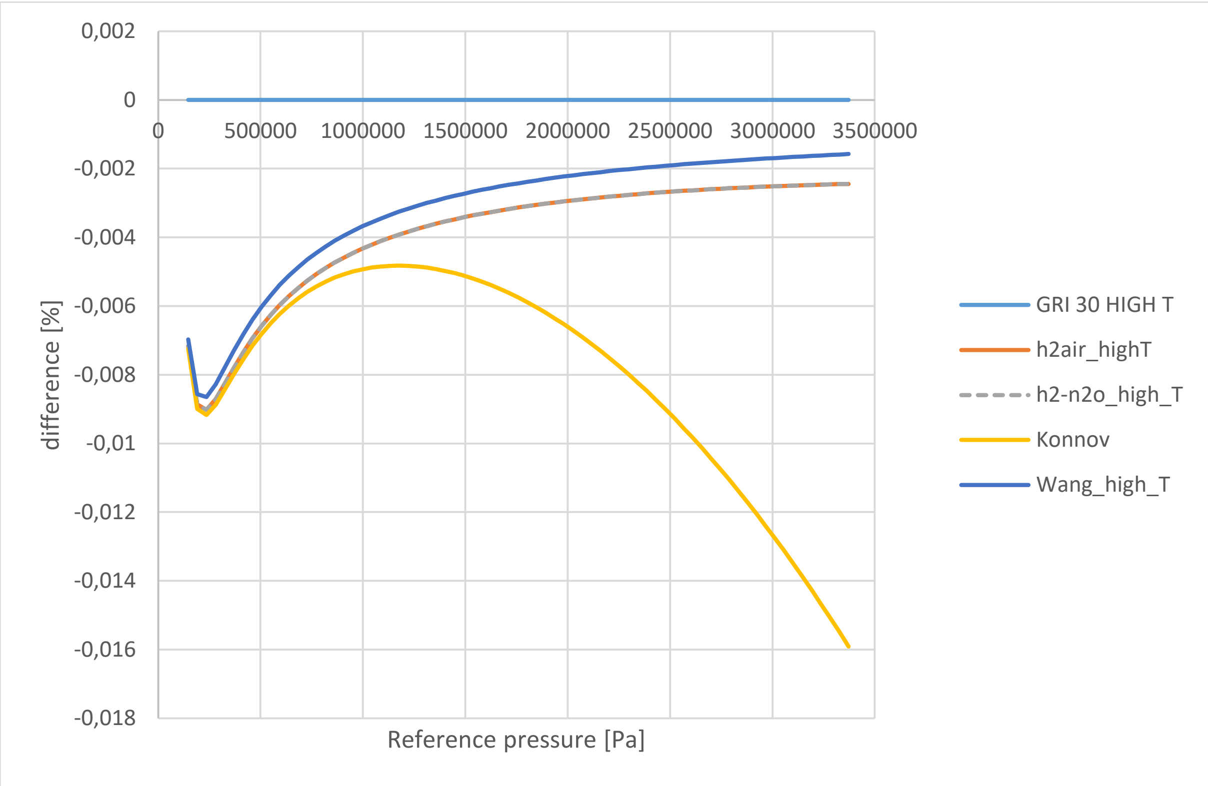

Figure 12: Pressure difference during combustion for initial temperature T0 = 493 [K] using gri 30 pressures as reference.

We can see that results from gri 30 highT are identical as in gri 30 mechanism. The rest of mechanisms behaves very similar to each other and the difference to gri 30 mechanism vary form -0,009% to -0,002%. Except form gri 30 highT all of the mechanisms shown decreased values comparing to the values form gri mech. We can also see anomaly in Konnov mechanism behavior, after 12 bar difference stars to increase up to -0,016%.

4. Conclusions

- All of the used chemical mechanisms showed difference lover than 0,03% which is very accurate to GRI 30.
- GRI 3.0 HIGH T behaves identically to GRI-Mech 3.0
- h2air_highT behaves identically to h2-n2o_high_T
- Konnov mechanism is the only one which showed anomalies
- The higher initial temperature is the greater temperature gradient is
- The higher initial temperature is the greater pressure gradient is