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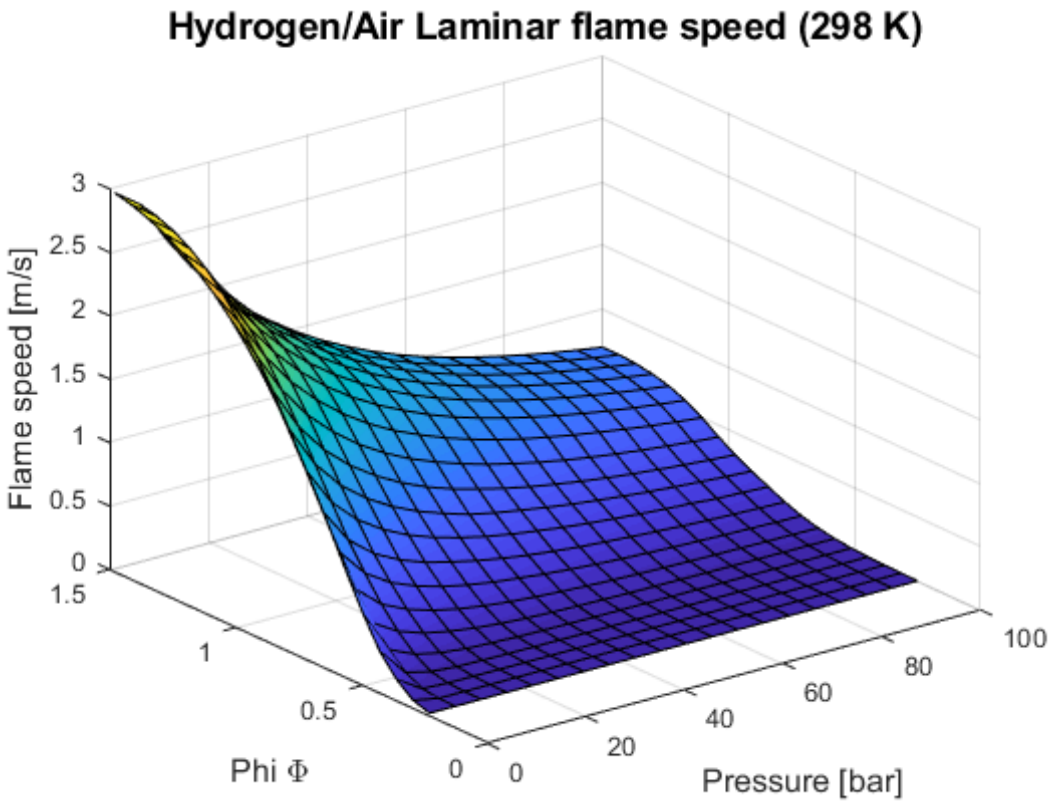

Laminar flame speed modeling for a 1-D hydrogen combustion model

Master's thesis in Automotive Engineering

HUGO GEFORS

Department of Mechanics and Maritime Sciences
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2020

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Cover: Surface plot for laminar flame speed of hydrogen/air depending on equivalence ratio and ambient pressure.

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Abstract

CO2 emissions from internal combustion engines is a world wide problem by being one of the sources contributing to global warming. While the internal combustion engine has proven to be a reliable and versatile mobile power source, ranging widely in size and power output, the most commonly used fuels are of fossil origin introducing new CO2 to the atmosphere. Upcoming legislation's will force new alternative fuels with reduced or zero CO2 emissions to the market. One of these alternative fuels is hydrogen which have the potential to be used in internal combustion engines. Volvo Penta have a lot of prior knowledge with diesel combustion but are taking a step into spark ignited engines with compressed natural gas (CNG) and hydrogen combustion to lower CO2 emissions.

By the use of 1-D simulation the potential of hydrogen as a fuel in an internal combustion engine (ICE) can be evaluated. While 1-D simulation software like GT-Power is commonly used when designing an ICE together with the traditional fossil fuels, gasoline and diesel, the potential to make simulations using hydrogen as the fuel is fairly unknown.

For a predictive combustion model many of the combustion characteristics for the fuel is described by the laminar flame speed model. How fast the combustion occurs and therefore the energy release rate is partially determined by the laminar flame speed. Hydrogen has very high laminar flame speed at stoichiometric conditions compared to gasoline and diesel. In combination with high laminar flame speed the fuel can ignite at a wide range of equivalence ratios. Due to limits in material strength and a need for highly controlled combustion it is interesting to run hydrogen at lean conditions and by doing so limiting the laminar flame speed.

By comparing the current laminar flame speed model used in GT-power to experimental data it was evident that the default laminar flame speed model did not give correct results near the lean limit for hydrogen. A chemical kinetics result based model was therefore created by using function fitting methods available in Matlab and then implemented into the predictive combustion model SITurb in GT-Power. The results when comparing the new kinetics-fit laminar flame speed model with the default GT laminar flame speed model showed similar results for lean combustion conditions until the very lean conditions occurred. For very lean conditions the kinetics-fit model showed more correlation to experimental results than the default GT-model did. While that was promising, the kinetics-fit model did not correlate well to the chemical kinetics results other than the points for which it was initially fitted for. In general the kinetics-fit model underestimated the laminar flame speed resulting in simulations showing inaccurate results.

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I would like to give a huge thanks to my supervisor Prajwal Shankaregowda at the Volvo Penta CAE department for both moral as well as technical support even at the more inconvenient times of the day. A big thanks to my other supervisor Alexander Ölén for providing an insight on the current development from Volvo Group and an expert opinion regarding hydrogen combustion. Also a big thanks to he whole CAE department at Volvo Penta, I really enjoyed our talks during coffee breaks and thank you for treating me just like another colleague.

Hugo Gefors, Gothenburg, June 2020

Abbreviations

EU	European Union
CNG	Compressed Natural Gas
ICE	Internal Combustion Engine
GT-Power	Engine performance 1-D simulation software
GT	Gamma Technologies
EGR	Exhaust Gas Recirculation
RON	Research Octane Number
MON	Motor Octane Number
MN	Methane Number
HHV	Higher Heating Value
AFR	Air-Fuel Ratio
BTDC	Before Top Dead Center
IVO	Intake Valve Opening
IVC	Intake Valve Closing
SI	Spark Ignited
PFI	Port Fuel Injection
DI	Direct Injection
AKI	Anti Knock Index
IMEP	Indicated Mean Effective Pressure
AHRR	Apparent Heat Release Rate

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1
Introduction

1.1 Background

Global warming has a big impact on mobile power source development and with increased concern sustainable solutions is of great interest. Alternative solutions to the fossil fuels gasoline and diesel with low or zero carbon content is popular due to their inevitable CO2 impact. Since the development of reciprocating internal combustion engines has a history of more than 100 years, the hardware as well as control software solutions have come far in development and are well proven. Fuels which combust with similar thermodynamics as diesel and gasoline and can be used with the same hardware are the most interesting due to their capability of being a direct replacement. Hydrogen is one of the combustible alternative fuels with zero carbon content.

1.1.1 Legislation

The emission legislation in the EU is pushing the manufacturers towards zero engine out emissions, in 2025 the average CO2 emissions from new heavy duty vehicles needs to be 15% lower than in 2019. Five years later in 2030 the next reduction step is introduced which is a 30% reduction in comparison to 2019[1]. While the vehicles running on fossil fuels are getting closer and closer to their efficiency limit alternatives are needed to reduce the fleet average for the vehicle manufacturers.

1.2 Purpose

The purpose of this thesis is to document and improve contingent shortcomings of the current hydrogen combustion model used in GT-Power. The laminar flame speed model, being the base of the predictive combustion model in GT-Power, is to be investigated as well as the knock model alternatives.

1.3 Limitations

The study will cover 30 ECTS-credits accounting for 20 weeks of work which is therefore the time frame limit. All the work is based around creating a hydrogen combustion model in GT-Power, no other engine simulation software is to be used.

No physical tests will be made and therefore the evaluation of the results will be based on other simulations or information gathered from prior investigations only.

Evaluation and consideration of emissions in terms of NOx and particulates will not be included in this study.

Effects of exhaust gas recirculation, EGR, will not be taken in to account during any part of the thesis.

2
Theory

2.1 Hydrogen as a SI ICE fuel

Hydrogen is a interesting substitute to the fossil fuels, gasoline and diesel, mainly due to the fact that it contains zero carbon content meaning that there will be no carbon footprint from the combustion. During combustion with hydrogen and air the main by-product is water.

2.1.1 Backfire, pre-ignition and knock during pure hydrogen/air combustion

Tests made using experimental test setups of hydrogen ICE describe problems of spontaneous ignition both during the intake stroke referred to as backfire as well as pre-ignition or superknock during the compression stroke. Normally this would be reflected in the octane rating of the fuel but the resistance to pre-ignition or knock heavily depends on the operating parameters when it comes to hydrogen. According to the Research Octane Number (RON) that for hydrogen is 130 or higher depending on equivalence ratio it seems as if it would have considerably higher resistance to knock than gasoline. Normally fuels are tested for determining their Motor octane Number (MON) as an additional indication of their resistance to knock. The test for MON ratings are made during harsher operating conditions usually making the value around ten points lower than the RON number for the same fuel. Unfortunately hydrogen does not have a MON rating but according to other studies it should be much lower than the RON rating[2]. The test conditions for determining the RON as well as the MON rating is stated in table 2.1. Due to the lack of a suitable number for an indication of the knock tendencies of hydrogen, some alternatives are suggested from prior studies. Methane number (MN) is the preferred reference to how well the resistance of knock hydrogen has and with a methane number scale of 0 to 100 hydrogen has methane number 0. Having a knock resistance number of 0 MN it is evident that hydrogen can be considered to have the worst knock resistance possible of the fuels presented in the MN scale[3].

Engine Parameter	**Reasearch Method (RON)**	**Motor Method (MON)**
Engine speed	600 RPM	900 RPM
Intake temperature	52°C	149°C
Spark Advance	13° BTDC	19 to 26° BTDC

Table 2.1: Engine parameters used while determining RON and MON rating[2].

The main characteristics making hydrogen so prone to pre-ignition is the high dilution coefficient together with low ignition energy. Both these values are significantly different to gasoline. Gasoline has a flammability region of 6,6% while hydrogen has 71% as seen in figure 2.1 and the ignition energy required is more than ten times higher for gasoline at normal ambient temperature and pressure, 0,25 mJ compared to 0,02 mJ[4][5]. The ignition energy needed is also almost constant over the dilution range making pre-ignition occurring even when only local parts of the of a highly diluted mixture face hot-spots[6].

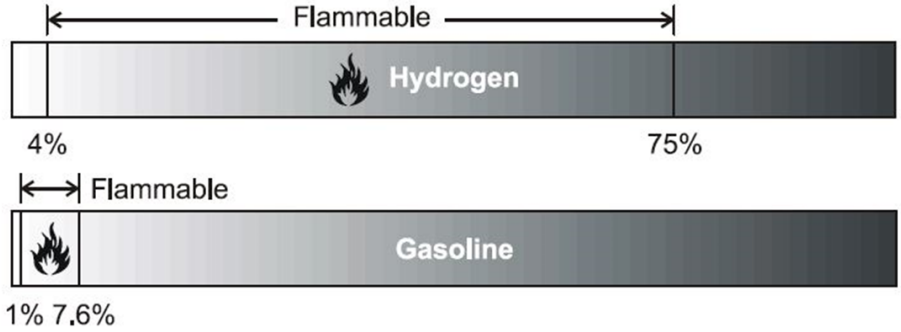

Figure 2.1: The flammability range for hydrogen and gasoline when mixed with air at 20 °C[4].

Prior studies mainly mention hot-spots to be the cause of pre-ignition but late ignition of trapped fuel mix in crevices during the intake stroke and therefore addition of new fuel mix has also been an explanation. After the exhaust stroke the potentially newly ignited crevice mix ignites the newly introduced mixture as soon as it enters the cylinder and due to hydrogen's low ignition energy, quenching distance and high flame speed stated in table 2.2 the flame propagates past the intake valve and into the intake manifold. By adjusting the inlet valve timing to give the crevice volume more time to ignite and burn off before introducing new mixture into the cylinder it is possible to prevent backfire[7]. It would work as a reversed miller cycle, and have late IVO instead of early IVC.

	Gasoline	**Hydrogen**
Stoichiometric AFR	15:1	34:1
Energy content LHV (Liquid)	44.5 MJ/kg or 31.150 MJ/m^3	119.93 MJ/kg or 8.491 MJ/m^3
Quenching Distance	2 mm	0.64 mm
Flame speed	0.42 m/s	3.46 m/s
Autoignition temperature	230–480°C	585°C

Table 2.2: Fuel characteristics for gasoline and hydrogen at stoichiometric conditions[4].

2.2 1D combustion model

In GT-Power the in-cylinder combustion model is chosen depending on the basic type of combustion, compression ignition or spark ignition, as well as if it is a predictive, semi-predictive or non-predictive model.

2.2.1 Chemical kinetics

Chemical kinetics is the science describing chemical reactions. By the use of chemical kinetics the rate of the chemical process and continuous transformation of reactants to products for a certain mechanism is defined. The change of species concentration in time is the rate of the chemical reaction[8].

By the help of chemical kinetics the chemical reaction process for a specific mechanism can be studied and used to evaluate the process depending on different conditions.

2.2.2 Cantera

Cantera is a toolbox that can be used together with Python and Matlab or through applications written in C/C++ or FORTRAN90. It is a tool that help automate chemical kinetic, thermodynamic and transport calculations[9].

2.2.3 Non predictive model

A non-predictive model uses a standard combustion rate which is not influenced by the in-cylinder conditions. If the objective is to evaluate engine parameters which are not directly influencing the burn rate of the combustion process, this is a viable alternative[10].

2.2.4 Semi predicitve model

A semi-predictive model have some variables that influences the burn rate, but instead of using a physical model the response is imposed by the use of lookups for calculating the suitible Wiebe parameters. The main advantage of using a semi-predictive model instead of a predictive model is that it can run much faster and be accurate for some cases[10].

2.2.5 Predictive model

A predictive model predicts the burn rate depending on a series of separate models. In terms of the Spark-Ignition Turbulent Flame Model, SITurb, the burn rate prediction is of a spark ignited homogeneous charge.

The burn rate is predicted using equation 2.1, 2.2 and 2.3. This prediction takes cylinder geometry, spark location and timing, air motion as well as fuel properties

into account[10]. The model determining the turbulent flame speed (S_γ) is proprietary and therefore not shared by GT.

$$\frac{dM_e}{dt} = \rho_u A_e (S_\gamma + S_L) \tag{2.1}$$

$$\frac{dM_b}{dt} = \frac{M_e - M_b}{\tau} \tag{2.2}$$

$$\tau = \frac{\lambda}{S_L} \tag{2.3}$$

M_e	Entrained mass
t	Time
ρ_u	Unburned density
A_e	Entrained surface area at the edge of the flame front
S_γ	Turbulent flame speed
S_L	Laminar flame speed
M_b	Burned mass
τ	Time constant
λ	Taylor microscale length

Table 2.3: SITurb predictive model variables[10].

2.3 Knock modelling

Models used for predicting the occurrence of knock is often based around the time of ignition delay which is also referred to as induction time.

K_c is the prediction of knock onset in the end gas when using the Livengood-Wu integral which is shown in equation 2.4. As seen in equation 2.4 when K_c reaches a value of 1 knock is apparent. This parameter does not signify the severity of the knock, only if it is present or not. For a PFI engine where the intake gas is containing fuel already during the intake stroke t is the time from start of compression, IVC, to the start of spontaneous ignition and τ is the ignition delay. In a DI engine t is instead calculated from the start of fuel injection[11].

$$K_c = \int_0^t \frac{1}{\tau} dt = 1 \tag{2.4}$$

2.3.1 Arrhenius function based knock prediction

While the Livengood-Wu integral is used to determine the knock onset the outcome is based on the ignition delay parameter. For knock models based on the Arrhenius equation τ is depending on the in-cylinder conditions pressure, p, and temperature of the unburned zone, t_u. A, n and B are constants which differ depending on the type

of fuel. The model must be calibrated using experimental data for all non-standard fuels where prior studies have not been performed[11].

$$\tau = Ap^{-n}exp(\frac{B}{T_u}) \tag{2.5}$$

To get a suitable ignition delay that rely on these as well as other influencing parameters a function describing the relationship is often used based on the Arrhenius function. It is known to capture what is called a negative temperature coefficient (NTC) behavior. Normally the ignition delay decreases with an increase in temperature but when burning hydrocarbon based fuels there is usually a region when the increase in temperature increase the ignition delay as seen in figure 2.2, this is what is referred to as NTC behavior[12].

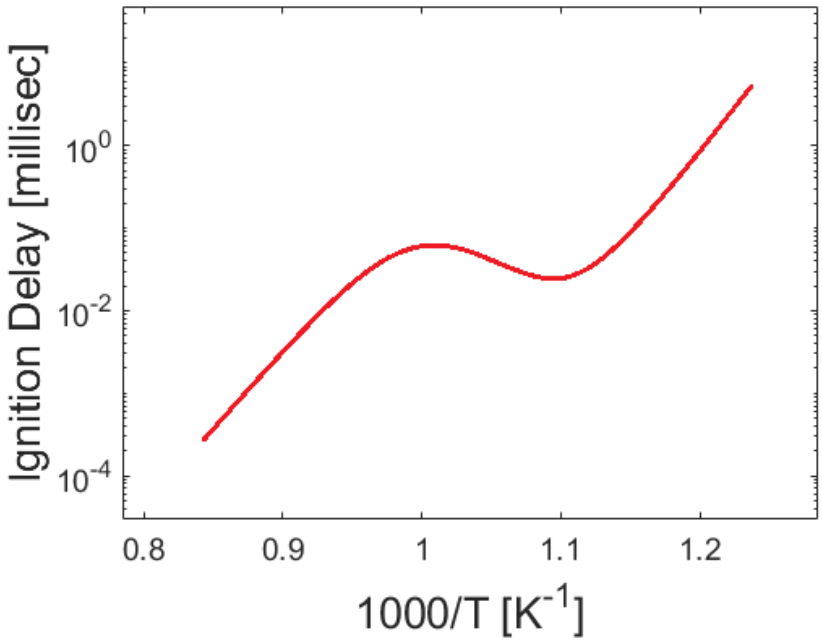

Figure 2.2: Example of Negative Temperature Coefficient (NTC) behavior.

2.3.2 Chemical kinetics based knock prediction

When using chemical kinetics for knock prediction the numerous concurrent chain reactions happening in an air-fuel mixture during certain ambient conditions are calculated. Because of the continuous chain reactions energy is distributed to the surroundings in the form of heat, but when the energy produced overcomes the amount that is distributed the mixture heats itself up and eventually auto-ignites[11].

3

Methods

The methods used to investigate the current model and how to create alternative model solutions for a hydrogen GT-Power combustion and knock model is presented in this chapter.

3.1 Combustion model

Since the model should not require any experimental data input to be used for evaluation of how suitable an ICE would be for hydrogen/air combustion as well as be a tool for sensitivity analysis it needed to be a predictive model. The SITurb model was chosen as a base since the investigations should treat a spark ignited base engine.

Due to lack of test data attempts to use test data as the base for the model evaluation and validation was discontinued. The default parameters for a predictive SITurb model was instead used and compared to tendencies shown in papers regarding hydrogen ICE.

In prior studies with experimental engine setups running a conventional ICE using hydrogen, the possibility of running at ϕ as low as 0.25 is mentioned. Theoretical studies based on the flammability capabilities of hydrogen also support the possibility of running very low equivalence ratios[13][14]. Therefore a case of running the default model between ϕ values 0.25-0.5 was made to evaluate the possibility to do so in GT-Power. The result showed that at ϕ-values lower than ≈ 0.35 no combustion was occurring. When contacting Gamma Technologies for an answer to why it is not possible to reach lower levels of equivalence ratio, the answer was that it is due to the default laminar flame speed model for hydrogen. As seen in figure 3.1 the model used by default shows that during ambient temperatures of 298 °K and atmospheric pressure there is no laminar flame speed after an equivalence ratio of $\phi \approx 0.36$.

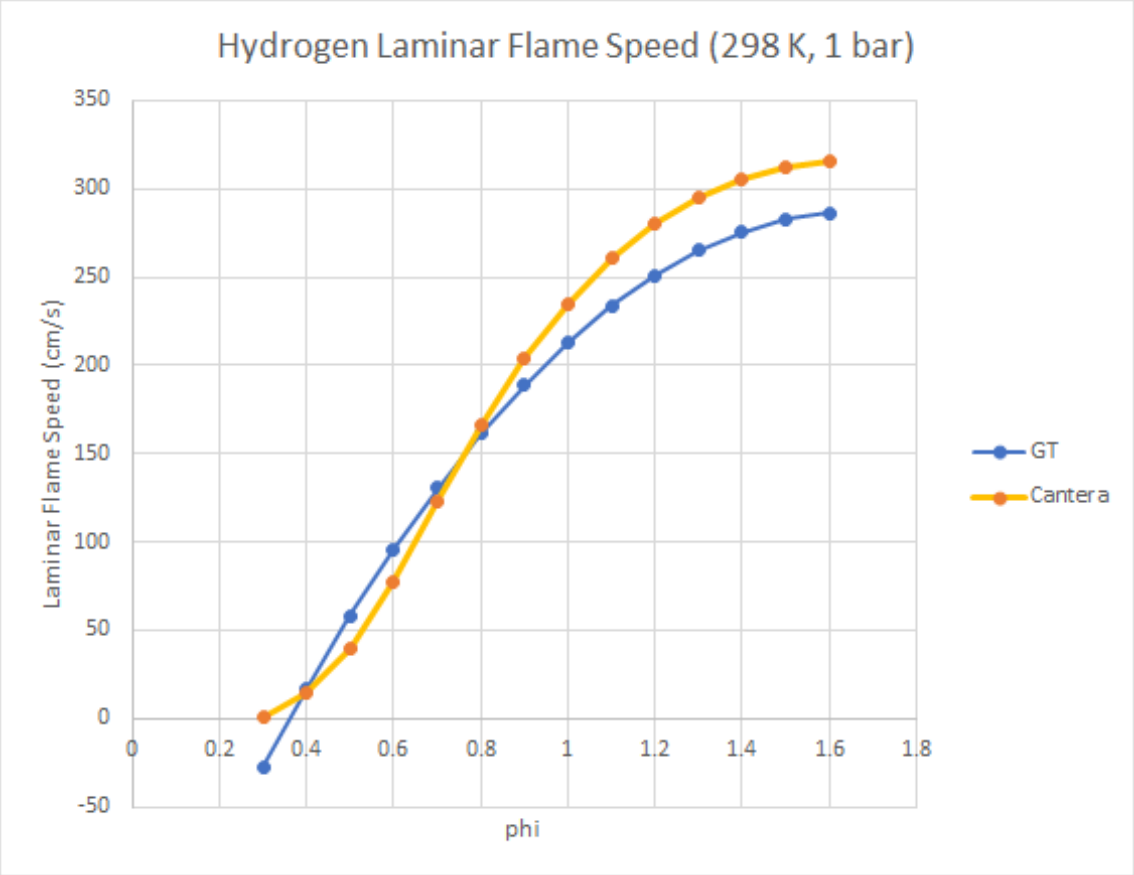

Figure 3.1: Comparison between Cantera kinetics model flame speed and GT default H2 flame speed model

3.1.1 Laminar flame speed model

The current laminar flame speed model used by Gamma Technologies is found in internal combustion engine fundamentals by John B. Heywood [15]. It is equation 3.1 and it is evaluated for gasoline and methane as well as some other fuels with similar characteristics. The dilution term, shown in equation 3.2, is added by GT in model version v75 and is not a part of the original equation. The current default hydrogen laminar flame speed model for SITurb combustion model is created using the same base model with coefficients that is proprietary and thus not available. By not using a dedicated and completely reconstructed model for the laminar flame speed for hydrogen simulation of very lean combustion is not possible.

$$S_L = (B_m + B_\phi(\phi - \phi_m)^2)(\frac{T_u}{T_{ref}})^\alpha(\frac{p}{p_{ref}})^\beta f(Dilution) \tag{3.1}$$

$$f(Dilution) = 1 - 0.75 * DEM(1 - (1 - 0.75 * DEM * Dilution)^7) \tag{3.2}$$

S_L	Laminar flame speed [m/s]
B_m	Maximum laminar speed [m/s]
B_ϕ	Laminar speed roll-off value
ϕ	in-cylinder equivalence ratio
ϕ_m	Equivalence ratio at maximum speed
T_u	Temperature of the unburned gas [K]
T_{ref}	298 °K
p	Pressure [Pa]
p_{ref}	101325 Pa
α	Temperature exponent
β	Pressure exponent
f(Dilution)	Dilution effect
DEM	Dilution effect multiplier
Dilution	Mass fraction of the residuals in the unburned zone

Table 3.1: Explanation of coefficients used in the default GT laminar flame speed model[10].

As earlier presented, in figure 3.1, GT uses the chemical kinetics simulation software Cantera as a tool for making comparisons with their own model. Since Cantera is used by GT to validate their own models it might be a good way to create results to base an alternative model on. Therefore a model of a flat free flame was created in Python using Cantera as the solver. The origin of the mechanism was a detailed chemical reaction model from Stanford University provided by Converge science which was used for the laminar flame speed model. The program was setup so that it calculates the laminar velocity of the H2/air free flame while iterating over different initial conditions.

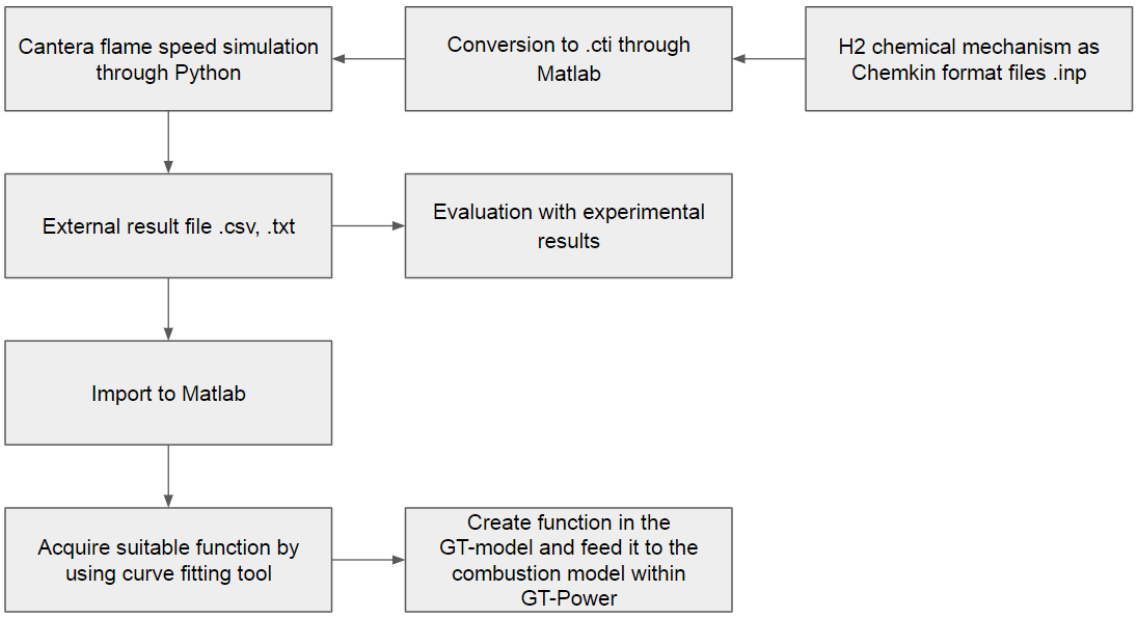

Figure 3.2: The workflow for creating a new laminar flame speed model based on a kinetics fit.

The result achieved by the free flame model seen in figure 3.3 which was created with the same initial conditions as GT used in figure 3.1 had a very similar overall shape to the GT Cantera model result. The response was calculated for $0.25 \leq \phi \leq 1.5$. Unfortunately the actual numerical results from figure 3.1 was not made available by GT, so therefore it was not possible to overlay the results in a combined graph. But only by looking at the graphs separately there is a distinctive difference between the two Cantera results. At $\phi > 1$ the GT Cantera model has higher predictions while it predicts lower values for $\phi < 1$. The difference might be due to the use of a different chemical reaction model.

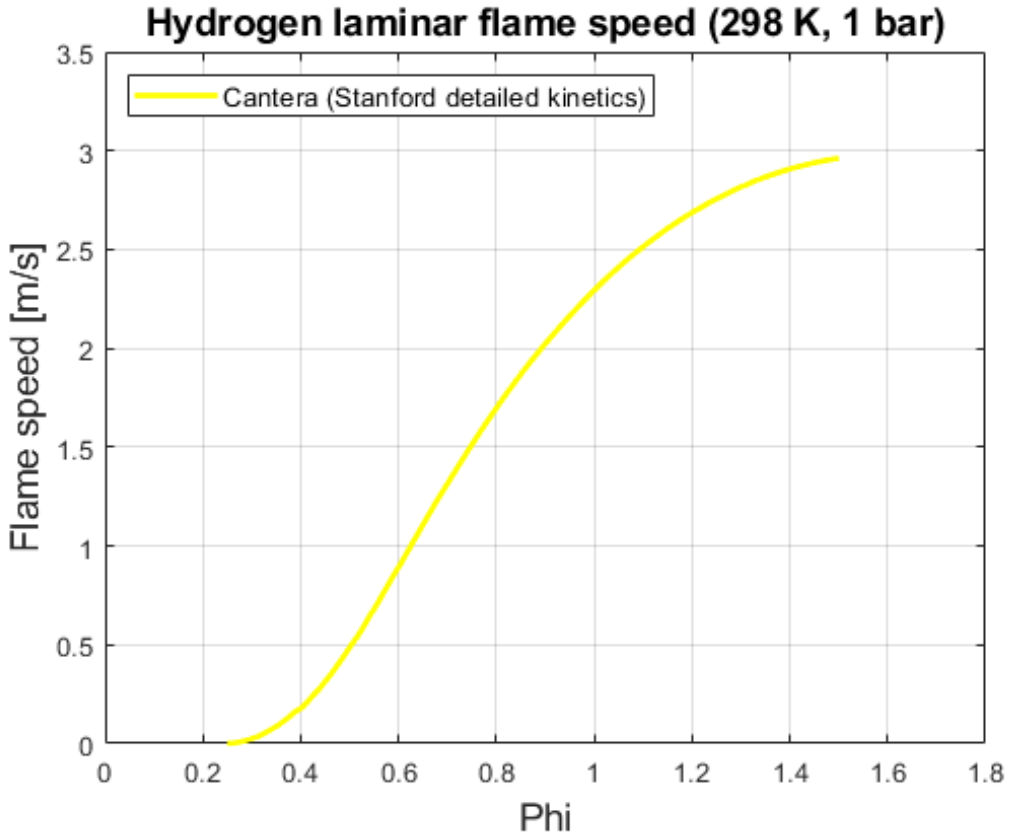

Figure 3.3: Cantera response using a detailed chemical kinetics model

While the similarity to GT's own Cantera model ensures that the free flame model is in the correct region of being accurate for flame speed calculations a comparison to real measured data were of particular interest. When measuring the laminar flame speed through experiments the resulting value is of the aerodynamic flame strain dependent speed. The flame strain is caused by mass, preferential and thermal diffusion as well as flow divergence. These values need to be corrected before getting the true, strain-free, laminar flame speed. While graphs of the true laminar flame speed are available in papers, tabulated values for making a direct comparison is scarce and therefore table 3.2 show a sparse amount of values possible to use for a direct comparison[16].

Equivalence ratio	Cantera [m/s]	Experiment [m/s]
4	1.64	1.44
1.6	2.99	3
1	2.29	2.1
0.3	0.025	0.059

Table 3.2: Comparison of Cantera simulation results and experimental results at 300 °K and atmospheric pressure.

From the comparison shown in table 3.2 the difference in flame speed is most significant near the lean limit, not because the results had an actual big value difference compared to the other equivalence ratio results, but because percentage wise the experimental result is 136% higher. It is the same part of the mixture range where the default GT laminar flame speed model does not produce realistic results.

By approaching the flame speed model described in Internal Combustion Fundamentals term by term it can be decomposed to each individual condition and their influence on the laminar flame speed. The first term describes the direct composition impact as seen in equation 3.3. The equivalence ratio is a part of the exponents α and β and so it does have an impact on the other terms as well. However the coefficients T_u and p only appear in their specific term as seen in equation 3.4 and 3.5.

$$\phi_{impact} = (B_m + B_\phi(\phi - \phi_m)^2) \tag{3.3}$$

$$T_{impact} = (\frac{T_u}{T_{ref}})^\alpha \tag{3.4}$$

$$p_{impact} = (\frac{p}{p_{ref}})^\beta \tag{3.5}$$

Since the method of keeping the influencing parameters apart and manage them term by term is proven and currently used for all SITurb-models in GT-Power it was the choice for creating a new model based on Cantera free flame model results. Since the equivalence ratio has an impact on all the three individual terms the separate equation for ϕ was made as the base. The Matlab application for curve fitting could create a fit of a polynomial equation as seen in figure 3.4 and equation 3.6. The resulting fit has an R-squared value of 0.9978.

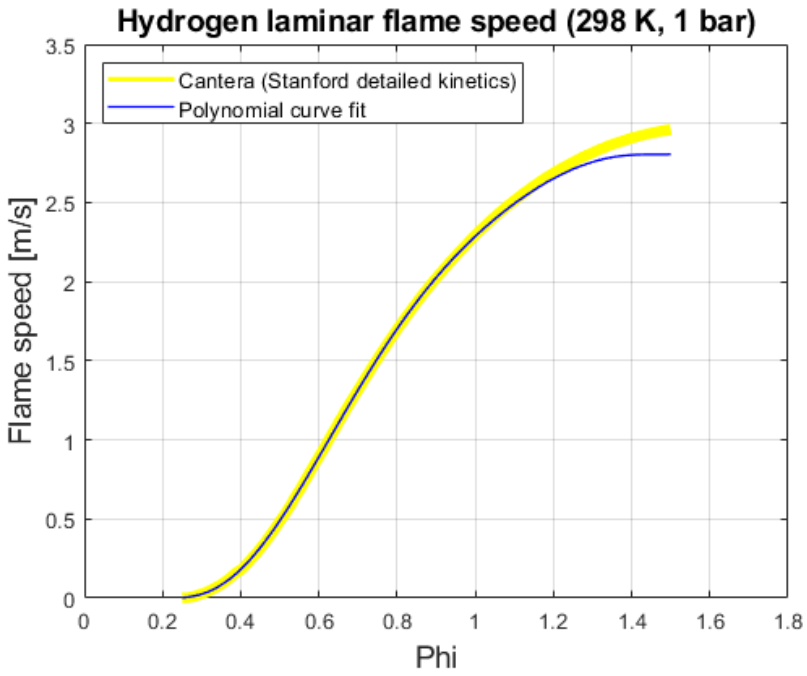

Figure 3.4: Comparison between Cantera kinetics model flame speed and polynomial fit.

$$\phi_{polyfit} = c_1 * \phi^7 - c_2 * \phi^6 + c_3 * \phi^5 - c_4 * \phi^4 + c_5 * \phi^3 - c_6 * \phi^2 + c_7 * \phi - c_8 \quad (3.6)$$

Where $c_1 - c_8$ *are constants.*

The Cantera model was only used for evaluation of initial conditions between 1-100 bar and 250-900 °K. This was due to the fact that the Cantera simulation showed inconsistent result at initial pressures above 100 bar and also for initial temperatures above 900 °K. A lowest initial temperature of 250 °K was based on possible cold start conditions.

The Cantera free flame model temperature response is shown in figure 3.5. The results are based on simulations between 250 to 900 °K and ϕ between 0.25 to 1.5 while keeping the ambient pressure as 1 bar.

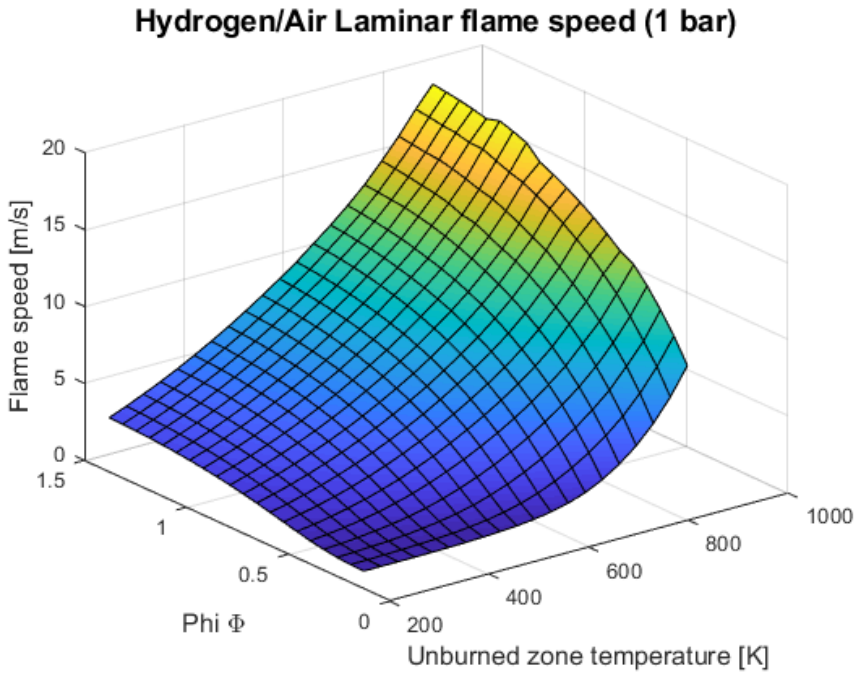

Figure 3.5: Cantera Laminar flame speed response for temperature and ϕ change.

The matlab curve fitting tool have several built in suggested functions for fitting 2d-curves where there is one variable and an associated response. When the fitting tool is used with two variables and a corresponding response the functions have to be custom made. The tool will help with achieving the best fit by changing constants incorporated by the user.

By choosing to use the default GT laminar flame speed model as a base for the temperature impact term the temperature exponent was the only thing that could be adjusted to make the fit. The resulting fit, equation 3.7, is shown in figure 3.6. For these specific initial conditions the fit has a good correspondence to the Cantera free flame model which is realised by the R-squared value of 0.9901.

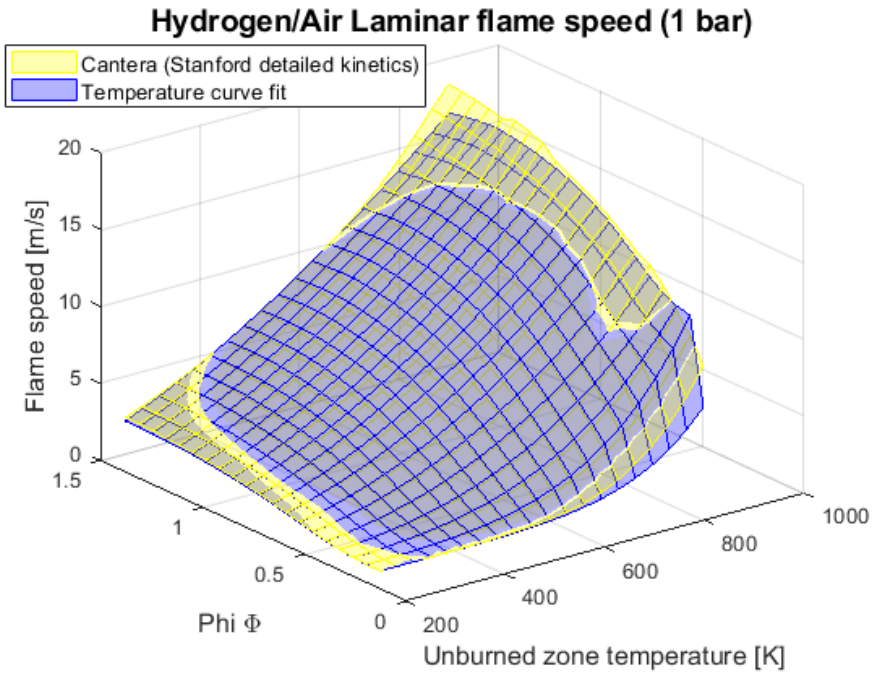

Figure 3.6: Cantera response vs. Temperature fit

$$T_{flamespeedfit} = (\frac{T_u}{T_{ref}})^{C_1+c_2*(\frac{-c_3}{\phi})+\phi^{-c_4}} \tag{3.7}$$

Where $c_1 - c_4$ *are constants.*

The Cantera free flame model response for change in pressure is shown in figure 3.7. It uses the same amount of data points as the temperature response.

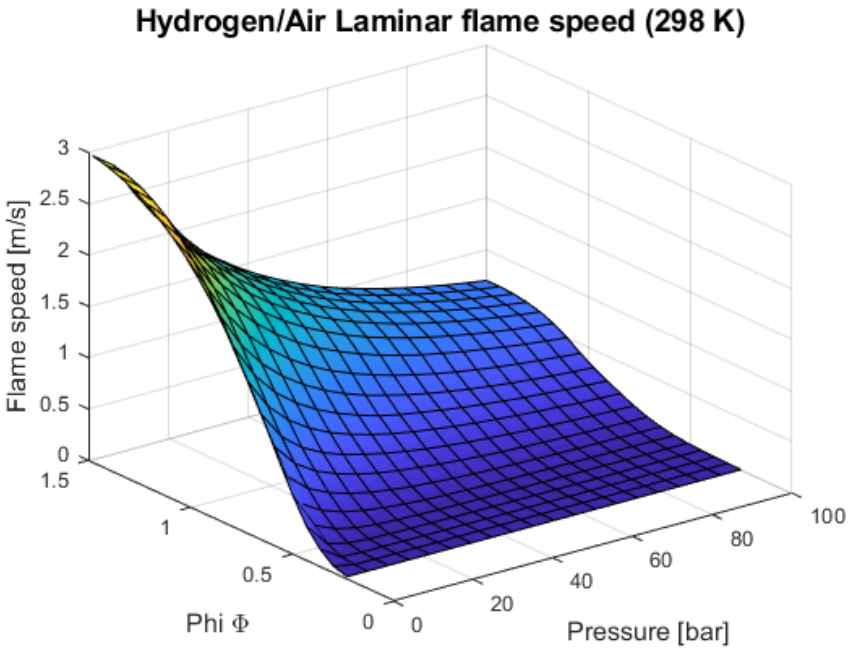

Figure 3.7: Cantera Laminar flame speed response for pressure and ϕ change.

The same approach as for the temperature term was used for the pressure impact term. The default GT model was used as the base and only the exponent was changed. The resulting fit did not show as good correspondence as for the prior fits as seen in figure 3.8 with a R-squared value of 0.9007. The resulting equation is equation 3.8.

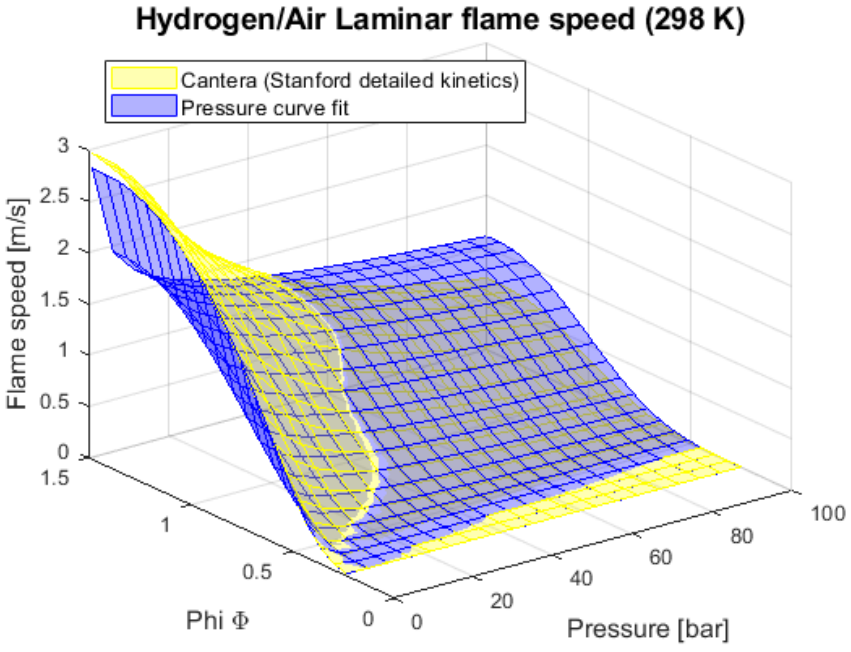

Figure 3.8: Cantera response vs. Pressure fit

$$P_{flamespeedfit} = (\frac{P}{P_{ref}})^{c_1 - c_2 * \phi^{-c_3} - c_4 * \phi^{c_5}} \tag{3.8}$$

Where $c_1 - c_5$ *are constants.*

3.1.2 GT-model implementation

The new kinetics-fit hydrogen flame speed model was implemented in a GT-Power model based on a 13 litre 6 cylinder SI CNG-engine. The model conversion to hydrogen was made by changing fuel type and laminar flame speed model.

Since the equation for the kinetics-fit laminar flame speed model uses ϕ as an instant variable that will have to be continuously updated for each time step of the GT simulation a RLTdependence reference object needed to be created for each cylinder and also for each term of the equation as seen in figure 3.9.

The air/fuel ratio variable was used as a wireless signal from each cylinder and then converted to equivalence ratio as in equation 3.9.

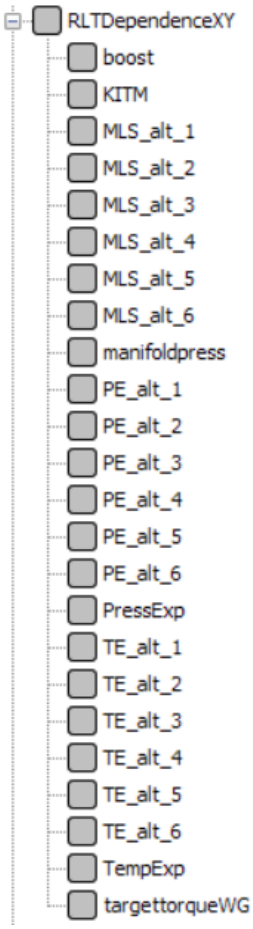

Figure 3.9: RLTdependence reference object in the GT-library

$$\phi = \frac{AFR_{stoichiometric}}{AFR_{cylinderX}} \tag{3.9}$$

The individual terms of the kinetics-fit laminar flame speed equation was divided into separate parts and added to the GT-library as XYFuntions as seen in figure 3.10. The temperature and pressure terms only needed the exponent created as a XYFunction since the rest of the terms were the same as for the default GT laminar flame speed model. To have updated cylinder specific ϕ the functions needed to be created for each cylinder. The XYFunctions must be selected as the dependency object for the corresponding RLTDependence reference object.

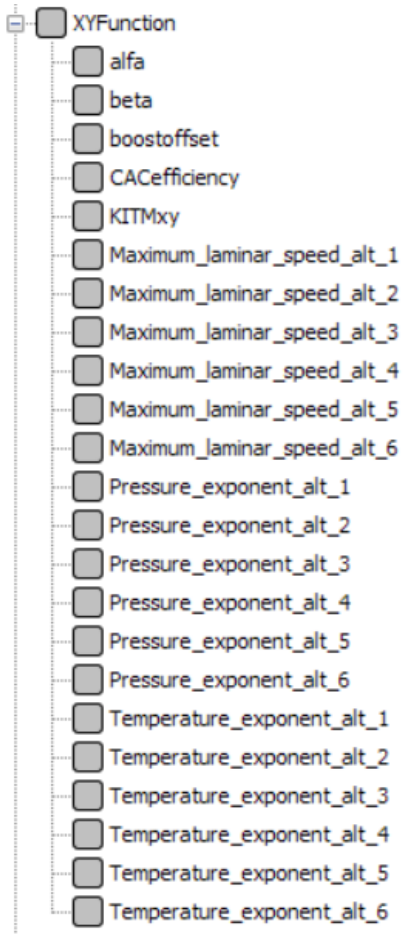

Figure 3.10: XYFunction reference object in the GT-library

Lastly a separate combustion object need to be created for each cylinder and the corresponding RLTDependence reference object must be added to the laminar flame speed tab. The Laminar Speed Roll-off Value must be set to zero so that it does not have any influence in the laminar flame speed equation. If the Laminar Speed Roll-off Value is set to zero the Equivalence Ratio at Maximum Speed value will have no impact on the rest of the equation due to them being multiplied with each other.

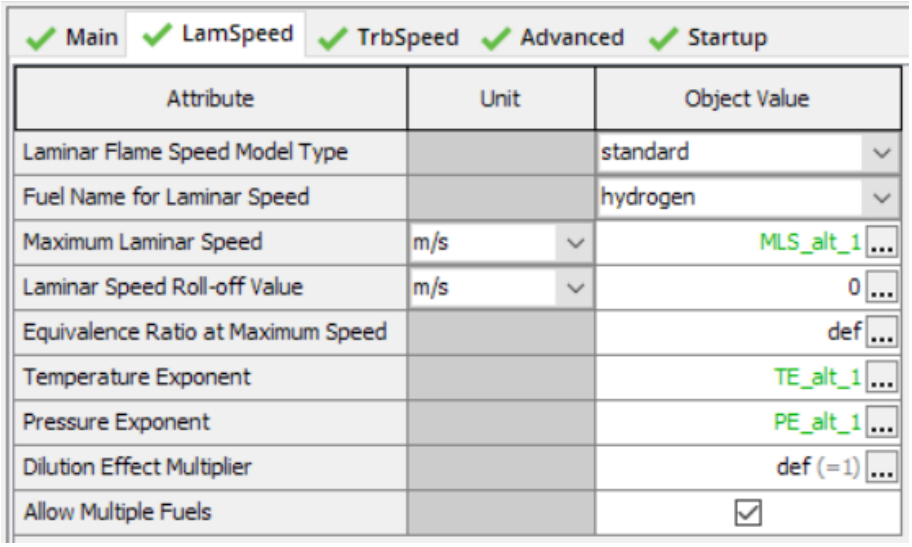

Figure 3.11: The laminar flame speed tab in the combustion object

3.2 Knock model

In GT-Power knock models from Douaud Eyzat, Frankze and Worret for carbon based fuels as well as their own dedicated kinetics-fit models for gasoline and methane gas combustion are available. There is no dedicated model for knock evaluation when running hydrogen combustion.

Since there is no possibility to calculate the octane number for hydrogen according to the AKI standard, the average of RON and MON, since the MON number is unavailable for hydrogen a comparison using any of the default models in GT-Power and expecting a relevant comparison is not possible. The only way would be to calibrate a model using experimental data to achieve a AKI which might reflect some of the knock characteristics of hydrogen.

With the use of Cantera the ignition delay was retrieved through chemical kinetic simulations. A constant volume reactor with the three initial conditions temperature, pressure and equivalence ratio was defined and used to evaluate the ignition delay time. The time defined as the ignition delay, τ, for Cantera simulations is the time it takes from the simulation start until a sudden increase of OH radicals occur.

4

Results

In this chapter the results and comparisons for the default GT laminar flame speed model and the kinetics-fit model are evaluated.

4.1 Laminar flame speed model - Validation

By running the kinetics-fit laminar flame speed model for conditions which differ from the initial conditions used when creating the model the overall compliance for different ambient conditions can be evaluated.

Figure 4.1 is a look of the response at an initial temperature sweep with stoichiometric conditions and three stages of initial pressure. It is clear that the temperature fit was made at 1 bar of ambient pressure. Except from the lower temperatures the correspondence at 50 and 100 bar is not very good.

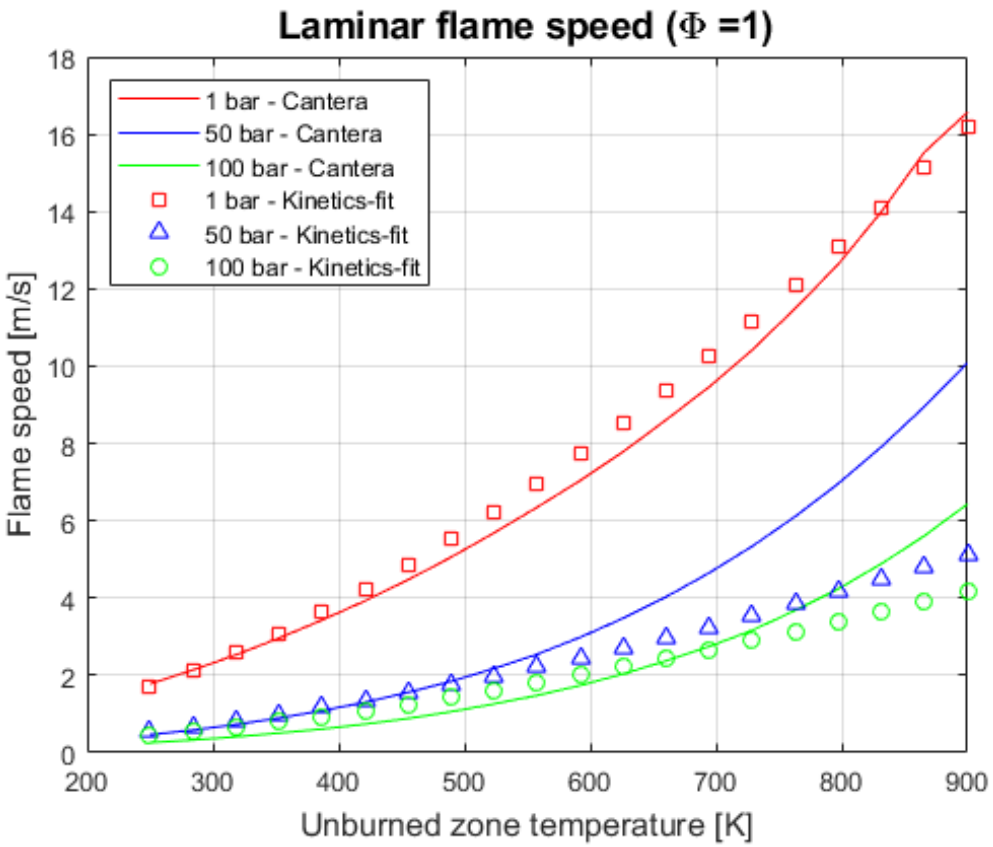

Figure 4.1: Comparison between Cantera and kinetics-fit laminar flame speed results for temperature sweep at ϕ=1

Pressure [bar]	R-squared value
1	0.9880
50	0.5587
100	0.8268

Table 4.1: R^2-value for temperature sweep at ϕ=1

Figure 4.2 instead shows a pressure sweep, altering the ambient temperature in three steps. Again the conditions for which the fit was created clearly shows much better correlation.

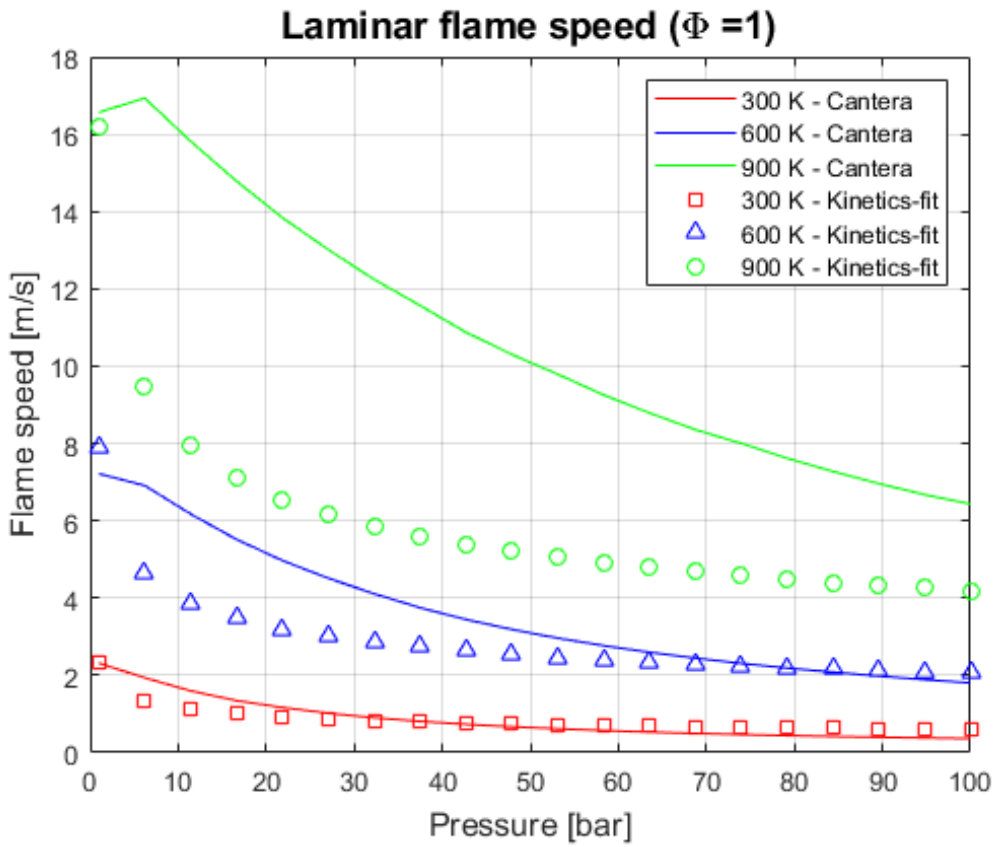

Figure 4.2: Comparison between Cantera and kinetics-fit laminar flame speed results for pressure sweep at ϕ=1

Temperature [K]	R-squared value
300	0.8114
600	0.5522
900	-1.3632

Table 4.2: R^2-value for pressure sweep at ϕ=1

The problem with the default GT laminar flame speed model is not necessarily at or near stoichiometric conditions but rather at the lean limit which is the main cause for a alternative model to begin with. Therefore results showing correlation at lean conditions is of interest. Figure 4.3 show a temperature sweep at very lean conditions. Notice that the y-scale is logarithmic. The R^2 shows worse correlation than for the results at phi=1.

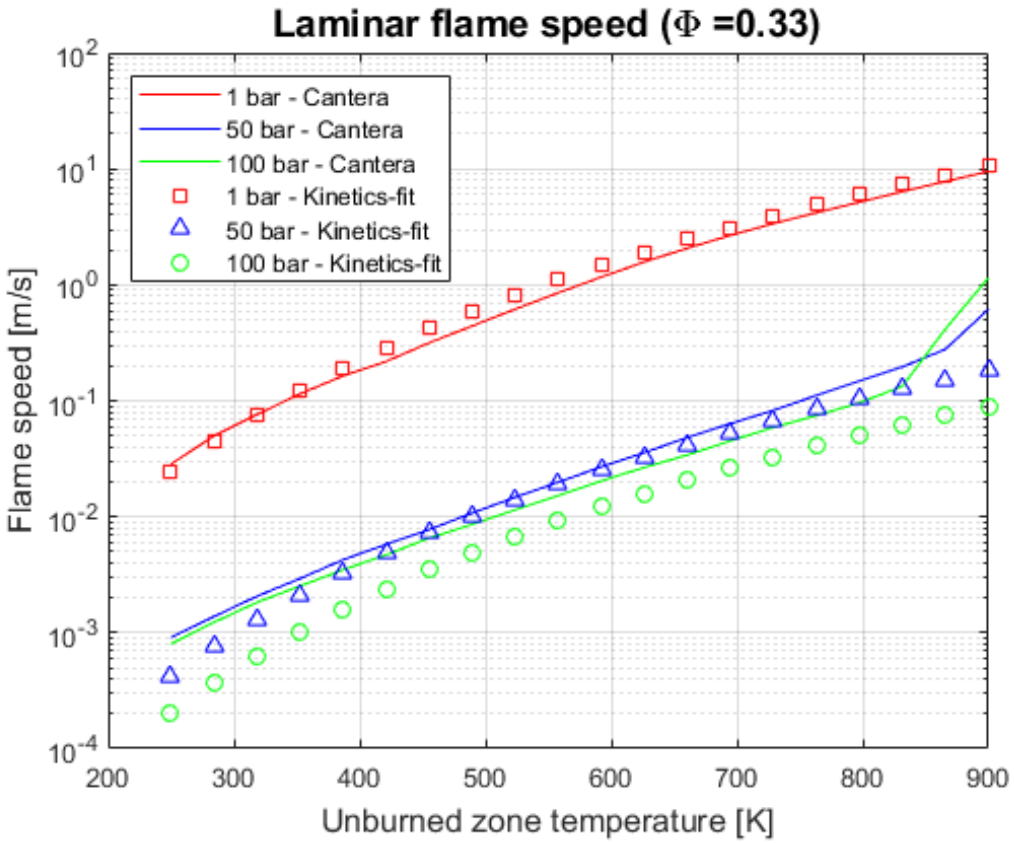

Figure 4.3: Comparison between Cantera and kinetics-fit laminar flame speed results for temperature sweep at ϕ=0.33

Pressure [bar]	R-squared value
1	0.9607
50	0.4774
100	0.0463

Table 4.3: R^2-value for temperature sweep at ϕ=0.33

The pressure sweep for lean conditions is shown in figure 4.4 and again the y-scale is logarithmic. These results show quite good correlation for all three cases. In general the kinetics-fit model shows tendencies of underestimating the laminar flame speed.

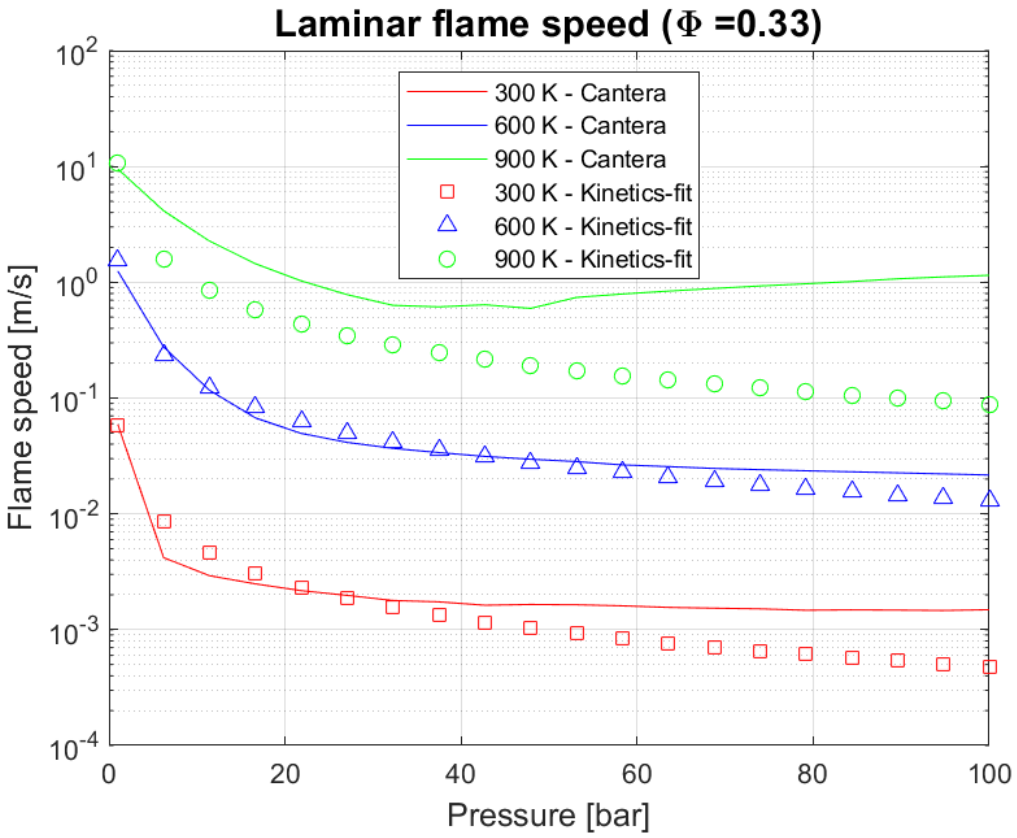

Figure 4.4: Comparison between Cantera and kinetics-fit laminar flame speed results for pressure sweep at ϕ=0.33

Temperature [K]	R-squared value
300	0.9893
600	0.9316
900	0.7588

Table 4.4: R^2-value for pressure sweep at ϕ=0.33

4.1.1 Default GT vs. Kinetics-fit laminar flame speed model

GT-simulation runs from a hydrogen converted 13L SI PFI CNG engine show the difference between how the default GT laminar flame speed model handles lean conditions compared to the kinetics-fit model. It is run at $0.33<\phi<0.5$ to capture the crossover where the default GT-model struggle with lean conditions.

Figure 4.5 show the average laminar flame speed during a complete engine cycle. Ignoring the actual values the graph shows an interesting point where the models cross each other. The crossing point corresponds very well to where the Cantera model crossed the GT-default model for 298 °K and 1 bar ambient conditions as seen in figure 4.6.

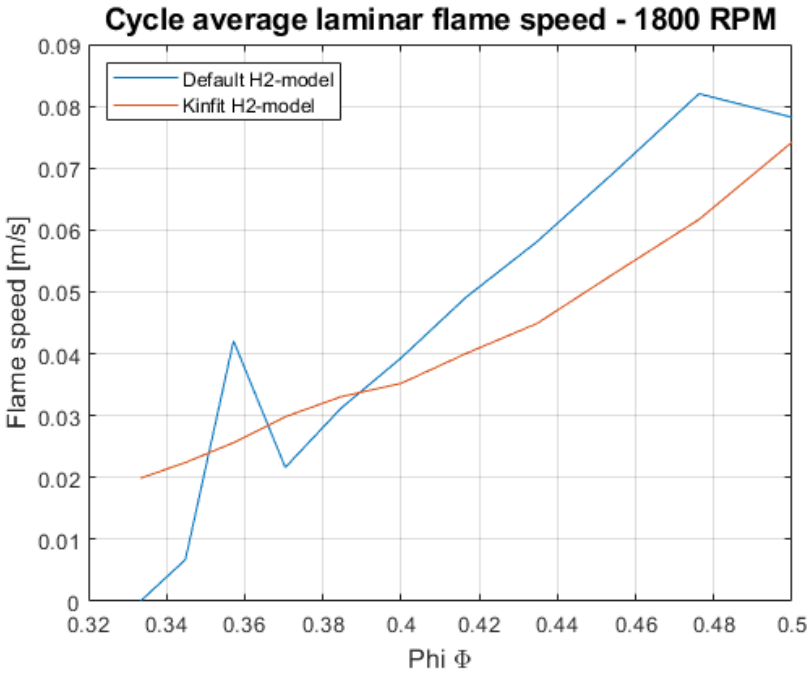

Figure 4.5: Cycle average laminar flame speed comparison, default GT-model vs. kinetics-fit

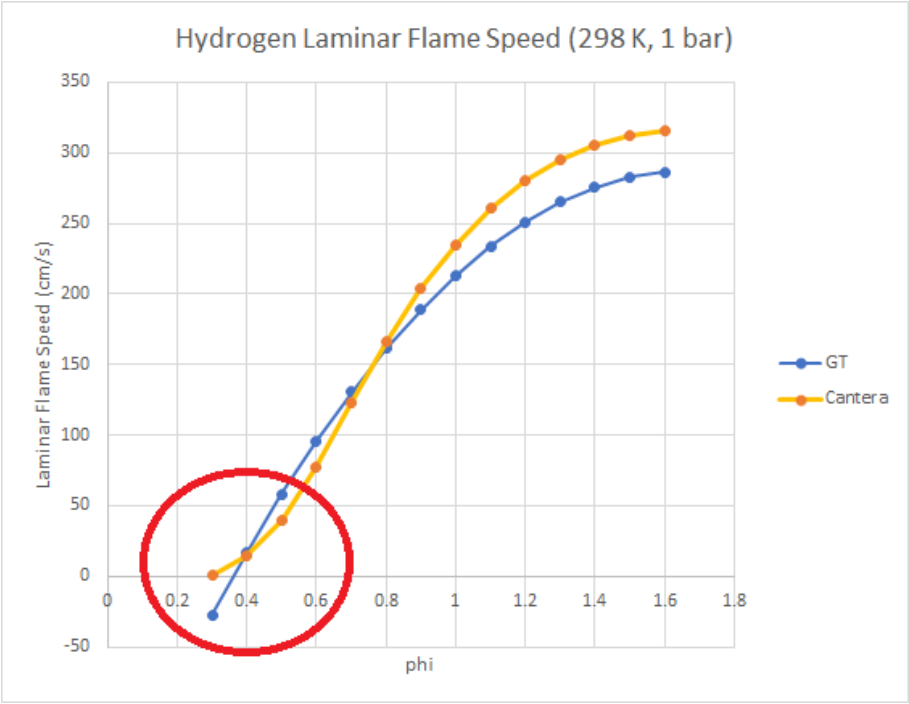

Figure 4.6: GT default laminar flame speed model compared to GT Cantera results highlighting the crossing point.

The maximum laminar flame speed per cycle, figure 4.7, shows a very similar trend as the cycle-average in figure 4.5.

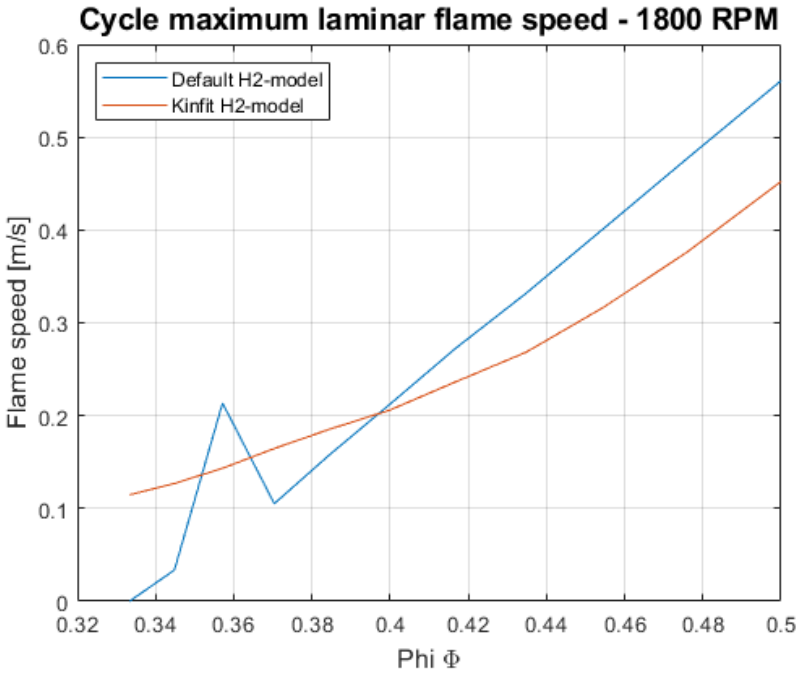

Figure 4.7: Cycle maximum laminar flame speed comparison, default GT-model vs. kinetics-fit

Figure 4.8 shows the IMEP which in the end is a result of the flame speed due to the flame speed being linked to the rate of energy release leading to an increase in temperature and pressure inside the cylinder. Again similar trends are shown, interestingly the IMEP of the default GT-model and the kinetics-fit is basically identical before the rapid drop for the default GT-model at $\phi \approx 0.38$.

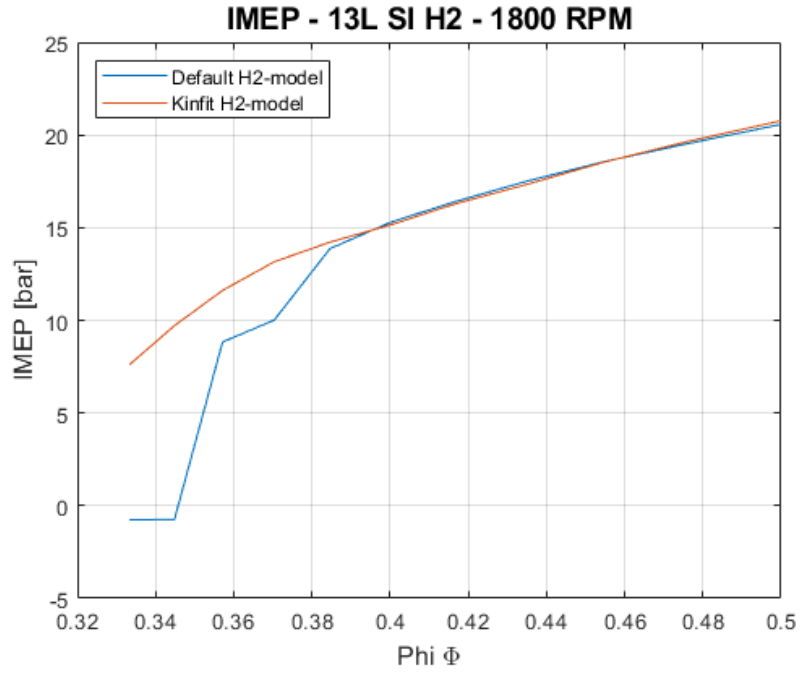

Figure 4.8: IMEP default GT-model vs. kinetics-fit

Apparent heat release shown in figure 4.9 and 4.10 show the similarities between the output from the models until the lean limit for the default GT-model.

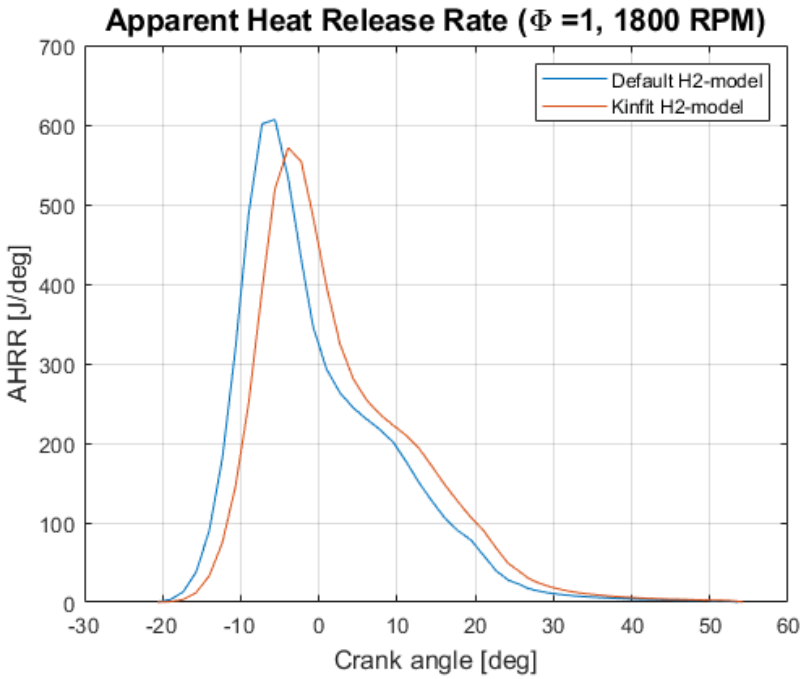

Figure 4.9: Apparent heat release comparison between flame speed models at ϕ=0.5

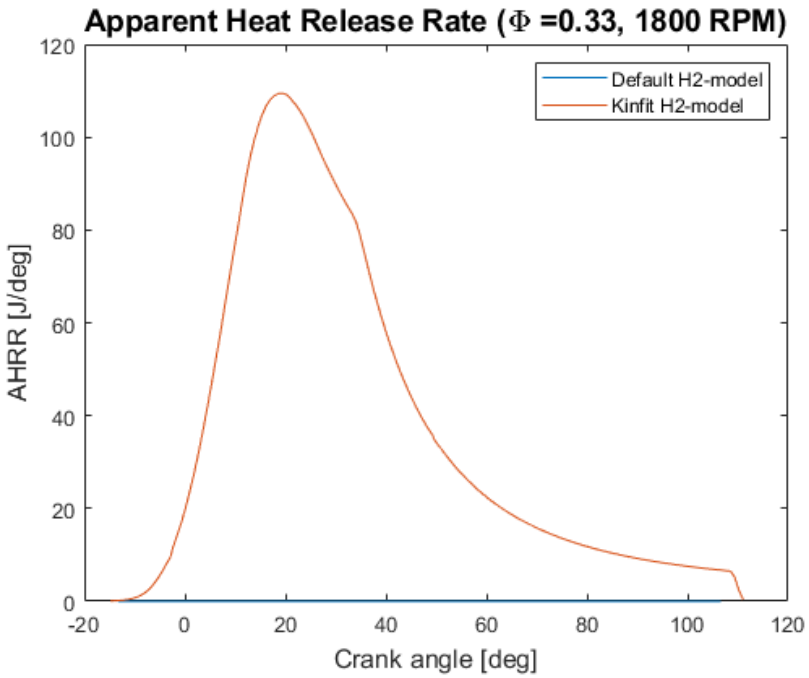

Figure 4.10: Apparent heat release comparison between flame speed models at ϕ=0.33

4.1.2 Turbulence multiplier impact

The laminar flame speed is only one of the inputs determining the burn rate for a predictive model, the actual flame speed is also depending on the turbulence induced in the cylinder air-fuel volume. The turbulence impact is defined by three multipliers, described in table 4.5, in the SITurb combustion model. These multipliers are adjusted when calibrating a model to fit experimental data. The default setting of 1 for all the multipliers has been used throughout this thesis but a case study was made to evaluate the impact for how the multipliers change the burned fuel fraction during lean combustion together with the kinetics-fit laminar flame speed model.

Flame Kernel Growth	Scales the value of the growth rate for the flame kernel. A higher value shortens the ignition delay.
Turbulent Flame Speed	Scales the turbulent flame speed which influences the overall duration of the combustion.
Taylor Length Scale	Modifies the time constant of the combustion for air/fuel mixture entrained into the flame zone by adjusting plume thickness.

Table 4.5: Turbulence multipliers available in the SITurb combustion object [10].

The upper limit for all the multipliers is 3 so therefore the evaluation range was set to 1-3. As expected both the kernel growth multiplier and the turbulent flame speed multiplier increase the burned fuel fraction the greater they get as seen in figure 4.11 and 4.12. The taylor length scale multiplier show very inconsistent results however the initial tendencies show a clear impact of reduced burned fuel fraction the higher the multiplier value becomes as seen in figure 4.13.

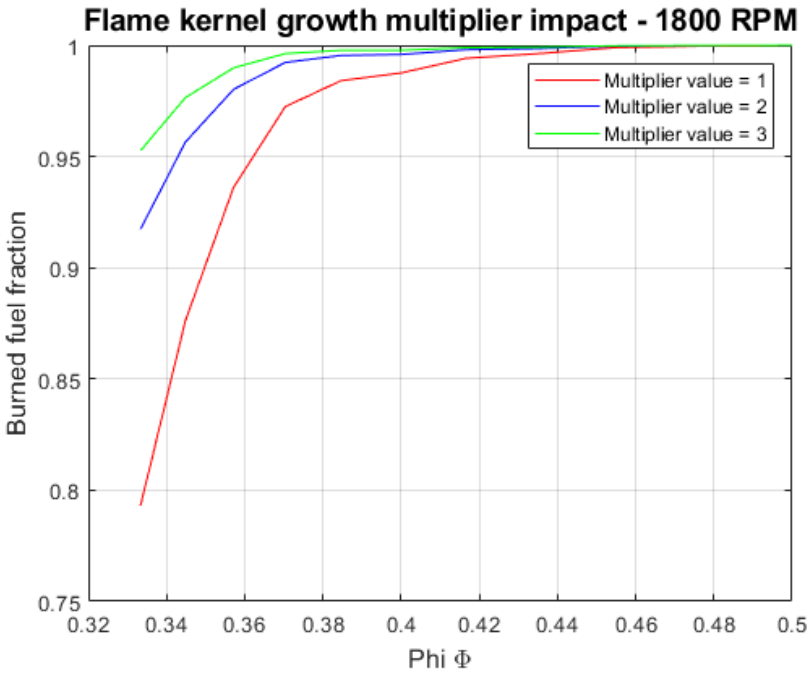

Figure 4.11: Kernel growth multiplier impact on burned fuel fraction

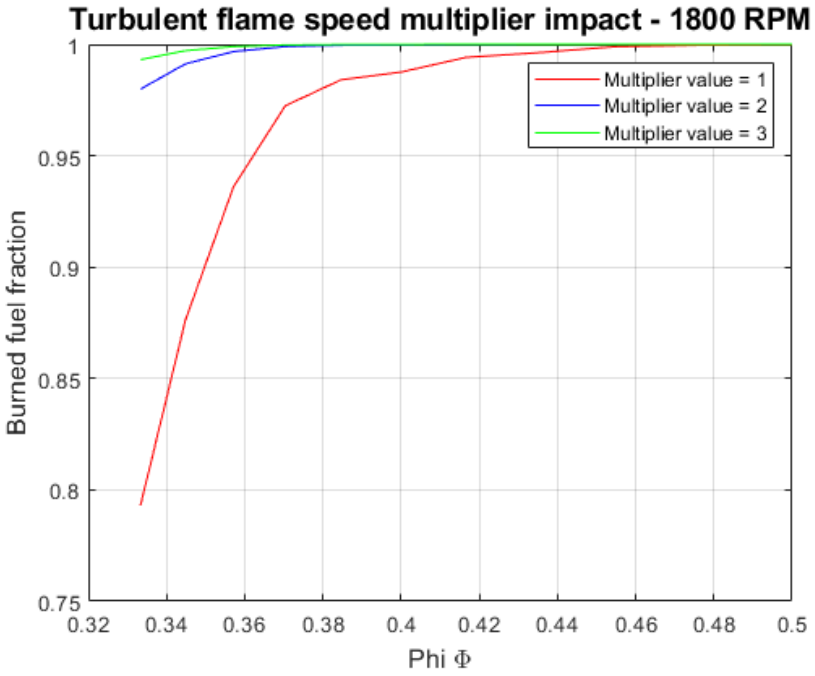

Figure 4.12: Turbulent flame speed multiplier impact on burned fuel fraction

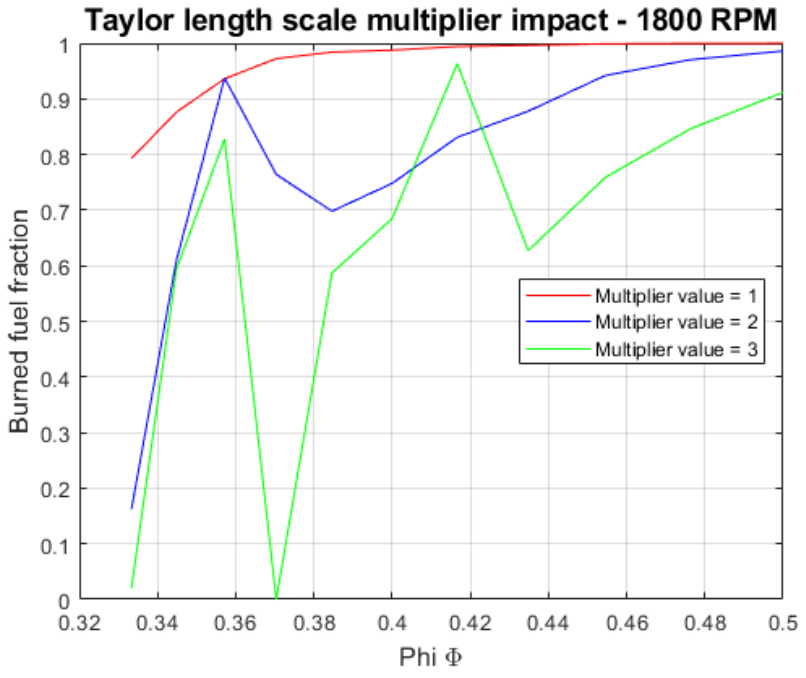

Figure 4.13: Taylor length scale multiplier impact on burned fuel fraction

4.1.3 Hydrogen vs. CNG

For Volvo Penta the question is if hydrogen could be a direct replacement in a SI PFI CNG-engine. The 13L CNG-engine needs to produce enough torque for a generator at given operating points. It is a comparison where the majority of the parameters

are the same. Ignition timing is optimized for each fuel to achieve enough torque and the best indicated thermal efficiency possible. The kinetics-fit laminar flame speed model is used for the hydrogen case. In table 4.6 the comparison results are shown, instead of throttling the hydrogen engine it can run lean helping to achieve a slightly higher indicated efficiency compared to the CNG-engine. Since there was no appropriate knock model for hydrogen it was not taken into consideration during this comparison.

Fuel	Engine speed [RPM]	Brake torque [Nm]	Phi Φ	Indicated efficiency [%]
CNG	1500	2400	1	42.76
CNG	1800	2000	1	42.44
H2	1500	2400	0.53	44.56
H2	1800	2000	0.53	43.73

Table 4.6: CNG and H2 steady state comparison

4.2 Knock model

By running chemical kinetic simulations for determining the ignition delay a comparison between hydrogen/air and CH4/air was made, the results show how much more sensitive hydrogen is to spontaneous ignition. Looking at figure 4.14 the results show not only the overall difference in ignition delay for hydrogen and methane but also the rapid decrease for hydrogen between ≈850 and 950 °K. The auto-ignition temperature for hydrogen is 860 °K which seems to correlate well with the point for the start of the rapid decrease in ignition delay.

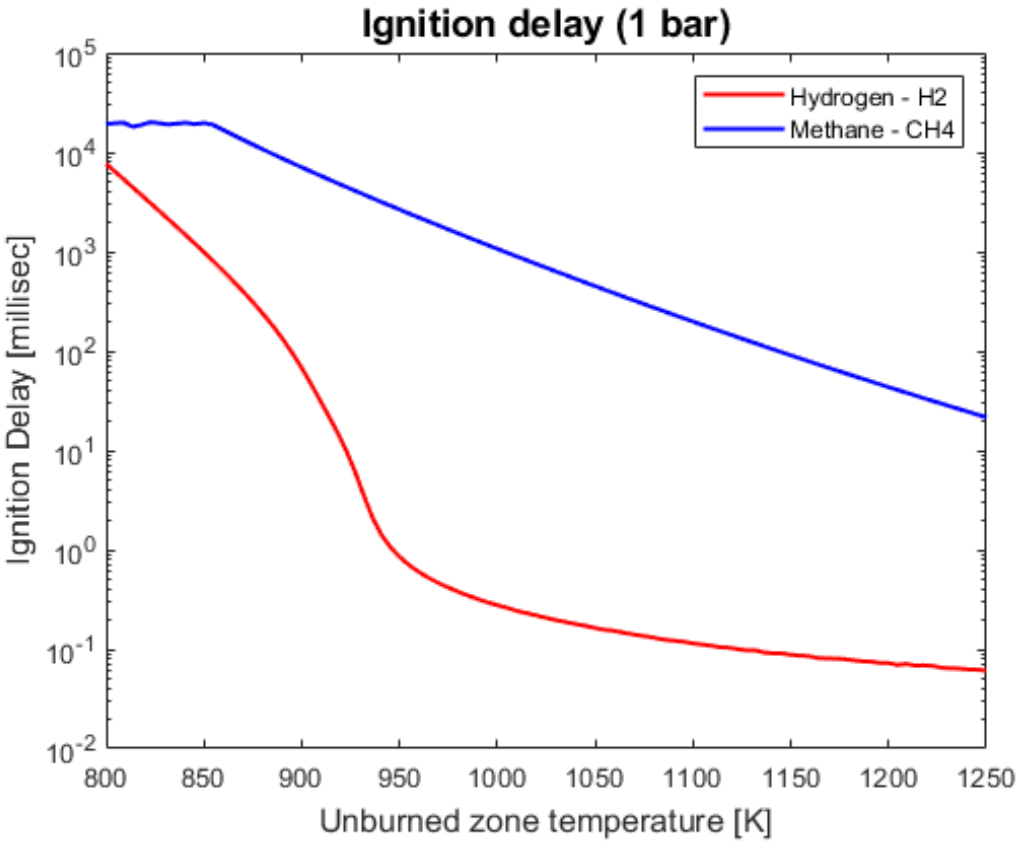

Figure 4.14: Ignition delay comparison between hydrogen and methane.

4.3 Discussion

Looking at the results for the kinetics-fit laminar flame speed model it is evident that there is a large improvement possibility. The idea of using multiple fitted equations for different in-cylinder conditions where the program interpolates between the equations to increase the usable range of the model seems valid. By the use of a XYZ map a different equation could be used depending on some chosen variable, for example in-cylinder pressure. This would greatly improve the possibility of getting a good fit for a wide operation range.

While using a chemicals kinetics model to achieve a reference for the equation fit was a success in terms of the amount of data available to make the fit, the reliability of the data must be considered. Not only can the calculations themselves be creating results that differ from reality, but the chosen chemical mechanism will have impact on the results.

5
Conclusion

Since the range of ignitable equivalence ratios is so much wider for hydrogen than the traditional fossil fuels, gasoline and methane, used in SI engines another dimension of accurate flame speed calculations are required. The way of how the hydrogen laminar flame speed respond to change in ϕ is also not as simple as with carbon based fuels because of the reduced impact near the lean limit. Hydrogen also includes a much wider spectrum of laminar flame speeds since the maximum is almost ten times faster than for gasoline. The bottom line is that a laminar flame speed model that shows accuracy both at stoichiometric conditions as well as near the limits of combustion will need to be more sophisticated than for the general carbon based fuel.

The end results show that the kinetics-fit laminar flame speed model still underestimates the flame speed at lean conditions ϕ<0.5, the possibility of running really lean as described in papers of actual experimental engine tests is still attainable in a 1-D simulation environment but it would need an updated fit of the kinetics-fit model or a complete redesign. While the kinetics-fit model shows more of a similarity to the Cantera responses, having usable combustion at as lean as ϕ=0.33 still will require higher laminar flame speeds. Not only does the Cantera model show higher flame speeds at lean conditions, the experimental results which the Cantera model was evaluated for show even greater laminar flame speeds at lean conditions ϕ<0.5. A comparison to CNG with a more accurate kinetics-fit laminar flame speed model would also show greater benefits.

In terms of the ignition delay results, describing the tendencies for knock, they further demonstrates the need for a calibrated knock model when doing hydrogen combustion simulations. Knock is widely discussed in papers about hydrogen as a ICE fuel. The ignition delay only brings forward the problems with spontaneous ignition due to the overall in-cylinder conditions. Hot-spots or late ignition of trapped fuel mix in crevices leading to backfire or pre-ignition is a different problem and is normally not discovered by 1-D knock models.

Volvo Penta can by using the method of achieving results from chemical kinetics simulations to use for a fitted equation improve the kinetics-fit laminar flame speed model or create a similar one. The implementation in GT-Power can be useful, not only for a laminar flame speed model but also for other custom models. Most importantly the exploration and identification that the problem exists is needed to make a valid decision to changing the model also.

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