Ignition delay and laminar flame speed calculations of ammonia/hydrogen mixtures

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As the world is transitioning away from the traditional hydrocarbon fuels, hydrogen and ammonia have emerged as promising alternatives. However, different fuels regularly have drastically different combustion qualities. Two parameters very frequently used to characterise combustion are ignition delay and laminar flame speed.

This thesis will explore common strategies to determine ignition delay and laminar flame speed, as well as the repercussions the two have for example in compression ignition engines. The manner in which they are influenced by various physical and chemical factors will also be investigated.

Finally, chemical kinetics simulations will be conducted using the open-source library, Cantera, to calculate ignition delays and laminar flame speeds for hydrogen and ammonia across a range of operating conditions.

Key words: ignition delay, laminar flame speed, hydrogen, ammonia, Cantera

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1 Introduction

1.1 Background

As the necessity of environmentally friendly technologies is becoming increasingly apparent, there has been a growing initiative within the industry to develop various types of internal combustion engines (ICE) with minimal greenhouse gas and other pollutant emissions. However, to achieve this, it’s evident that the traditional hydrocarbon fuels must be replaced with carbon-free alternatives.

Some of the more promising options of such include hydrogen as well as different hydrogen carriers, such as ammonia. Excitement regarding hydrogen stems from its remarkably high heating value combined with zero carbon emissions. Consequently, numerous applications have been identified for both, ranging from ICEs to the aviation industry. [1, 2]

While some commercially available products have already been launched [3], the large-scale adaptation has yet to materialize. Contributing factors to this include the challenges involved in the distribution and storage of hydrogen and ammonia. In addition to the question of practicality, many engineering considerations arise from the use of these fuels due to their vastly different combustion characteristics. [1]

Two properties that are significantly affected by the choice of fuel are ignition delay and laminar flame speed. In the context of ICE design these have been found to have a considerable effect on both performance and NOx emissions, the former remaining as a substantial environmental challenge facing engines powered by hydrogen. [4]

The objective of this work is to first present a brief literature review into existing research on ignition delay and laminar flame speed evaluation for hydrogen-air and ammonia-air mixtures. Then chemical kinetics simulations will be conducted using the Cantera library [5] to determine ignition delays and laminar flame speeds in various conditions and chemical compositions.

1.2 Ignition delay

The principle that facilitates compression ignition in the first place is hydrocarbon-air mixtures’ tendency to spontaneously ignite in specific conditions in a process called autoignition. That is, ignition without an external heat source, such as a spark.

Even prior to the ignition there are various reactions continuously taking place in which highly reactive radicals are produced. A stable state is maintained as long as a sufficiently large portion of these radicals are reduced in radical recombination. However, if the so-called ignition limits are exceeded by a sudden change in either pressure or temperature, the quantity of the radicals begins to increase exponentially. As the concentration of the free radicals reaches a critical value, an ignition occurs after a brief period. It is this period that is signified as the ignition delay.

Its duration can range from microseconds to minutes depending on the physical conditions and the chemical composition of the system. For most applications it’s generally advantageous to keep ignition delay quite low since shorter overall combustion time allows for a larger number of these processes to take place in the same time window. [6]

Furthermore, for compression ignition engines ignition delay can be formulated simply as the time between fuel injection and the start of combustion [7].

1.3 Laminar flame speed

After an ignition has occurred, the flame front begins to propagate through the unburnt gases at a specific speed also defined as flame speed. Flame speed is generally categorized into two types depending on whether the conditions are laminar or turbulent [6].

It’s important to note that when analysing flame speed, the flame type is generally assumed to be laminar, and the fuel-oxidizer mixture is fully premixed. Having said that, real-world conditions are almost exclusively turbulent and non-premixed when dealing with e.g. compression ignition engines. The aforementioned assumptions are made to facilitate the flame speed calculations solely using the chemical kinetic simulation library, Cantera, without Computational Fluid Dynamics (CFD) simulations. Furthermore, Cantera’s one-dimensional flame configurations do still account for fluid flow and diffusion processes [5].

Laminar flame speed does still provide a valuable insight into any combustion process since under most circumstances turbulent flame speed is higher than the laminar kind. Higher flame speed leads to faster combustion, and by applying analogous reasoning as with ignition delay, moderately high flame speed is usually preferred.

Also, to facilitate complete combustion in internal combustion engines, the whole process from autoignition to the total consumption of the fuel needs to take place within a certain time frame dictated by the speed of the pistons. If the flame speed is too low, there isn’t enough time for all the fuel to burn and the remainder is wasted, drastically reducing efficiency. [1, 6, 8]

However, excessively high flame speed may also cause unwanted effects, including flashback, elevated NOx-emissions and instabilities [1, 9].

1.4 Evaluation

In most cases combustion is an extremely difficult phenomenon to describe analytically due to the intrinsic complexity of the chemical kinetics involved. Oxidation of both hydrogen and ammonia are intricate mechanisms with many intermediate reactions [6]. For example, the reaction between hydrogen and air is often represented as the simple single step reaction $2H_2 + O_2 \rightarrow 2H_2O$. A detailed mechanism for hydrogen oxidation (Conaire et al., 2004) on the other hand, considers 19 unique reactions and 10 species [10]. Another mechanism developed by University of California San Diego considers 57 species and 268 reactions [11].

Consequently, exact quantitative analysis of combustion isn’t usually practical or even feasible. Therefore, when approximating ignition delay and laminar flame speed it is necessary to resort to various experimentally derived relationships and numerical simulations. Computational analysis can be carried out using numerous different methods. Most comprehensive results are yielded by CFD simulation methods. For example, in a Direct Numerical Simulation (DNS) the governing Navier-Stokes equations are completely solved numerically without turbulence models. In the present work, however, the primary focus will be on 0D and 1D reactors. [6, 8]

An emerging strategy expected to gain popularity in the coming years is the utilization of machine learning and artificial intelligence. Existing research has already shown that advanced neural networks are capable of high precision prediction of ignition delay [12, 13] and laminar flame speed [14] even when trained on rather small datasets.

1.4.1 Ignition delay

To derive accurate correlations conventionally, a lot of data must first be gathered from experiments. Ignition delay is commonly analysed with a setup comprising of a shock tube equipped with highly sensitive pressure sensors. In such case the start of combustion can be designated by for example the moment of highest rise in pressure. Eventually correlations may then be obtained with multiple regression analysis. [15]

This general workflow with slightly different implementations has been applied in numerous studies. While some research focuses on diesel and other hydrocarbon fuels [16], other papers have exclusively explored hydrogen's and ammonia's ignition delay [15, 17].

Many of the relationships developed for ignition delay are based on the Arrhenius equation [16]. The general form of the Arrhenius type equation for ignition delay is presented in Equation 1. This correlation is presented in a study (Miron et al., 2020) that examines ignition delay for a large variety of hydrocarbon fuels.

$$\tau = kp^{-n}\exp\left(\frac{E_a}{RT}\right) \tag{1}$$

Here τ is ignition delay, k and n are constants specific to each mixture condition, E is the activation energy, R is the universal gas constant, p is pressure and T is temperature. From this dependency alone, valuable conclusions can be made regarding how ignition delay responds to changes in thermodynamical conditions. Namely, one can expect exponentially decreasing ID with increasing temperature as well as inverse proportionality with pressure (as $n > 0$).

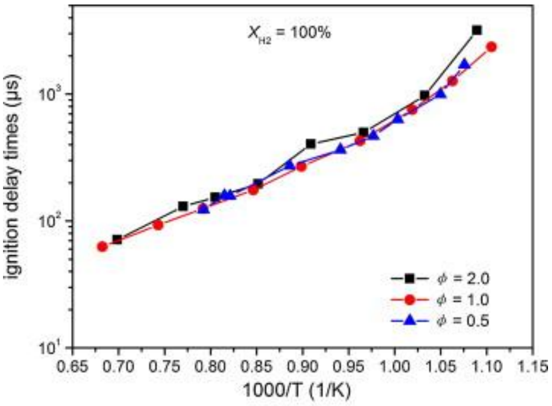
The values of both k and n, on the other hand, are dependent on the chemical compositions of the fuel and the oxidizer as well as the respective amounts of the two. Since it can be rather impractical to describe the composition of a system by exact masses or moles of each molecule, it is preferred to express this by equivalence ratio. Equivalence ratio, generally denoted as φ, is the ratio of the fuel-oxidizer ratio to the stoichiometric ratio.

The following empirical correlation incorporates equivalence ratio explicitly.

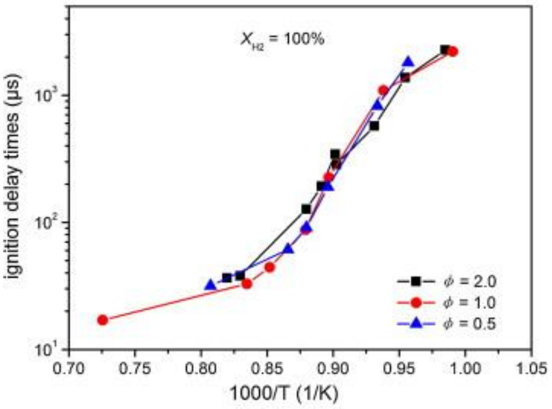
$$\tau = A\varphi^{\alpha}p^{\beta}\exp\left(\frac{E_a}{RT}\right) \tag{2}$$

Included in Equation 2 are correlation parameters A, α and β (here $\beta < 0$). This relationship was introduced in study (Tang et al., 2013) that set out to examine the effects of equivalence ratio on ignition delay. The mixtures in question were comprised of propane, hydrogen, oxygen and argon. Hydrogen's mole fraction of the propane-hydrogen fuel blend was also varied at 0%, 70%, 95% and 100%. It was found that the ignition delay ceases to showcase Arrhenius type dependency with temperature once hydrogen's fraction of the fuel is higher than 95%. Hence, the correlation parameters for Equation 2 were determined only for the mixtures with 0% and 70% of hydrogen.

Figure 1 presents the experimentally obtained ignition delay figures for mixtures with pure hydrogen as the fuel. While not quite matching the exponential temperature dependency, it is still quite evident that ignition delay shortens extremely rapidly as the initial temperature is increased. At 10 bars for instance, the ignition delay of the stoichiometric mixture decreased from approximately 20 ms to under 20 µs as the temperature was raised from ~1000K to around 1380K. [15]



(a) P = 1.2 bar



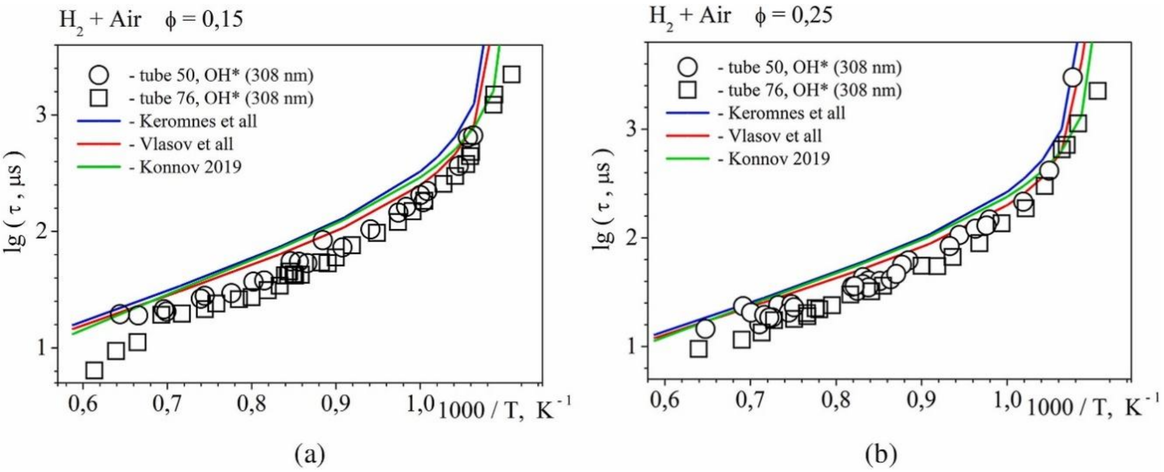
(b) P = 10 bar

Figure 1: Ignition delay times of pure hydrogen at various equivalence ratios and pressures of 1.2 and 10.0 bar. Adopted with permission from [15].

The experiments conducted in the previously discussed study demonstrate well that while correlations can be obtained for specific conditions, and they are very convenient when applicable, combustion cannot be comprehensively modelled with them only.

This is why numerical simulations have become such an essential tool in combustion analysis. As a result of extremely accurate modelling techniques, extensive thermodynamical data, and improvements in computational power, the evolution of the thermochemical state can be precisely determined for virtually any system. In practice, the only remaining major source of error is attributed to insufficient level of detail in the chemical mechanisms. [18]

Determination of these mechanisms by hand is a tedious and error-prone process, but over the last years there have been improvements in this area as well. A program by the name Reaction Mechanism Generator (RMG) [18] developed by Gao, Allen, Green, and West can construct complex mechanisms very quickly.



(a)

(b)

Figure 2: Comparison between experimental and simulation results. Adopted with permission from [17].

Despite the incredible effectiveness displayed by the various simulation models, it is still important to keep validating the results by comparing it to experimental data.

Multiple studies have been conducted with such approach, each with different ranges of temperature and pressure, equivalence ratios and mixture compositions. Notable interest has been on how adding hydrogen into other fuels, such as ammonia, propane or diesel, affects ignition delay. [15, 17, 19]

An example of a comparison between experimental and simulated ignition delay results for a hydrogen-air mixture at two equivalence ratios is shown in Figure 2.

1.4.2 Laminar flame speed

Analysis of ignition delay and laminar flame speed share many common elements regarding the general workflow. Correlations can be obtained as best fits for experimental data but, as in the case of ignition delay, most accurate results are yielded by numerical simulations.

The experimental setups and the simulation methods can differ in many ways, however, as laminar flame speed analysis requires examination of all the transport phenomena. Previously with ignition delay and 0D reactors this wasn't necessary. [6, 9, 20]

Experimental laminar flame speed assessments can be conducted in many different flame configurations. These include counterflow/stagnation flame, Bunsen flame, burner-stabilized planar flame and Outwardly Propagating spherical Flame (OPF). Studies cite OPF as the preferred method. [9, 20]

In contrast to most ignition delay correlations, laminar flame speed relationships are regularly expressed using some reference temperature, pressure or the laminar flame speed at those reference conditions. Usually this would refer to the NTP conditions, that is, a temperature of approximately 298 K and an atmospheric pressure. [9]

Compact expressions for laminar flame speed in the literature usually assume the following general form,

$$S_L = f(x_i)(T/T_0)^{\alpha(x_i)}\,(P/P_0)^{\beta(x_i)} \tag{3}$$

where, S_L is laminar flame speed, T and P are temperature and pressure, T_0 and P_0 are the reference temperature and pressure, and f, α and β are parameters that are expressed as a function of one or more independent variables, such as equivalence ratio, temperature or pressure. Determination of f, α and β can be performed using numerical simulations. [21]

A study published in 2012 by Sankaranarayanan Ravi and Eric L. Petersen derived the parameters as a function of equivalence ratio for a wide range of conditions. Following polynomial functions were conceived:

- $f(\varphi) = a_1 + a_2\varphi + a_3\varphi^2 + a_4\varphi^3 + a_5\varphi^4$
- $\alpha(\varphi) = b_1 + b_2\varphi + b_3\varphi^2 + b_4\varphi^3$
- $\beta(\varphi) = c_1 + c_2\varphi + c_3\varphi^2$

The pressure dependency was then eliminated from the analysis by evaluating parameters a_i and b_i at various fixed pressures. Thus Equation 3 reduces to

$$S_L = [a_1 + a_2\varphi + a_3\varphi^2 + a_4\varphi^3 + a_5\varphi^4](T/T_0)^{(b_1+b_2\varphi+b_3\varphi^2+b_4\varphi^3)} \qquad (4)$$

Through detailed Chemkin chemical kinetic simulations the parameters at different pressures were then calculated and compiled into Table 1. [21]

Table 1 Correlation parameters to be used with Equation 4. Adopted with permission from [21].

	H_2/air ($0.5<\varphi<2.0$)					H_2/air ($2.0<\varphi<5.0$)				
	1atm	**5atm**	**10atm**	**20atm**	**30atm**	**1atm**	**5atm**	**10atm**	**20atm**	**30atm**
a_1	−3	161	232.9	259.3	272.8	355.8	481.8	378.9	492.5	450.5
a_2	−234.7	−970.8	−1228.7	−1281.3	−1316.4	16.2	−87.2	−31.2	−184.1	−190.6
a_3	998.4	1902.6	2131.7	2081.5	2079.4	−24.7	−5.3	−20.8	21.1	25.9
a_4	−673.4	−1111.7	−1197.3	−1147.1	−1141.8	2.53	1.38	2.8	−0.59	−1.05
a_5	136.1	209.8	220.7	209.5	208.6	0				
b_1	5.07	5.52	5.76	6.02	7.84	1.405	1.091	1.64	0.84	0.81
b_2	−6.42	−6.73	−6.92	−7.44	−11.55	0.053	0.317	−0.03	0.56	0.64
b_3	3.87	3.88	3.92	4.37	7.14	0.022	0	0.07	0	0
b_4	−0.767	−0.728	−0.715	−0.825	−1.399	0				
T_0						320				

Similarly, as in the case of ignition delay, laminar flame speed can be determined using numerical simulation methods only. Figure 3 presents a comparison between experimental results and 1D chemical kinetics simulation with Chemkin PREMIX. [9]

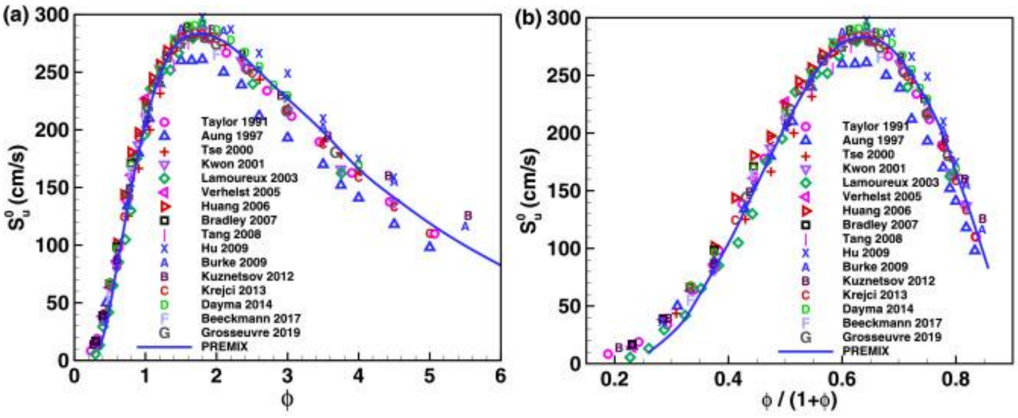


Figure 3: Simulation and experimental laminar flame speed results as a function of equivalence ratio (left) and normalized equivalence ratio. Adopted with permission from [9].

2 Considerations for Cantera simulations

2.1 Ignition delay

Before getting further into the Cantera simulations it’s useful to establish which assumptions and conditions are going to be applied.

For the ignition delay computations Cantera’s zero-dimensional constant pressure reactor for ideal gases will be utilized [5]. As the name suggests, it presumes ideal gas behaviour for homogeneous fuel-oxidizer mixture as pressure is kept constant. The oxidizer in this case is air with 21% of oxygen and 79% nitrogen (mole-%).

Two built-in Cantera mechanisms will be applied, *h2o2.yaml* for hydrogen oxidation and *example_data/ammonia-CO-H2-Alzueta-2023.yaml* for ammonia. The former considers ten species and twenty-nine unique reactions and the latter forty-two species and 281 reactions.

With the selected mechanism one can then set the initial mixture composition, temperature, and pressure. The relative amounts of fuel and air will be assigned in terms of equivalence ratio. Unless otherwise stated, for each case the equivalence ratio $\varphi = 1$, corresponding to the stoichiometric ratio.

The state of the system can be determined at pre-determined time intervals Δt and the over-all real-time duration of the simulation is generally 2000 – 50000 times longer than Δt. The ability to control Δt provides a convenient way to influence the computational cost of the simulation.

It’s crucial for the accuracy of the results that Δt is always much smaller than the ignition delay. However, if the ignition delay can be expected to be rather high, then Δt can be increased and it turn the over-all simulation time can be decreased from for example $10000 \times \Delta t$ to $5000 \times \Delta t$. This essentially halves the number of states that will be calculated for the system, thus reducing the computation time.

The states at each moment in time are stored into a large array making it easy to plot any of the properties as a function of time. An example of this is shown in Figure 4. It presents temperature evolution of stoichiometric hydrogen-air mixture at 50 bars. It also illustrates how the start of combustion, and consequently ignition delay, is defined going forward.

Hereon, ignition delay will be specified as the time it takes for the temperature to rise by half of the eventual temperature change.

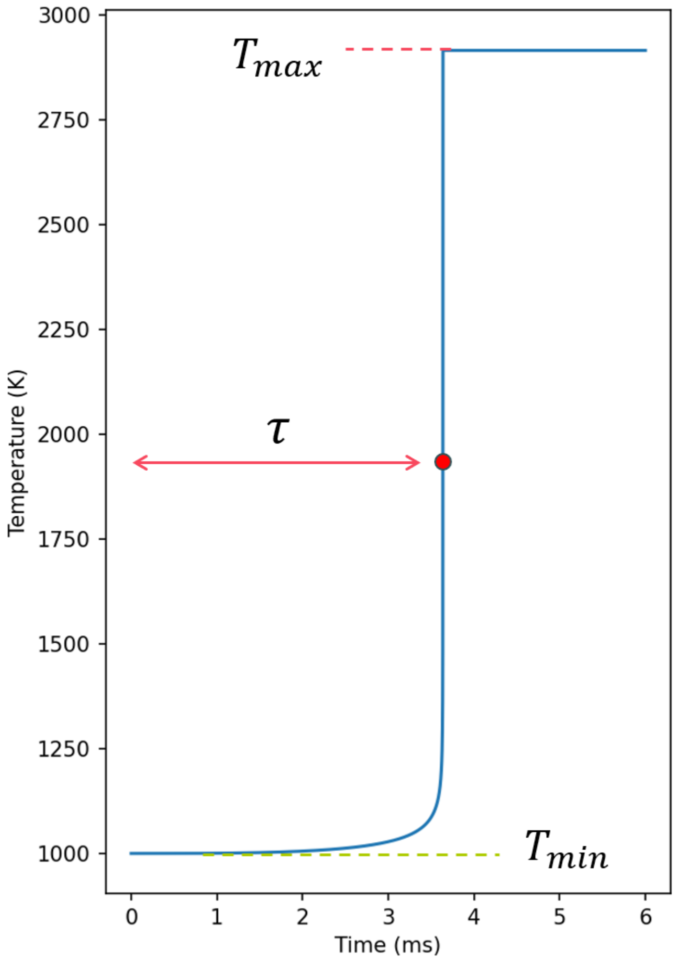


Figure 4: A sketch of how ignition delay is defined from here on out

Evaluating ignition delay at some very specific conditions isn't particularly interesting, however. A lot more useful results can be obtained when inducing variation to one or more of the initial properties and then plotting the relationship between ignition delay and the property in question. A schematic of this process is shown in Figure 5, exhibiting the temperature dependency of ignition delay for hydrogen.

All original plots in this text are made using the Matplotlib library.

An example of the Cantera code used to determine ignition delays is provided in Appendix 1 and 2. It was utilised to make Figures 6 and 7.

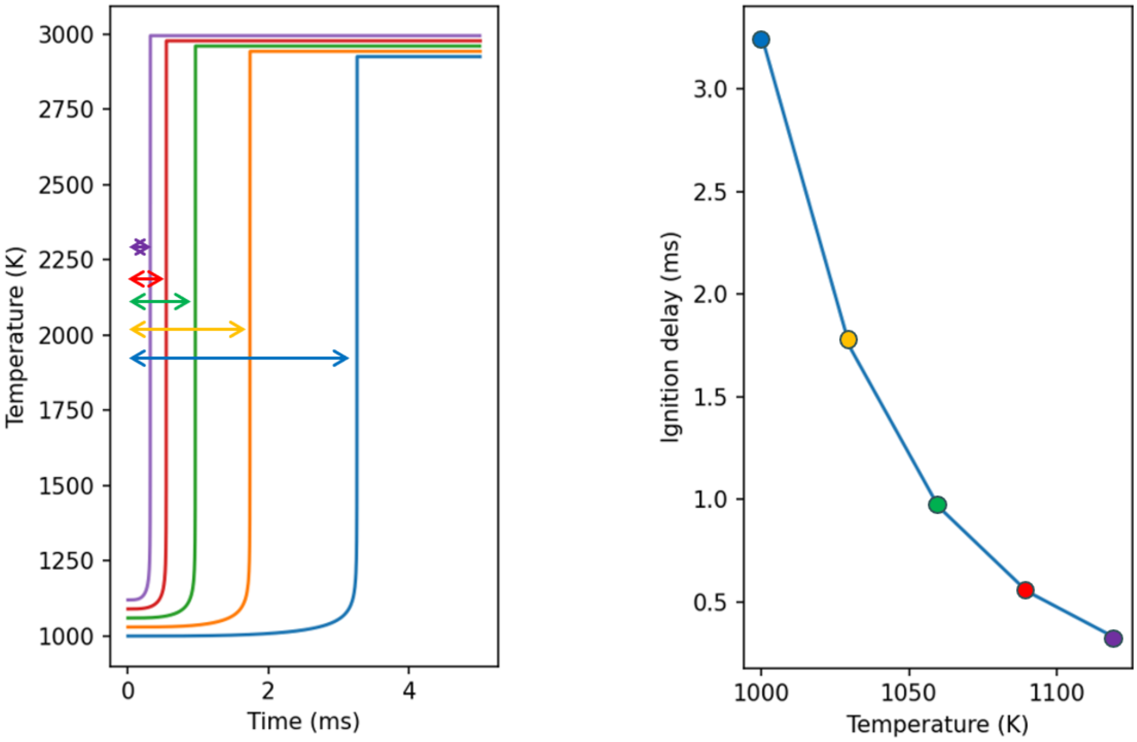


Figure 5: Plotting ignition delay as a function of the initial temperature

2.2 Laminar flame speed

While the 0D-reactor framework was sufficient in the case of the ignition delay calculations, laminar flame speed considerations require using Canteras 1D-reactor networks. The initial conditions and composition can still be defined in a very similar manner as previously.

In contrast to ignition delay, laminar flame speed is a quantity that is directly calculated by Cantera without a need to explicitly define it ourselves.

An example of the code used to determine laminar flame speeds is provided in Appendix 3. It was utilised to make Figure 11.

3 Results

3.1 Ignition delay

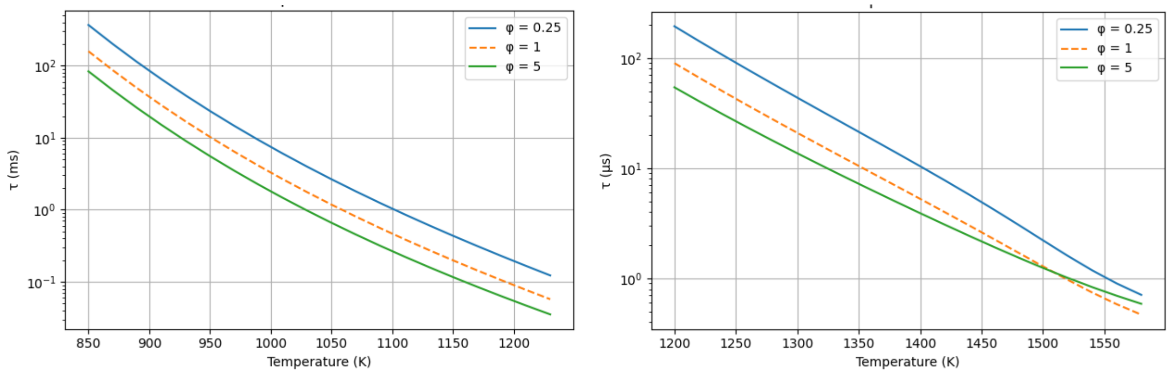


Figure 6: Hydrogen’s ignition delay as a function of temperature at three different equivalence ratios. Temperatures range from 850 K to 1230K (left) and from 1200 K to 1580 K. Pressure is 60 bars.

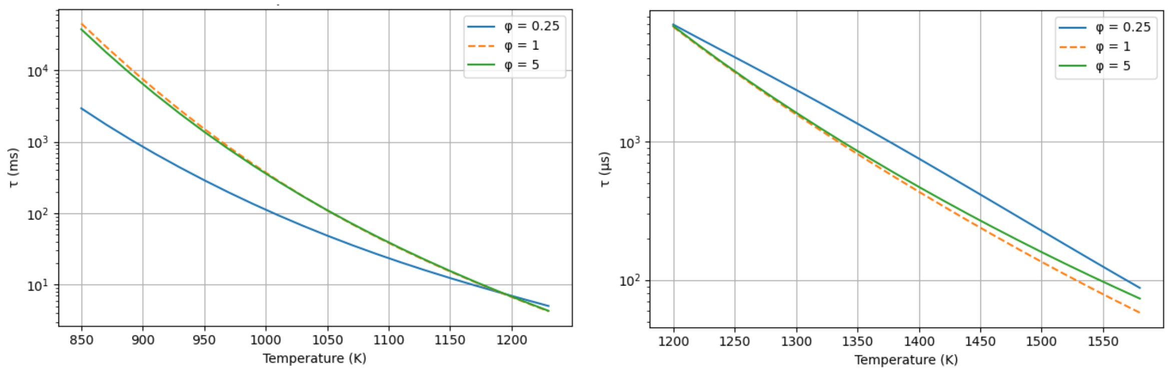


Figure 7: Ammonia’s ignition delay as a function of temperature at three different equivalence ratios. Temperatures range from 850 K to 1230K (left) and from 1200 K to 1580 K. Pressure is 60 bars.

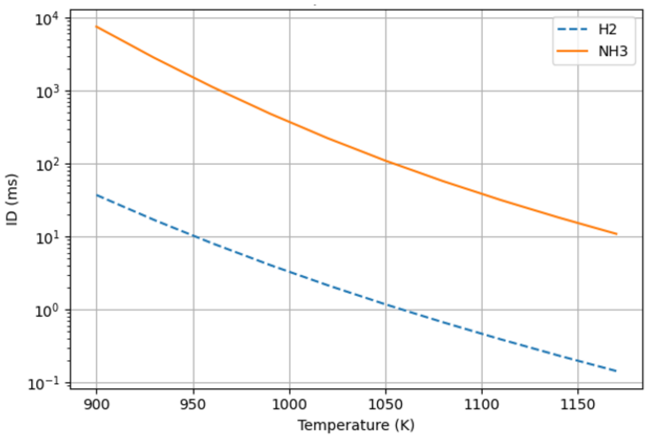


Figure 8: Ignition delay of stoichiometric hydrogen and ammonia mixtures. Pressure is 60 bars.

Figures 6, 7 and 8 showcase ignition delay's temperature dependence for both hydrogen and ammonia mixtures. As expected, ignition delay appears to decrease exponentially as a result of an increase in temperature. Something to note is the considerable disparity between hydrogen's and ammonia's ignition delay at similar conditions. For example, at 900 K with $\varphi = 1$ ammonia's ID is almost 8 seconds while for hydrogen it's just under 40 ms.

Another noticeable difference between the two fuels is the nature in which they respond to changes in equivalence ratio. Hydrogen's ignition delay appears to slightly decrease the richer the mixture is, especially at lower temperatures. For ammonia on the other hand, at lower temperatures the ignition delay is quite significantly shorter for the very lean mixture of $\varphi = 0.25$. This discrepancy between lean and rich mixtures then keeps narrowing as the temperature approaches approximately 1200 K, and from this point forward the lean mixture has a higher ignition delay.

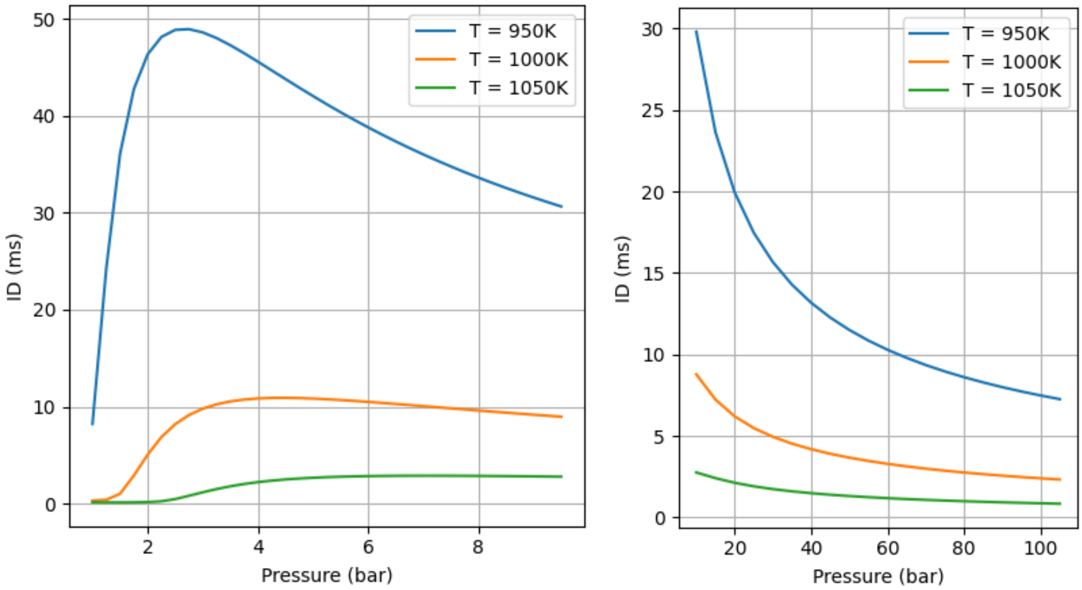


Figure 9: Hydrogen's ignition delay as a function of pressure at three different temperatures. Pressures range from 1 bar to 10 bars (left) and from 10 bars to 110 bars. Stoichiometric mixture.

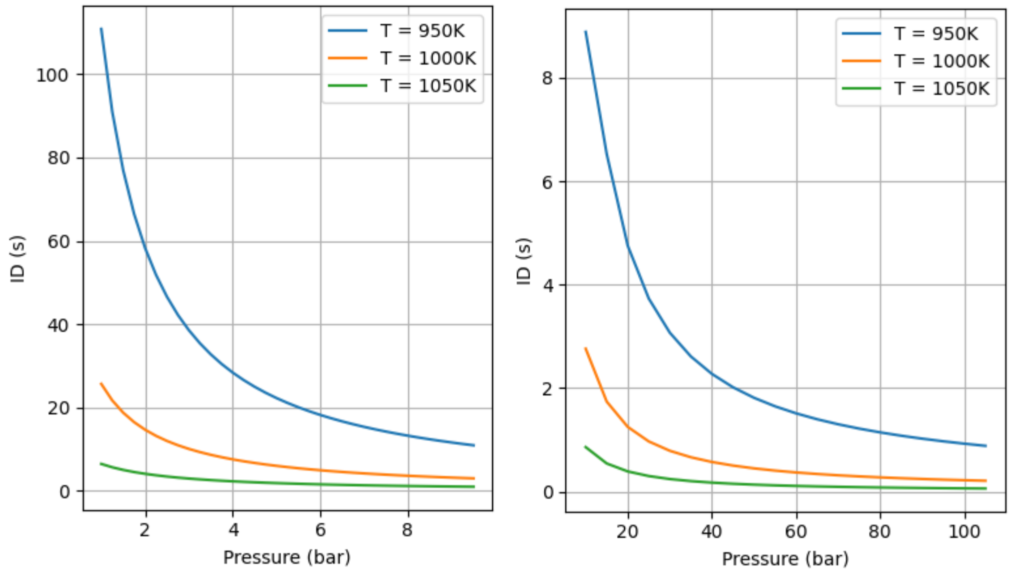


Figure 10: Ammonia’s ignition delay as a function of pressure at three different temperatures. Pressures range from 1 bar to 10 bars (left) and from 10 bars to 110 bars. Stoichiometric mixture.

The effect of pressure on ignition delay is shown in Figures 9 and 10. Both hydrogen’s and ammonia’s ignition delays evidently display a predominant inverse proportionality with increasing pressure. For hydrogen, however, at low pressures this trend reverses and the ignition delay begins to rapidly decrease when pressure is further lowered.

3.2 Laminar flame speed

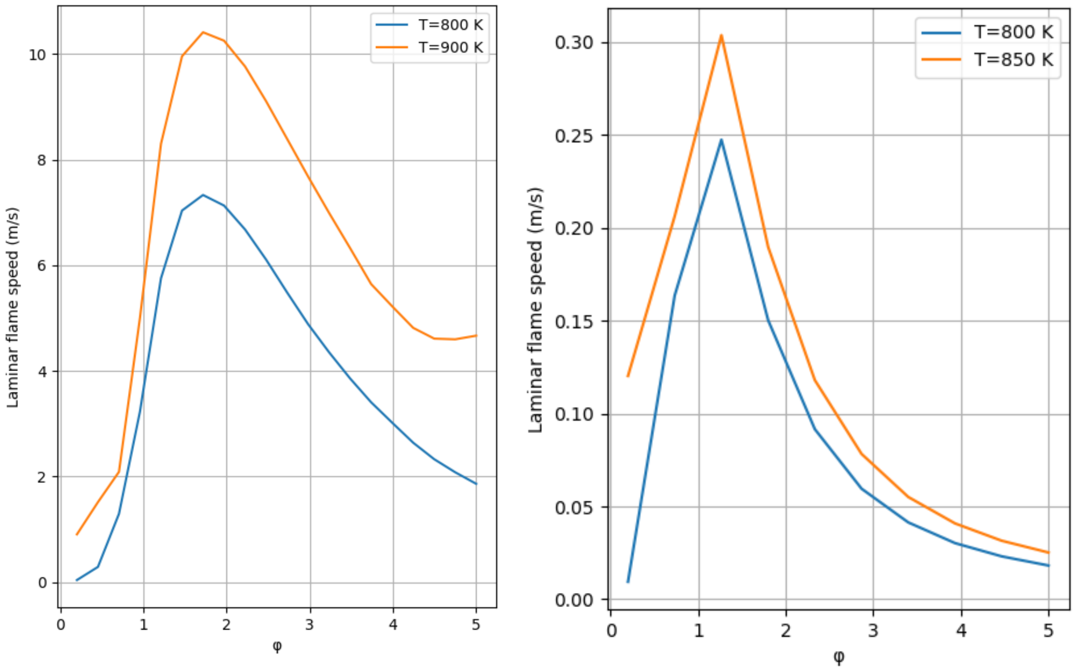


Figure 11: Laminar flame speed of hydrogen (left) and ammonia as a function of equivalence ratio

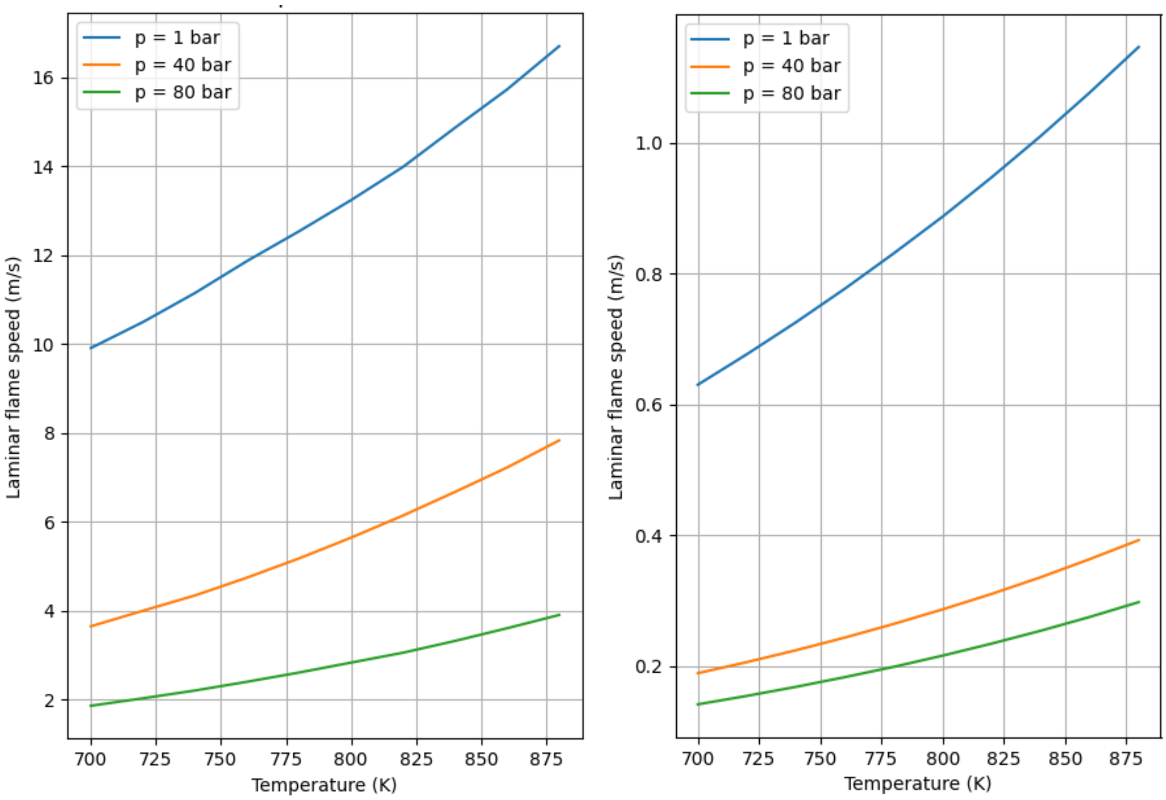


Figure 12: Laminar flame speed of hydrogen (left) and ammonia as a function of temperature

Figures 11 and 12 illustrate the effect of equivalence ratio and temperature on laminar flame speed. In Figure 11 the pressure was set at 60 bars and in Figure 12 the equivalence ratio is 1.

The maximum laminar flame speeds for hydrogen and ammonia appear to be achieved with equivalence ratios of approximately 1.7 and 1.3, respectively. The temperature dependency is seemingly very close to linear. Pressure instead has an inverse effect: as it closes in on atmospheric pressure levels, laminar flame speed increases rapidly.

4 Conclusions

The graphs presented in Section 3 appear to mostly indicate behaviour that is in-line with the studies discussed in Section 1. Based on the numerical Cantera calculations hydrogen expectedly shows mostly preferrable combustion characteristics compared to ammonia. In identical conditions compared to ammonia, hydrogen always had shorter ignition delay and faster laminar flame speed. Hydrogen’s indicated laminar flame speed at low pressures with an equivalence ratio of 1-2 actually appears to be overly high for many applications.

Ammonia mixtures, on the other hand, would need to be pre-heated quite a lot more to accomplish reasonable combustion characteristics. However, not only has this approach been found to increase NOx emissions, but it would also be quite unpractical [2, 4].

Therefore, the optimal fuel wouldn’t necessarily be either hydrogen or ammonia, but rather a blend of the two.

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Appendices

Appendix 1

```
import cantera as ct
import numpy as np

def statemachine(temp = 1000, pressure = ct.one_atm, i=1):
    air = "O2:1,N2:3.76"
    #gas = ct.Solution('example_data/ammonia-CO-H2-Alzueta-2023.yaml')
    gas = ct.Solution('h2o2.yaml')
    gas.set_equivalence_ratio(i, fuel="H2", oxidizer=air)
    gas.TP = temp, pressure
    r = ct.IdealGasConstPressureReactor(gas)

    sim = ct.ReactorNet([r])
    sim.verbose = True

    delta_T_max = 20.
    r.set_advance_limit('temperature', delta_T_max)

    dt_max = 1.e-5
    t_end =  5000 * dt_max
    states = ct.SolutionArray(gas, extra=['t'])

    while sim.time < t_end:
        sim.advance(sim.time + dt_max)
        states.append(r.thermo.state, t=sim.time)
    return states

def ignition_delay(states):
    return np.interp((max(states.T) + min(states.T)) / 2, states.T, states.t)
```

Appendix 2

```
import matplotlib.pyplot as plt
from simthing import statemachine
from simthing import ignition_delay

plt.subplot(1,1,1)

d_t = 20
n_temp_states = 20

ER = [0.25, 1, 5]

for comp in ER:
    temp = 850
    pressure_bar = 60
    states = []
    delays = []
    initialtemps = []

    no = 0
    while no<n_temp_states:
        initialtemps.append(temp)
        s = statemachine(temp, pressure_bar*10**5, comp)
        states.append(s)
        delays.append(ignition_delay(s))
        temp += d_t
        no += 1

    if comp == 1:
        plt.plot(initialtemps, delays, label=f"φ = {comp}", linestyle="dashed")
    else:
        plt.plot(initialtemps, delays, label=f"φ = {comp}")
```

```
plt.xlabel('Temperature (K)')
plt.ylabel('τ (ms)')
plt.yscale("log")
plt.legend()
plt.grid(visible=True)
plt.tight_layout()
plt.show()
```

Appendix 3

```
import numpy as np
import matplotlib.pyplot as plt
import cantera as ct

p = ct.one_atm * 60
T_list = [800, 850]

eq_ratios = np.linspace(0.2, 5, 10)
air = "O2:1,N2:3.76"

width = 0.03
loglevel = 0

#gas = ct.Solution('h2o2.yaml')
gas = ct.Solution('example_data/ammonia-CO-H2-Alzueta-2023.yaml')

plt.clf()
plt.subplot(1, 1, 1)
```

```
for T in T_list:

    Fuel = []
    speeds = []

    for i in eq_ratios:
        gas.set_equivalence_ratio(i, fuel="NH3", oxidizer=air)
        gas.TP = T, p

        f = ct.FreeFlame(gas)
        f.set_refine_criteria(ratio=3, slope=0.06, curve=0.10)

        f.transport_model = 'mixture-averaged'
        f.solve(loglevel=loglevel, auto=True)

        Fuel.append(i)
        speeds.append(f.velocity[0])

    plt.plot(Fuel, speeds, label=f"T={T} K")

plt.xlabel('φ')
plt.ylabel('Laminar flame speed (m/s)')
plt.legend()
plt.grid()
plt.tight_layout()
plt.show()
```