Measuring ON in Fuels

James Harris

When a petrol car is operating normally you will hear a continuous low-pitched engine noise. However, under some circumstances, an engine can make a pinging noise that is quite different from normal. This is known as knocking, and the burning process which leads to this knocking noise can be very damaging to an engine.

Petrol is made from many different components. When a mixture of components is blended to make a fuel, it is important to understand under what conditions this fuel will cause knocking before it is sold to the public. This is done by comparing the test fuel with a reference fuel. If the test fuel knocks with the same intensity as a reference fuel under the same conditions, the test fuel is said to have the same *octane number* as the reference fuel. Reference fuels are simple mixtures of two hydrocarbons, iso-octane and n-heptane, hence the name octane number; a reference fuel with 95% iso-octane has an octane number of 95. High octane number fuels have a low propensity to cause knocking.

During a normal cycle of an internal combustion engine, the spark plug initiates a flame which propagates like a wave through the cylinder. Experiments show that, during a knocking cycle, there is an autoignition in the unburnt gas ahead of this flame. It is generally agreed that this is caused by the compression of the unburnt gas by the flame itself, which increases the temperature sufficiently to cause the gas to explode. The autoignition tends to be local, so a small amount of the unburnt gas starts reacting rapidly, rather than the whole of the unburnt gas burning at once.

To reduce the environmental impact of petrol cars, companies such as BP are starting to blend components from sources other than fossil fuels into their petrol, such as ethanol derived from sugarcane. In this context, a key question is how the different components of a fuel affect its propensity to cause knocking, and thus its octane number. Our overarching aim is to develop a mathematical model to link knocking with fuel composition in order to expedite the development of new, more environmentally friendly, fuels.

Model

As a first step towards understanding knocking, we consider fuel combustion in a 1D tube with closed ends, as shown in Figure 1. It is necessary for the tube to have finite length with closed ends as we want to allow for the compression of the unburnt gas between the end of the tube and the flame. We consider a simple, single-species, exothermic reaction.

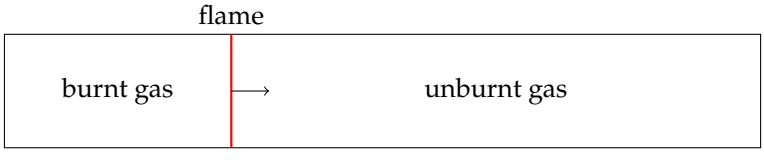

Figure 1 – Schematic of a flame in a tube with closed ends.

At first we model the flame front as a discontinuity, or shock. We specify that the mass, momentum and energy of the gas entering the shock are preserved as the gas leaves the shock. In our case of a reactive gas, we modify the energy condition, so that there is a jump in energy across the shock, corresponding to the energy release due to consumption of reactants. In general, two different behaviours are possible: the flame could propagate supersonically or subsonically relative to the gas in front of it. The flame front observed in an engine is the latter, and is known as a *deflagration*.

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On either side of the deflagration we have to choose how to model the burnt and unburnt gas. One possible assumption is that the gas on either side is unreactive. This makes sense for the burnt gas, since we can assume all the reactant has been used up. In the unburnt gas, the speed of sound in the gas is much larger than the speed of the flame, so we can think of the unburnt gas as being uniformly compressed by the flame, with small pressure fluctuations due to sound waves.

However, this assumption is too restrictive to model knock. Modelling the gas in front of the flame as unreactive precludes the possibility of autoignition. To bring in the possibility of autoignition, we must consider the reaction in the unburnt gas. We assume the rate of reaction is very sensitive to temperature, with faster reaction at higher temperatures. As the reaction is exothermic, this leads to positive feedback, with faster and faster reaction until the reactant starts to deplete. We assume that pressure waves sent into the the unburnt gas raise the temperature. This increases the rate of reaction, thus increasing the amplitude of the pressure disturbance.

The effect of chemical amplification on pressure waves travelling in one direction has been studied before, and, for example, a simple model for the amplification of small amplitude pressure disturbances in a reactive atmosphere has been made by J. F. Clarke in *The Mathematics of Combustion, 1985*. We solve this model numerically and present the results in Figure 2. We assume that the pressure is initially uniform and equal to zero, before the pressure at $x = 0$ is rapidly increased and then sustained. The resulting shock wave in an inert atmosphere, plotted in red, does not grow in amplitude, whereas the shock wave in the reactive atmosphere, shown in blue, grows.

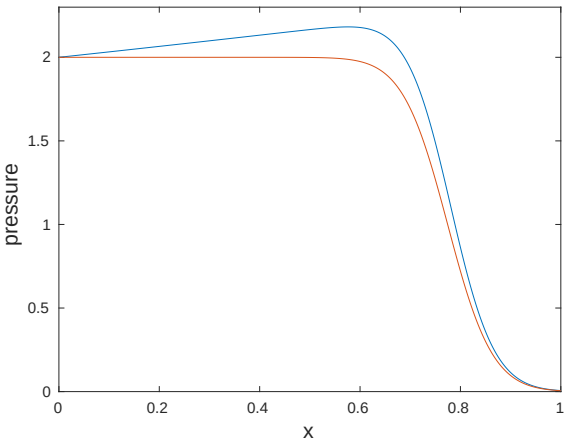

Figure 2 – Growth of a shock due to chemical amplification.

It is important to note that this model is for unidirectional waves. As the gas in our problem is confined, pressure waves will reflect off the closed end of tube and interact with incoming waves. Extending the existing models to incorporate reflected waves presents an interesting mathematical challenge and careful consideration will be needed to incorporate the effects of the boundaries, as well as the interactions between the flame and the sound waves.

Conclusions and Discussion

As an initial building block towards understanding knock, we have implemented a numerical solution of a simple model for pressure waves in a reactive gas. We found that these pressure waves are amplified by the exothermic chemical reaction. We believe this amplification is instrumental in the autoignition which causes knock. Further analysis of this simple 1D model will allow us to determine which parameters influence the onset of knock, and its intensity. These will be related to the physical parameters in the problem. We will then have to adjust our model to consider multi-component fuels by incorporating additional chemical species, as well as reviewing the processes before the engine to determine the correct initial conditions. Insights gained from this model will help further our understanding of how fuel components affect the octane number of a fuel mixture.

Brian Macey, Fuels Advisor at BP, commented:

> *Understanding how new bio components affect octane number is critical to permitting the transition from fossil derived fuels to low carbon fuels. The primary purpose of this mini project is to assess if mathematical modelling methods can be applied to combustion so that the effect of changes in physical and chemical properties of these new components can be predicted. This project has shown us that the development of a 1D model is feasible and the key input conditions are in agreement with inputs identified during previous empirical studies. Further work is required to validate the model with the known effects of bio components such as ethanol.*