# KNOCK PREDICTION WITH REDUCED REACTION ANALYSIS

**Master's thesis**
performed in **Vehicular Systems**

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**TOMAS LIDHOLM**

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**Titel** KNACKPREDIKTION MED HJÄLP AV REDUCERAD REAKTIONSANALYS

Title KNOCK PREDICTION WITH REDUCED REACTION ANALYSIS

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**Sammanfattning**
Abstract

In the report a model using a reduced reaction analysis has been used to see if it is possible to predict knock. The model is based on n-heptane combustion, but it is used for iso-octane. The model was supposed to be able to adapt to different fuels, but it is shown to be unable to do so. Further, the model has been compared to an existing method for predicting knock, known as knock index, to see if any improvements could be made.

When comparing the model to the knock index, it has shown that no big advantages can be found using the new model. It is more time consuming and is not able to work with simulated input, instead of measured. It can however predict if knock occurs with a good reliability, but compared to the knock index it is not an improvement.

**Nyckelord**
Keywords Knock, Combustion, Kinetics, Prediction, Reactions, Engine

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## Thesis outline

This thesis consists of five chapters. The first chapter is an introduction to the problem, and to combustion engines and knock. The second chapter deals with the chemistry that most of the model is based on, explaining the theory used in the model. In the third chapter, the model as it has been used is described, together with a description of how it was implemented in MatLab. The fourth chapter shows the validation of the model, and also different adaptions that was tried to improve the model. In the last, fifth, chapter the results of the model, and a comparison with an existing model, is shown and discussed.

## Acknowledgment

I would like to thank everyone who has helped me get this through to the end. Specially, I want to thank my supervisors, Ylva and Gunnar, for all the help and ideas they have come up with. Further, I would like to thank the people at the Division of Combustion Physics, Lund Institute of Technology, for supplying the model to get me started. I would also like to thank all the people at the Department of Vehicular systems, Linköpings university, for all the help and company they have given me.

# Contents

# Chapter 1

# Introduction

The purpose of this masters thesis is to evaluate the possibilities to use a reduced reaction analysis to predict knock in internal combustion engines. The objective is to find a model that can predict if and when knock occurs for a given pressure curve. This method will be compared to an existing method, known as knock index, to see if the older method can be improved.

There is also an interest to find out more about models of reduced reaction analysis, and whether these can be used without to much loss of accuracy. The method used in this thesis is one of the simplest possible, reducing the number of different reactions taking place to four. Totally there are eight different substances involved.

A notation with all abbreviations and symbols used can be found in the end of the report.

## 1.1 SI-engines

A spark ignited (SI), engine, is the most common type of engine used in modern cars. Other engine types are diesel and Homogeneous Charge Compression Ignition (HCCI), though the HCCI engine is only for research and has not yet reached production. In an SI-engine, self ignition of the fuel is a limiting factor. Self ignition in an SI-engine is commonly referred to as knock. This will be described in section 1.2 but to understand the consequences better, it is best to know the basics of how an SI-engine works. A short description of the basics of an SI engine will be provided, for more information see [10].

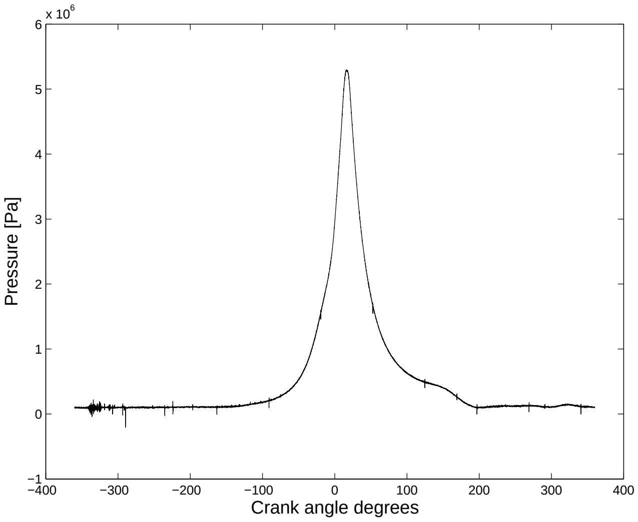

Figure 1.1: A typical plot of the pressure in the cylinder for the four-stroke cycle.

### 1.1.1 The working principle of an SI-engine

The four-stroke cycle is a way of describing the functionality of an SI-engine. The cycle is divided into four parts, taking two full revolutions of the piston. The four parts are intake, compression, expansion and exhaust.

In the intake phase (TDC-BDC) the piston moves down while the inlet valve is open and a mixture of gasoline and air is inhaled into the cylinder. When the piston reaches its lowest position the compression phase starts.

In the compression phase (BDC-TDC) the inlet valve is closed and the piston is moving up, compressing the fuel/air mixture. At a certain point, about 25° BTDC (before TDC), a spark ignites the fuel. As the flame expands through the cylinder the temperature, and hence also the pressure, rises.

When the piston reaches its top position the expansion phase (TDC-BDC) begins. The combustion continues through the beginning of this phase, giving more energy to the system. This is the phase where useful work is put out from the engine. The high pressure in the cylinder pushes the piston down, creating a force that moves the vehicle forward. At the end of this phase the exhaust valve is opened to let all the residual gases out of the combustion chamber.

In the last phase, the exhaust phase (BDC-TDC), of the combustion, the piston moves up, pushing all the residual gases out of the

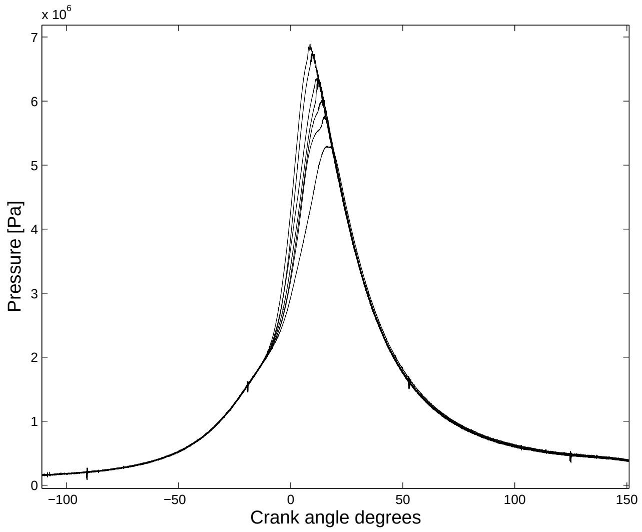

Figure 1.2: Cycle to cycle variations in the cylinder, under steady state conditions

cylinder. When the piston reaches TDC, a new cycle begins. In figure (1.1) a plot of the pressure as a function of crank angle degrees is shown. It starts at −360° (TDC) and is completed two revolutions later, at 360°. The different phases do not have to start exactly at BDC or TDC. These angles are just an approximation. The valves do not open and close at exactly BDC or TDC, but rather close to them.

### 1.1.2 Cycle to cycle variations

The pressure varies a lot between different cycles. This occurs even when the engine is working under steady state conditions, i.e. all controllable parameters are held constant. In figure 1.2, a number of consecutive cycles are shown, and as can be seen, the pressure varies between cycles. According to [10] there are three major reasons why this occurs.

- Variations in the gas motion in the cylinder.
- Variations in the amount of fuel, air and recycled gases causes the amount of energy in the cylinder to vary from one cycle to another.
- Spatial variations in the concentration of air, fuel and recycled gases.

These variations are a problem since they limit engine efficiency and makes it harder to control the engine. Even though the engine is running safely, at operating points that should not cause knock, occasional

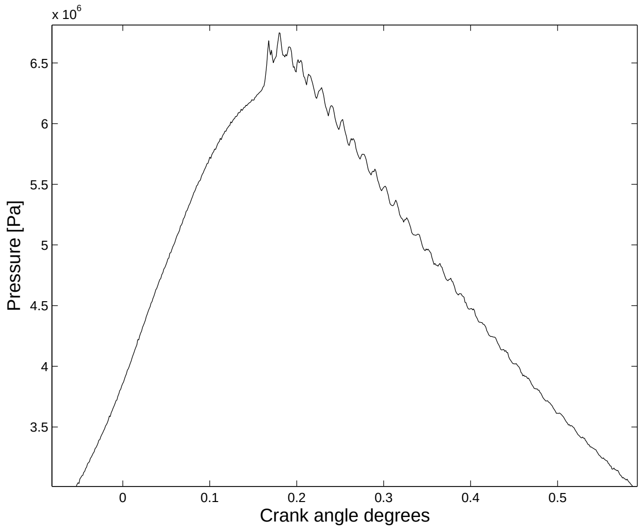

Figure 1.3: A zoomed in pressure curve, where the knock phenomenon is clearly visible.

cycles may have a pressure high enough to cause knock, as explained in section 1.2.

## 1.2 Knock and its consequences

Knock is one phenomenon that is most limiting to engine efficiency. It occurs when the temperature of the unburned gas in the cylinder increases to much, and causes the fuel to self ignite. This will result in an oscillating pressure wave in the combustion chamber. For the driver, this sounds as a number of low thuds. This can be both stressing and agitating, and are therefore dangerous, since the driver will be less focused on his or her surroundings. Knock is also very strenuous for the engine. The high oscillating pressure, as seen in figure 1.3, can cause damage that will in the end lead to a shorter lifetime for the engine. Really severe knock can damage the engine even after only one or a few self-ignitions.

The reason why knock is so interesting is because the optimal operating point of the engine is often in the area where knock will occur. Therefore the ability to predict when knock will occur will make it easier to control the engine towards the optimal operating point.

Running an engine at its optimum has a lot of advantages. The most obvious being that the more efficient the engine runs, the more you can get out of it for the same input. The input in this case is of course gasoline, and therefore an efficient running engine will reduce the amount of gasoline it uses. This will lead to a reduced oil consumption, which is a must since the earths fuel supplies are being depleted. A reduced fuel consumption will also reduce the discharge of pollutants such as $NO_x$ and $CO_2$, which is very good for the environment, and will reduce the contribution to the green house effect.

### 1.2.1 Two-zone models

When modeling knock, a common way is to use a thermodynamic two-zone model. The two zones are for the burned and unburned parts of the air/fuel mixture. The zones are separated by the propagating flame front, that is assumed to be infinitesimal. The two zones have the same pressure, but different temperature and chemical composition. The models include heat and mass transfers between the zones as well as heat transfer to the surroundings. The model used in this thesis is a two-zone model, but since the only interest is in the unburned zone, no model for the burned zone is made. However, when knock occurs, and the fuel in the unburned zone ignites, the gas will no longer be unburned, but it is still treated as a separate zone to simplify the model.

### 1.2.2 Octane and cetane numbers

The octane number is a measure on how likely the fuel is to self-ignite. A fuel that is prone to knock will have a low octane number, and a fuel that is not as likely to knock will have a higher. The number is defined after the two fuels iso-octane and n-heptane. Iso-octane is defined as 100 and n-heptane as 0 on the octane scale. If a fuel has an octane rating of 95, the fuel is as likely to knock as a mixture of 95% of iso-octane and 5% of n-heptane.

The cetane number is the opposite to the octane, in the sense that it has a higher value the more prone a fuel is to self-ignite. There is not, however, any easy correlation between the two values. The cetane number is defined as the octane number, but instead of iso-octane and n-heptane, the definition uses cetane, $C_{16}H_{34}$, a substance that ignites very easy, and alpha-methylnapthalene, $C_{10}H_7CH_3$, a substance that is very hard to ignite. According to [14] , the cetane numbers for iso-octane and n-heptane are about 5 and 60 respectively , but the relation is not linear. More information about the correlation between octane and cetane numbers can be found in [14].

# Chapter 2

# Chemistry

The combustion process can be well described with chemistry and thermodynamics. In this chapter there will be an introduction to the different parts of the chemistry involved. In section 2.1 the non-steady state chemistry, or chemical kinetics, will be brought up, while in section 2.2 the steady state chemistry is discussed. In section 2.3 the more combustion specific chemistry will be discussed. A more thorough explanation of the chemistry involved in combustion can be found in [5].

## 2.1 Chemical kinetics

Chemical kinetics are used to describe a reacting system, where changes occur constantly. A reaction is described by the reactants and products, and a reaction rate, that is a measurement of the speed with which a reaction occurs. A reaction is often written as:

$$A + B \rightleftarrows C + D \tag{2.1}$$

In some cases, the reaction is not very likely to occur in both directions. In these cases, the reactions can be written as one-way reactions on the following form:

$$A + B \rightarrow C + D \tag{2.2}$$

A, B, C and D are arbitrary chemical substances.

The reaction rates are calculated using the Arrhenius function. The forward reaction is described by:

$$k_f = AT^n e^{-\frac{E}{RT}} \tag{2.3}$$

where A, n and E are tabulated values. E is the reactions activation energy, an energy level that the substances must reach to start.

The backward reaction rate can be calculated using the forward reaction rate and the equilibrium concentration for the substance as:

$$k_b = \frac{k_f}{K} \tag{2.4}$$

### 2.1.1 From reaction to equation

To be able to calculate concentrations as a function of time, a method to transform the reactions into differential equations must be used. This method is described at length in [5].

The rate with which the reactions occur depends on two things. The first is the reaction rate, k, from the Arrhenius equation (2.3). The other factor is the concentration of the reacting substances. The higher the concentration the more they react. For an arbitrary reaction

$$A + B \rightleftarrows C \tag{2.5}$$

with reaction rates $k_f$ and $k_b$ the differential equations for the concentrations are formed as

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = -\frac{d[C]}{dt} = -k_f[A][B] + k_b[C] \tag{2.6}$$

As an example, consider the (one-way) reaction:

$$H_2 + M \rightarrow 2H + M \tag{2.7}$$

Here, the substance $H_2$ reacts, or rather collides, with a neutral substance $M$ and splits into two $H$ atoms. $M$ is usually used to represent the total of all molecules in a system and are often a part of a reaction as a catalyst, since many reactions will not occur unless a collision has taken place. The change in concentration of $H_2$ and $H$ molecules can in this case be written as:

$$\frac{d[H_2]}{dt} = -k[H_2][M] \tag{2.8}$$

$$\frac{d[H]}{dt} = 2k[H_2][M] \tag{2.9}$$

where k is the reaction rate for the reaction.

The total reaction rate with which the reaction occurs, in this case $k[H_2][M]$ are often denoted with the Greek letter $\omega$. This is only defined for one-way reactions, and therefore the arbitrary reaction (2.5) will have two different $\omega$-values. One for the forward reaction, $\omega_f$ and one for the backward, $\omega_b$. With this definition equations (2.8) and(2.9) can be written as

$$\frac{d[H_2]}{dt} = -\omega \tag{2.10}$$

$$\frac{d[H]}{dt} = 2\omega \tag{2.11}$$

but equation (2.6) is written as

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} = -\frac{d[C]}{dt} = -\omega_f + \omega_b \tag{2.12}$$

For a more complex system, containing more than one reaction, the differential equation will contain one element for each reaction the substance is partaking in. For example a system with two reactions, 1 and 2. In the first reaction, one molecule of $H_2$ is a reactant, and in the second, one molecule is produced. The expression for calculation of the concentration would then be:

$$\frac{d[H_2]}{dt} = -\omega_1 + \omega_2 \tag{2.13}$$

## 2.2 Chemical equilibrium

If a reaction, or a number of reactions, can go on for a long time, the system will reach chemical equilibrium. Long being from mere milliseconds up to thousands of years, depending on factors such as temperature, pressure and the reacting substances. Chemical equilibrium means that the concentration of the substances are constant. This is not equivalent with a system where no reactions are taking place. There can be a lot of reactions happening, but they will not change the concentration of any substance. That is, for every reaction 'taking' from a substance, another reaction must be 'giving'. The system in equilibrium is affected by outer factors, such as pressure and temperature. Therefore, a system in chemical equilibrium will probably not be in chemical equilibrium if the temperature changes. For more information on how to calculate chemical equilibrium, see [2].

## 2.3 The chemistry of combustion

The combustion of iso-octane is a very complex chemical system. The reactions included in the model in chapter 3 might seem easy and few but in such a reduced system most of the interim stages are disregarded since the substances thus created only exist for a very short time. In total there are over 2500 of these interim substances and they take part in several thousands of reactions. A system this big will be very time-consuming to solve, and therefore a reduction of the system is necessary. There are several possible ways to reduce the reactions, and some of those are discussed in [11, 13]. The model used here are even simpler than those discussed in the mentioned articles. A full review of the chosen model is given in chapter 3.

# Chapter 3

# Model and structure

## 3.1 The model

The model chosen for this application is one of the simplest possible when modeling combustion. It is the four step method found in [9]. This model is based on the combustion of n-heptane and the demands set by Müller [9] is to describe the kinetics of n-heptane combustion as good as possible. The main goal is however to describe diesel fuels, and to do this the cetane number has been included in the model to be able to adapt the model for different types of fuel. Thus it should be possible to use the model when modeling iso-octane combustion. The goal is to have a physically correct model that can discover knock through a change in the chemical concentrations. Especially the amount of burnt fuel should be very different between the cycles with and without knock.

The model involves only four reactions, containing eight substances, and thus giving rise to eight differential equations. The reactions are:

$$n - C_7H_{16} \rightarrow 3C_2H_4 + CH_3 + H \tag{3.1}$$

$$3C_2H_4 + CH_3 + H + 11O_2 + M \rightarrow 7CO_2 + 8H_2O + M \tag{3.2}$$

$$n - C_7H_{16} + 2O_2 \rightleftarrows HO_2C_7H_{13}O + H_2O \tag{3.3}$$

$$HO_2C_7H_{13}O + H_2O + 9O_2 \rightarrow 7CO_2 + 8H_2O \tag{3.4}$$

In addition to the eight differential equations formed from the reactions, a ninth is formed for the temperature. This is a very important part of the model, since the reaction rates are very dependent on the temperature.

There are several different isomers of the substance $HO_2C_7H_{13}O$ but in this model the isomer $n - HO_2C_7H_{13}O$ has been used.

### 3.1.1 Modified Arrhenius expressions

This model does not use the Arrhenius expression described in section 2.1, but a slightly modified version of it, to calculate the reaction rates of the system. For easier overlook, the reactions (3.1) to (3.4) are here denoted reaction 1 to 4, with reaction 3 being split into 3f and 3b, for its forward and backward reaction.

There are two major differences in this model compared to the original Arrhenius expression. The first is that instead of the temperature the pressure is used in the factor that is not in the exponent. The other difference is that in reaction 4 a factor $(\frac{CN}{60})^2$ is included. This is because the model is based on n-heptane combustion, and to simulate another fuel, Müller [9] states that this can be done by changing the cetane number. The cetane number of the fuel is used as input to the CN factor. The cetane number of n-heptane is 60, so in that case the factor is one, but since this model is used for iso-octane combustion, it will have an effect.

The total reaction rates for the reactions are:

$$\omega_1 = [n-C_7H_{16}]A_1e^{-E_1/\tilde{R}T} \tag{3.5}$$

$$\omega_2 = [C_2H_4][CH_3][H][O_2][M]A_2e^{-E_2/\tilde{R}T} \tag{3.6}$$

$$\omega_{3f} = [n-C_7H_{16}][O_2]p^{-1.75}A_{3f}e^{-E_{3f}/\tilde{R}T} \tag{3.7}$$

$$\omega_{3b} = [HO_2C_7H_{13}O][H_2O]p^{-1.75}A_{3b}e^{-E_{3b}/\tilde{R}T} \tag{3.8}$$

$$\omega_4 = [HO_2C_7H_{13}O][H_2O][O_2]\left(\frac{CN}{60}\right)^2 A_4e^{-E_4/\tilde{R}T} \tag{3.9}$$

The values $A_i$ and $E_i$ are

| Reaction | $A$ | $E[kJ/mol]$ |
|---|---|---|
| 1 | $9.0 \cdot 10^{8}$ | 150.0 |
| 2 | $7.0 \cdot 10^{15}$ | 60.0 |
| $3f$ | $1.0 \cdot 10^{20}$ | 160.0 |
| $3b$ | $5.0 \cdot 10^{25}$ | 310.0 |
| 4 | $1.0 \cdot 10^{13}$ | 110.0 |

where the unit of $A$ depends on which reaction it is. The unit of $A_i$ is adapted so that the unit of $\omega_i$ is $mol/(m^3 \cdot sec)$. Thus the unit of $A_i$ is $\left(\frac{m^3}{mol}\right)^{x_i-1}\frac{1}{sec}$, where $x_i$ equals the number of reacting substances in reaction $i$.

### 3.1.2 Temperature

The temperature model is very important, as explained earlier, and it is also the most complex part of the total model. The model used can be found in [1]. The expression for calculation of the temperature is:

$$\rho_u c_{p,u} \frac{dT_u}{dt} = \frac{dp}{dt} - \sum_{j=1}^{N_s} h_j M_{j,u} \sum_{k=1}^{N_r} \nu_{j,k}\omega_k + \alpha \frac{A_w}{V_u}(T_w - T_u) \tag{3.10}$$

In this model the last part, $\alpha\frac{A_w}{V_u}(T_w - T_u)$, is neglected to simplify the model further. The term is a model for the heat loss from the unburned section to the wall of the cylinder. By removing this term, the model probably gets less accurate, and a further improvement of the model might include adding this term back to the equation.

The density of the unburned zone, $\rho_u$ is calculated as:

$$\rho_u = \frac{m_u}{V_u} = p\frac{M_u}{\tilde{R}T_u} \tag{3.11}$$

### 3.1.3 Initial temperature

In the beginning, the initial temperature was set to 400K. The initial temperature can, however, vary and can not be set as constant in a more precise experiment. Such considerations as residual gases must be taken when calculating the temperature. For this experiment this was not of a major importance, and tests were made with different initial temperatures and it was shown that it did not effect the important parts of the model.

### 3.1.4 Specific heat

The specific heat, $c_p$, of a substance is defined as:

$$c_p = \left(\frac{\partial H}{\partial T}\right)_{p,m} \tag{3.12}$$

where H is the free energy of the substance. Due to the definition the specific heat for an entire system is a bit complex to calculate. The correct way to calculate the total $c_p$ for the unburned gases is:

$$c_{p,u} = \left(\frac{\partial}{\partial T}\left(\frac{\tilde{h}_u}{M_u}\right)\right)_{p,m} = \frac{1}{M_u}\left(\frac{\partial \tilde{h}_u}{\partial T}\right)_{p,m} - \frac{\tilde{h}_u}{M_u^2}\left(\frac{\partial M_u}{\partial T}\right)_{p,m} \tag{3.13}$$

where

$$\begin{aligned}
\left(\frac{\partial \tilde{h}_u}{\partial T}\right)_{p,m} &= \sum_i \left(\tilde{x}_i \tilde{c}_{p,i} + \tilde{h}_i\left(\frac{\partial \tilde{x}_i}{\partial T}\right)_p\right) \\
\left(\frac{\partial M_u}{\partial T}\right)_{p,m} &= \sum_i M_i \left(\frac{\partial \tilde{x}_i}{\partial T}\right)_p
\end{aligned}$$

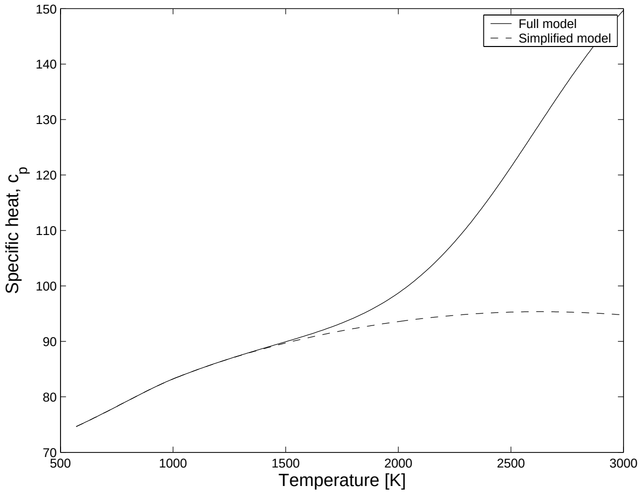

Figure 3.1: Plot of the two models for calculation of $c_p$, where the dashed line is the simplified model

where the symbol  is used to represent the mole fraction. However, for low temperatures this can be simplified to a sum of the specific heat values of the substances multiplied with the fraction of the substance, as

$$c_{p,u} = \sum_i x_i c_{p,i} \tag{3.14}$$

The difference between the models can be seen in figures (3.1) and (3.2). As can be seen the two models are very similar for low temperatures. The relative error of the simplified model is less than 0.01% for temperatures below 1200 K. Temperatures below 550 K are not included in the model since no interesting reaction will take place at such low temperatures.

## 3.2 The program

The program is divided into four distinct parts. The first is a shell, that calls on the other parts, and evaluates the results. The second part is the definition part. This is where all substances and reactions are defined. It also defines which substances and what the concentration of these substances are, when the program starts. The third part takes the information from the definition part and turns it into a number of differential equations, one for each substance and another for the temperature, and the fourth, solver, part uses a numerical solver to

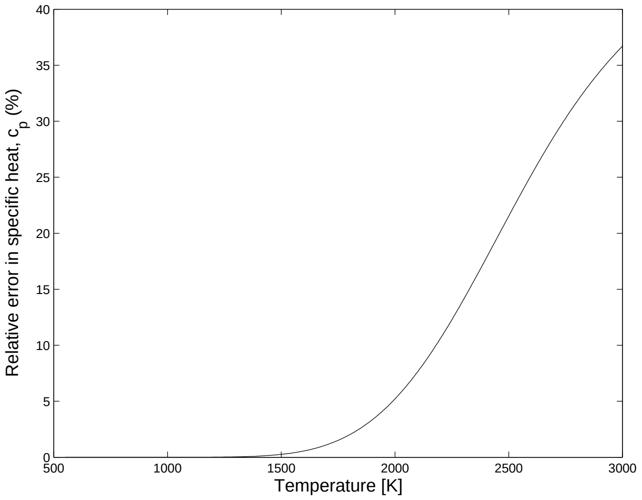

Figure 3.2: Plot of the relative error of the reduced model. As can be seen the models differ very little for temperatures below 1500K and even for temperatures below 2000K the relative error is less then 5%

solve the differential equations. It is the results from these equations that are evaluated by the shell. A scheme of the program is included in figure 3.3.

The program is made to be able to work for any set of reactions and substances selected. It can therefore be used to simulate any model of combustion, not only the one shown in this report. in appendix A a manual on how to use the program can be found.

### 3.2.1 CHEPP

For calculation of chemical equilibrium, CHEPP or CHemical Equilibrium Program Package has been used. CHEPP uses the NASA polynomial form, see [8], to calculate the thermo chemical properties. CHEPP can also be used for calculation of enthalpy, specific heat values and derivate of the concentration, all of which are used in the model described in chapter 3. For more information on CHEPP, see [4].

CHEPP had to be extended slightly for this application, since it did not contain any higher order hydrocarbons. One new specie, the fuel, was added and the molecule parser was expanded to handle more complex molecules. The parameters added was found at [7].

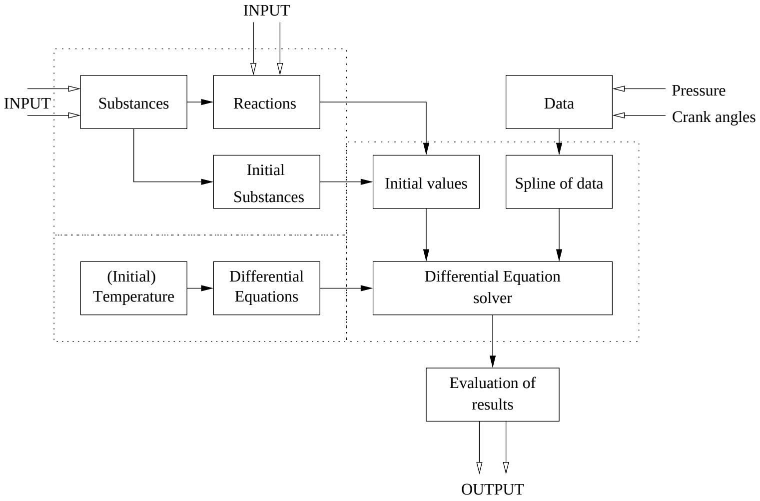

Figure 3.3: Diagram of the basic layout of the program. Boxes within dotted lines are parts of a subsystem.

### 3.2.2 The shell

The shell of the program is dividable into a before and an after part. The first (before) part is the startup of the entire program. The main responsibilities for this part is to make sure that everything is the way it should be. This includes formatting of the data the simulation needs, and starting of external sources, such as CHEPP. When this is done it calls the function that initializes the substances and reactions, and then it calls the solver.

The second (after) part of the shell is where the data from the solved differential equations are evaluated.

### 3.2.3 Definition of substances and reactions

This part of the program is quite straight forward. The substances are set into two vectors. One that contains all the substances taking part in the reactions and nitrogen, $N_2$. The other vector contains the substances that form the initial system, before any reactions have taken place. All substances in the second vector are also included in the first one. In addition to the defined substances, the substance 'M' is added in the end of the first list. This is not a single substance, rather 'M' is used to define the total number of particles in the system. The M-particles are used for calculating the possibility of colliding as described in 2.1.

The reactions are defined using the function `add_reac`. The function is called once for every reaction added. The arguments of the functions are the reacting substances (including their amount), the produced substances (including their amount) and a vector containing the numerical values used to calculate the transfer rates. The function can handle two types of vectors. One with the A, n and E values for the modified Arrhenius function, and one with A, n, E and the cetane-number of the fuel. These are then stored in matrices and vectors. One matrix for all the reacting substances, containing one row for each reaction, and one column for each substance. One similar matrix is created for all the produced substances. Further, there are three vectors, one each to store the A, n and E values of the Arrhenius expression. For the reactions that use the cetane number, that factor is multiplied to the A value and therefore not stored in a separate vector. The big advantage with using this function is that the program becomes easy to supervise, and the adding or removal of new reactions, if the program should be expanded or altered, become much easier. One matter of importance is the definition of reactions that can react in both directions. In the current state of the program, they must be added twice, once for each direction. The function is not defined to understand a two-way reaction.

All of the matrices and vectors created in this file are defined as global variables in Matlab. The reason for this is to give easy access to the stored data from other parts of the program, especially the part that defines the differential equations.

### 3.2.4 Differential equations

The major responsibility of this part is to transform the information from the matrices and vectors created in the previous part into differential equations describing the system. The first step is to calculate the reaction rates, using the A, n and E vectors. This is done by using the modified Arrhenius expression as in section 3.1.1.

The reaction rates was the used together with the two matrices for reacting and produced substances to create a number of differential equations. These equations were created with a number of matrix operations in Matlab. The number of differential equations created is equal to the number of reacting substances. The big advantage with this type of calculation, is that there is no need to change anything in this file when substances and/or reactions are added or removed.

In addition to the differential equations that are defined for each substance, another equation, for calculation of the temperature, is created. It calculates the temperature using equation (3.10). As said in section 3.1.2, the wall heat transfer is not included in the model. The density is calculated using equation (3.11). The enthalpy, specific heat and molar mass are calculated using CHEPP.

The derivate of the pressure is approximized with the function $\frac{dp_k}{dt} = \frac{p_{k+1}-p_k}{t_{k+1}-t_k}$. This is possible since the measured pressure, that is the input to the model, has a very high sample rate, thus creating very small steps $t_{k+1} - t_k$.

### 3.2.5 Solver

The solver contains all the calculations to create initial values for the differential equations. These are calculated using the list of substances created in the definitions part. The initial concentrations of these substances are calculated using the air/fuek ratio determined by the input to the program. It is assumed that the entire cylinder is filled with a mix of the substances found in table 3.1 and the total mass of the different substances can then be calculated. This is then used to calculate the initial concentration, which is considered to be constant throughout the cylinder. The substances chosen are the ones considered to exist pre-reaction. The initial substances are listed in table below.

| Substance | Chemical formula |
|---|---|
| Oxygen | $O_2$ |
| Nitrogen | $N_2$ |
| Fuel | $N_7H_{16}$ |

Table 3.1: Table of the initial substances in the model.

When the initial values for the system have been calculated the solver calls on the differential equations with a numerical solver in Matlab. In this case a stiff solver was used, since there are a lot of different time factors involved. The reaction rates vary very much, and using a non-stiff solver would lead to calculation problems. The solver used in this case is `ode15s`. The results of this operation are then sent back to the shell for evaluation.

# Chapter 4

# Evaluation of model

In figure 4.2 and 4.3 the output from the program is shown, using the original model as defined in section 3.1. In these plots, and in all other plots of this chapter, unless stated otherwise, the same input data has been used. The data is shown in figure 4.1, and it consists of two pressure curves, one with a clear knock and one without. Even though the model has been adapted to be used for iso-octane combustion, these data series, and all other data used to validate the model is generated from combustion of gasoline. The simulation is run with a cetane number of 5, which is the cetane number for iso-octane. These curves are used to be able to get a clear view of the program, since it is very important to be able to separate the cases where knock do and do not occur. When evaluating the results from these two cycles, a distinct difference in the end concentration of n-heptane should be noticeable. The knocking cycle should burn more fuel than the cycle without knock. In the knocking cycle, allmost all fuel should be burnet. The model will later be further validated with data that does not have the clear knock as the one used here in the beginning.

As can be seen in figures 4.2 and 4.3 the two cycles are not easy to tell apart. Both the temperatures and n-heptane concentrations differ only slightly, where they should have a large difference between them. However, in figure 4.3 it is obvious that the two cycles differ in a very important way. The amount of burned n-heptane is greater for the cycle that have knock than for the cycle without. The difference is clear, but it is not what was expected, since the knocking cycle should have nurnet more fuel. The difference can be enough since allmost twice as much fuel is burnt in the knocking cycle. If this is consistent for other cycles this might be a way to detect knock. If a way can be found to increase the gap between the two cycles, this would improve the model.

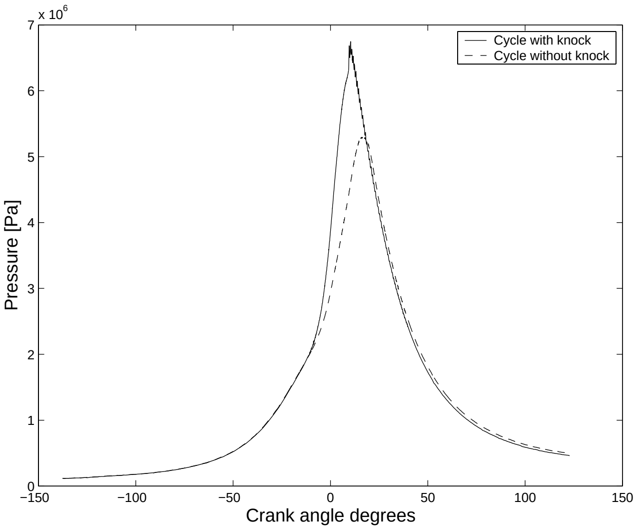

Figure 4.1: Plot of the data used to validate the model, in an initial stage.

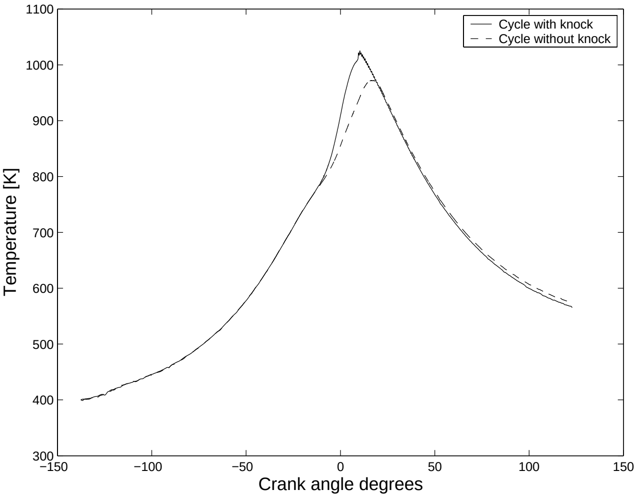

Figure 4.2: Comparison of two temperature curves using the original model. The dashed line, symbolizing a cycle where knock does not occur, should be considerable lower than the other curve, symbolizing a cycle with high knock intensity.

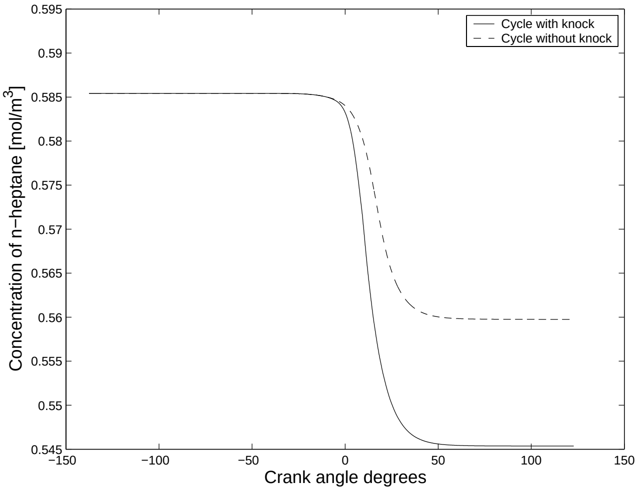

Figure 4.3: Comparison of two curves of the concentration of n-heptane, using the original model. The full line should tend towards zero, since it is a cycle with knock, where the fuel in the unburned section should have self ignited.

## 4.1 Changing parameters

Since there are needs to improve the model, it is important to look at how this can be done. A change of the model itself, by changing the reactions seems rather harsh, and will remove the model very far from its original state. That leaves the parameters of the reactions. If the model is not adapted to use iso-octane as fuel, several parameters may have to be changed, but it is important to try to keep the model as close to its original state as possible.

The parameters of the model that are easiest to change, in the sense that they have the least substantial foundation are the factor $p^{-1.75}$ in equations (3.8) and (3.9) and $\left(\frac{CN}{60}\right)^2$ in equation (3.9). These are factors that Müller [9], without much deduction, have included in the model to correct the errors that occur due to the simplification of the model. Of these two parameters the cetane number is the one that is, according to Müller, the instrument that can be used to adapt the model for another fuel, besides n-heptane. This is therefore the parameter that should be modified before any other.

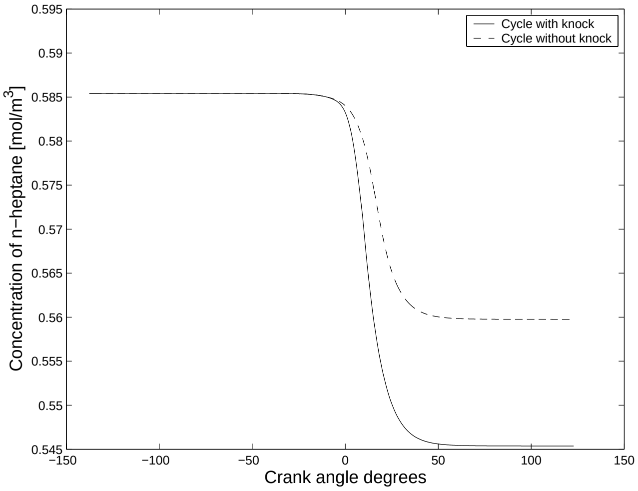

Figure 4.4: Concentration of n-heptane when the cetane number of the model is changed to 1. The other parameters were set to their original values.

### 4.1.1 Changing the cetane number

The initial value of the cetane number, 5, gives a model that is not fully satisfactory since the two curves showing the n-heptane concentration are to similar. As it is now, the two curves differ about 2.5%. Taking into account that these cycles represent the extreme cycles this difference should be greater. For a more satisfactory model the concentration of n-heptane in the knocking cycle should be less than half the concentration in the cycle without knock. Therefore attempts to further adapt the model by varying the cetane number can be done. As can be seen in figures 4.4 and 4.5 changing the cetane number to 1 and 20 does not effect the model.

The concentration of n-heptane is almost unchanged in comparison to the original model, and therefore these changes have no effect. In figures 4.6 and 4.7 a more radical change of the cetane number has been made to further investigate the effect of the cetane number on the model. As can be seen in the figures, even an extremely small or high cetane number has only a marginal effect on the model and therefore the conclusion can be made that the cetane number is not enough to adapt the model for another fuel. The cetane number can work to make small adjustments though, and can be used as a fine-tuning device to make the model good in the end.

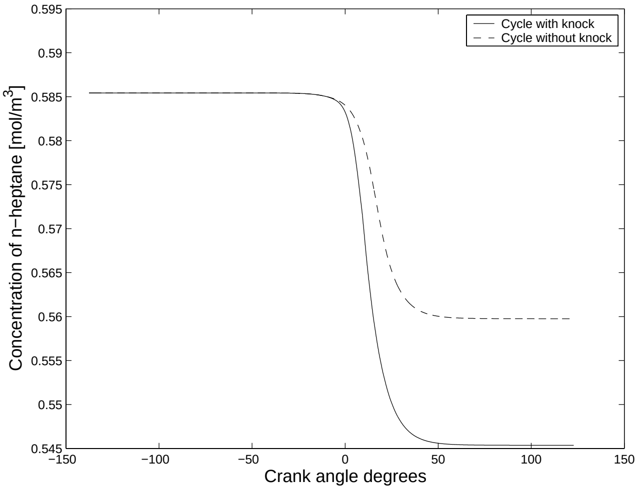

Figure 4.5: Concentration of n-heptane when the cetane number of the model is changed to 20. The other parameters were set to their original values.

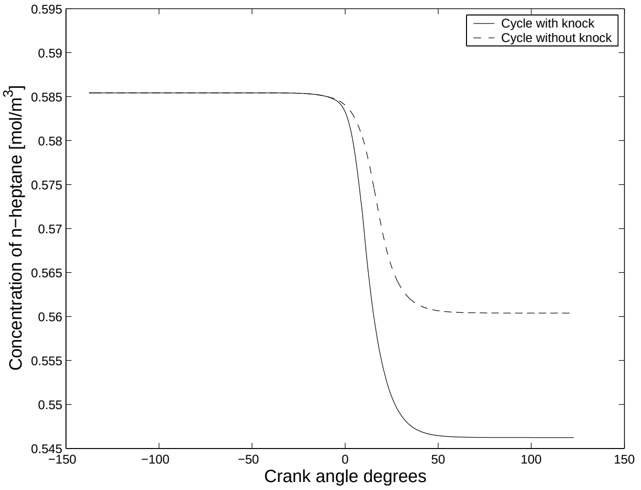

Figure 4.6: Concentration of n-heptane when the cetane number of the model is changed to 0.0001. The other parameters were set to their original values.

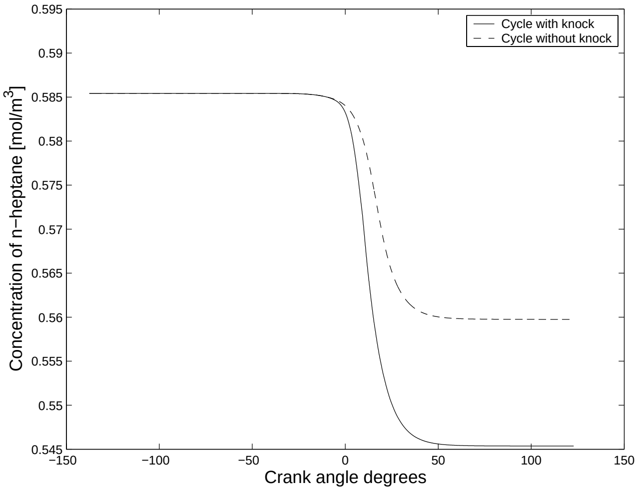

Figure 4.7: Concentration of n-heptane when the cetane number of the model is changed to 10000. The other parameters were set to their original values.

### 4.1.2 Further changes

Since the cetane number had little or no effect when changed, some other parameters have to be modified in order to improve the model. As previously stated the most obvious parameter to change is the pressure exponential in reactions $3_f$ and $3_b$.

By reducing the exponent of the pressure term in reactions $3_f$ and $3_b$ only slightly, from $-1.75$ to $-1.65$ a prominent change is taking place. Not only is the amount of burned n-heptane increased, but the difference between the cycles with and without knock becomes larger. This is shown in figure 4.8. There is also a small difference in the temperature, increasing the maximum temperature for the knocking cycle with approximately $5K$. The temperature increase is not greater since the amount of burned n-heptane is only slightly increased.

In figure 4.9 the pressure exponent has been further reduced to $-1.3$. This has the effect that both the cycles used for examples react to fast, thus burning out all the fuel at a very early stage. This is especially bad for the cycle without knock, since only a limited amount of n-heptane, if any, should be burned there. This fast reaction rate is also clearly visible in the temperature, figure 4.10, where a powerful increase of temperature takes place.

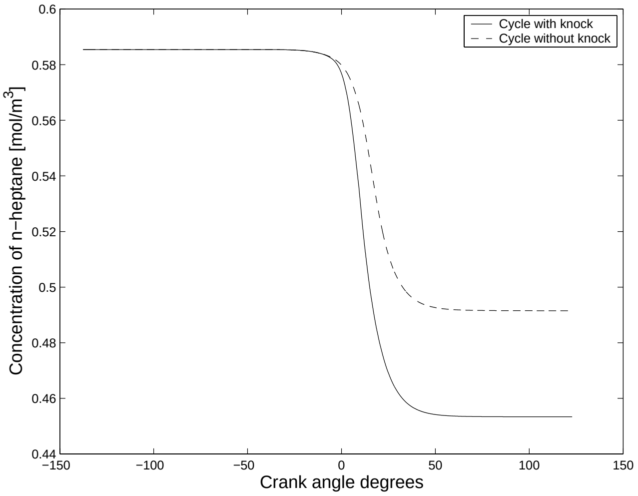

Figure 4.8: Concentration of n-heptane when the pressure exponent in reactions $3_f$ and $3_b$ has been reduced to $-1.65$, but all other parameters are set to their original values. Compared to the original model, a clear difference is noticeable.

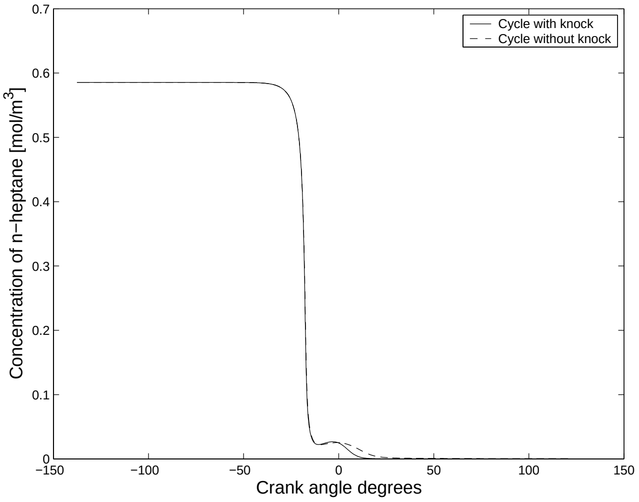

Figure 4.9: Concentration of n-heptane when the pressure exponent in reactions $3_f$ and $3_b$ has been further reduced, but all other parameters are set to their original values. As can be seen the reactions now take place to fast for both the cycles, since all fuel is burned out, even for the cycle where knock does not occur.

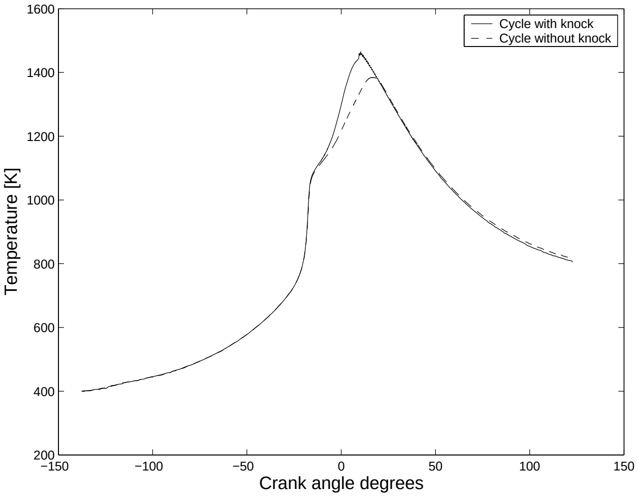

Figure 4.10: Temperature when the pressure exponent in reactions $3_f$ and $3_b$ has been further reduced. A clear self ignition can be spotted for both the cycles, but should only be seen on one of th cycles.

### 4.1.3 Parameter optimization

To optimize the parameters of the model the program `lsoptim` [3] was used. An error function with three parameters was created. The three error parameters was defined as follows:

- Difference between end concentration of n-heptane and a control concentration of n-heptane for the cycle without knock.
- Difference between end concentration of n-heptane and a control concentration for the cycle with knock.
- Time of the knock in the knocking cycle.

To represent the fact that the cycle without knock might consume some n-heptane, and the cycle with knock might not burn all n-heptane, the levels for the optimization was not set to the initial concentration and zero. These levels are not in any way scientifically determined, they are only ad hoc. The levels are chosen only to loosen the demands on the cycles and are therefore set to 0.5 (compared to the initial concentration 0.5856) and 0.1 (compared to 0).

The measured time when knock occurs in the knocking cycle was determined with a function called `knockfcn`, and the time of knock in the model was estimated in MatLab as:

```
min(diff(diff(C_1(:,9))./diff(t_1)));
```

where `C_1(:,9)` is the concentration of n-heptane and `t_1` is the time. The reason for the min operator is because the concentration has a negative slant. Thus the function estimates the biggest difference between two samples of the derivate to the n-heptane concentration. The reason for this modeling of knock time is purely observational. When observing a number of plots on the n-heptane concentration there is a similarity in that there is a break, or direction change, in the curve at the same time as the temperature rises clearly. This break in the concentration curve is able to find using the command line above. The problem with this method is that if there is no break, or bend, in the curve the estimation can place the time of the knock anywhere on the curve. One other problem is that the method is only a variation of detecting knock on the pressure curve itself. This will be described in section 5.2. This can be avoided by using good starting points for the optimization. There is also the factor that if there is no clear time for the knock, the concentration of n-heptane has not been reduced very far, and thus creating a much larger error than the time. Therefore it is a usable method in this case.

### 4.1.4 Optimization method

As described in [3], the method used for optimization of the error function can be described as a minimization of the following expression:

$$V_N(\theta) = \frac{1}{2}\sum_{1}^{N}(y_i - f(x_i,\theta))^2 = \sum_{1}^{N}\epsilon_i(\theta)^2 \tag{4.1}$$

where $N$ is the number of parameters in the model, $\theta$ the values of the parameters, $y_i$ the control values and $x_i$ a penalty vector. The parameters, $\theta$, must have an initial value, $\theta^0$, where the optimization starts.

The function `lsoptim` takes a function that creates the errors $y_i - f(x_i,\theta)$ as an argument as well as the initial values, $\theta^0$.

### 4.1.5 Optimization results

Running the optimization problem with all twelve parameters (the A, E and n values, as well as the cetane number) as variables are a very time consuming process. Therefore a limitation on the number of variables must be made. To begin with, the optimization was run with the two parameters previously tested, to see if there was an optimum that could satisfy the demands. The parameters in the optimization were the cetane number, CN, and the pressure exponent in equations 3.8 and 3.9. The other parameters were set to the original conditions. The initial values of the two parameters were set to the original values, $-1.75$ and 5. To limit the time of the process the program was limited

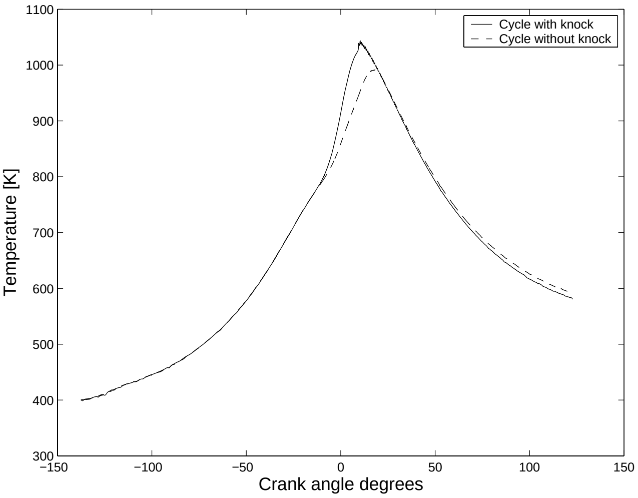

Figure 4.11: Temperature for the optimized model, with 35 iterations

to 35 iterations on the first run. The optimal values produced were:

$$\begin{aligned} n &= -1.6101 \\ CN &= 4.9841 \end{aligned}$$

The results of these values is found in figure 4.11 and 4.12.

The optimization procedure had to run all 35 iterations and because of this probably was not in its optimum. A new optimization was made, allowing the program to run 100 iterations instead, and the optimal values of this run were:

$$\begin{aligned} n &= -1.5744 \\ CN &= 5.2418 \end{aligned}$$

As can be seen in figures 4.13 and 4.14 this gives a different result. The absolute difference between the two curves are almost zero, but the latter optimization values has pushed both curves slightly down, allowing them both to burn more fuel.

The result from 100 iterations was the same as when the program was run with 250 iterations thus giving a good estimate of the optimal values for the program.

### 4.1.6 Changing the A and E values

As stated in section 4.1.3, changing the A and E values are the last thing that should be tried when adapting the model. But since the results in

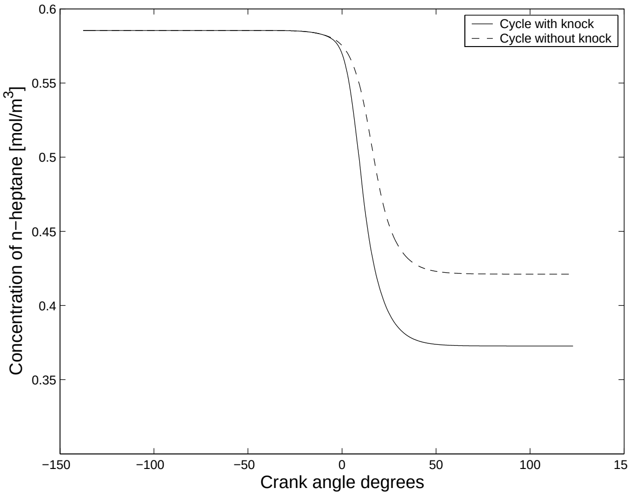

Figure 4.12: Concentration of n-heptane for the optimized model, with 35 iterations

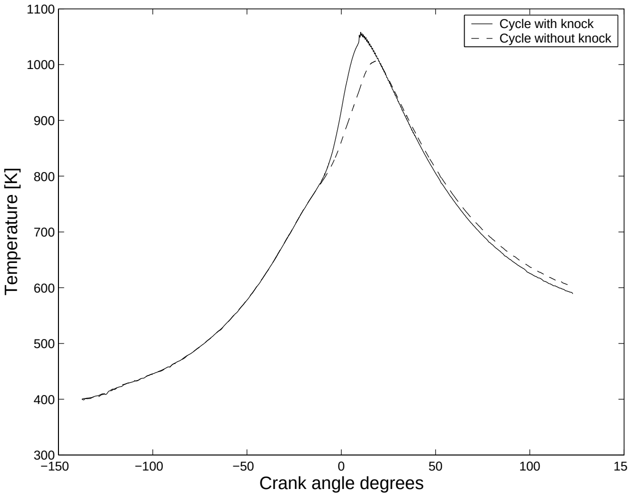

Figure 4.13: Temperature for the optimized model, with 100 iterations

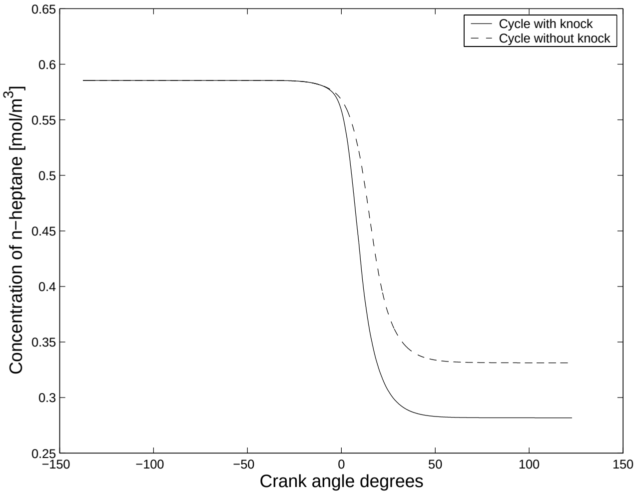

Figure 4.14: Concentration of n-heptane for the optimized model, with 100 iterations

the previous sections are not good enough, the method should at least be evaluated. This could be done using the same optimization method as above, but instead of changing the n and CN values some of the A and/or E values should be parameters to the optimization model. This is however not a satisfactory way of dealing with the problem, since the model contains a large amount of local minima that will stop the optimization process. This is a problem since the model requires large changes in the A and E values to make any difference, and therefore the optimization process will not be effective enough.

The other way of adapting the A and E values is by making a lot of runs, manually changing the values, learning by trial and error method which values that effect the model. But before doing this a plan has to be made on what to change. To do this there consideration to all the factors must be made.

The primary goal of the model is to detect knock. Therefore a wider gap between the n-heptane concentrations of the cycles with and without knock must be created. Since previous tests have shown that changing the parameter $A_4$ (which is the same as changing the cetane number) does not give any large effect on the output, this should be considered stationary. Furthermore, when studying plots of the different interim species, especially $HO_2C_7H_{13}O$ and $CH_3$, the conclusion can be made that most of the fuel is burned by reactions $3_f$, $3_b$ and 4. It is also apparent that the reactions 1 and 2 do not have that big effect on the system and therefore these should be made faster.

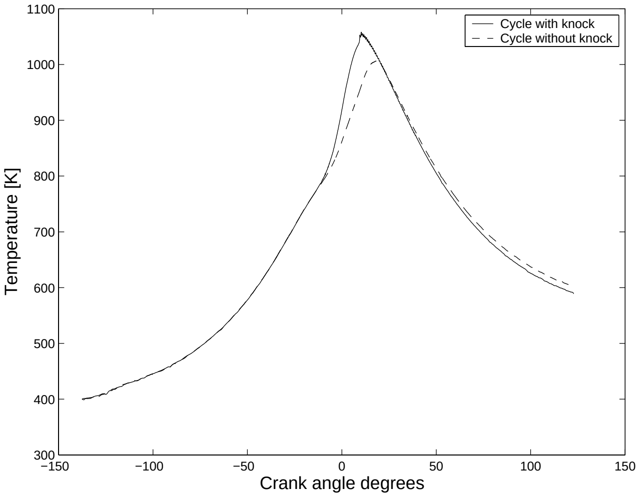

Figure 4.15: Temperature of the adapted model, where $E_1 = 156 * 10^3$ and $A_1 = 4.5 * 10^1 0$

Several tries with different values were made, with both small and big increases of the values and after a while it became apparent that the factors that had the most effect on the system were $A_1$ and $E_1$. A small increase in $E_1$ with only 4% and a bigger change in $A_1$, with a factor 50. Attempts to change the other parameters were made, but the changes in the result were very small, even for very large changes in the parameters. Therefore these parameters were not changed, since it would take the model further away from the original model. The results from this model are shown in figures 4.15 and 4.16.

The optimization program described earlier was tested on this adapted model to find the optimal cetane number and pressure exponent.

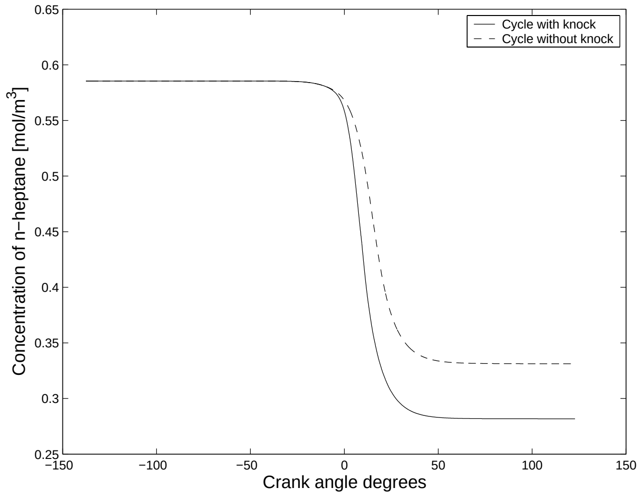

Figure 4.16: Concentration of n-heptane of the adapted model, where $E_1 = 156 * 10^3$ and $A_1 = 4.5 * 10^10$

# Chapter 5

# Analysis

Since the original model gives a clear, if not big, difference between cycles that knock and cycles that do not, it was finally chosen as the model to use. The main reason for this is the fact that in order to get the model better, a big change has to be made to some of the parameters, thus taking the model very far from it's original state. So instead of marginally changing the parameters with no or little effect, the original model is kept. The model should be able to do two things. First it should be able to detect if knock occurs (section 5.1), and second to decide at what time it occurs (section 5.2). In section 5.3 the model is compared to another model for determining knock to see if this is an acceptable method.

## 5.1 Detection

The detection is solved by a check on the concentration of n-heptane at the end of the cycle. If this concentration is below a certain value the cycle knocks. The detection level was decided by looking at several different cycles, figures 5.1, 5.2 and 5.3 show some of these cycles. The level was then set to a values between the cycles with and without knock. The value chosen was a linear function depending on the compression ratio, since the levels of ignited n-heptane was very different for different $r_c$. Thus the level was set to $0.427 + 0.01r_c\ mol/m^3$. Any cycle that has a concentration of n-heptane equal to or higher than this values at the end of the cycle is considered not to have knocked. Cycles with values below this level have knocked.

This method is however not bulletproof. In the border between cycles that knocks and cycles that don't, some cycles will end up on the wrong side of the line. These cycles are the ones with a very marginal knock and since this is barely noticeable the model is set so that all

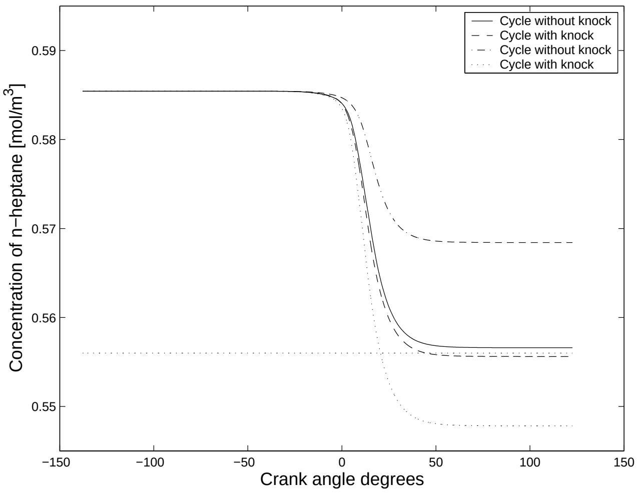

Figure 5.1: Cycles used to validate the model and to decide where the level for knock should be. The dotted vertical line is the limit for knock. $\theta_i = 18°BTDC$, $r_c = 12$.

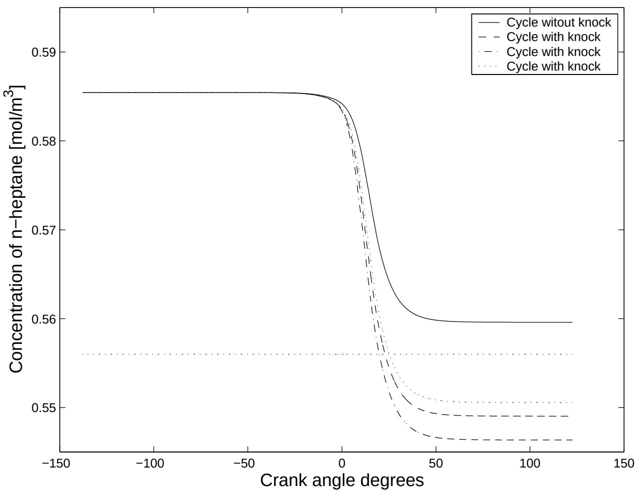

Figure 5.2: Cycles used to validate the model and to decide where the level for knock should be. The dotted vertical line is the limit for knock. $\theta_i = 16°BTDC$, $r_c = 13$.

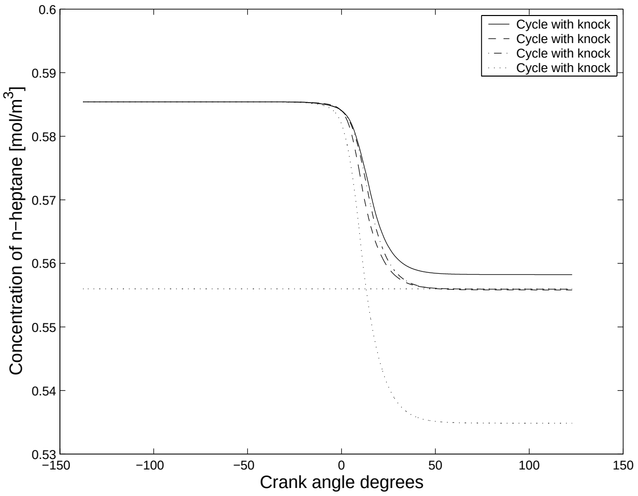

Figure 5.3: Cycles used to validate the model and to decide where the level for knock should be. The dotted vertical line is the limit for knock. As can be seen, one cycle with knock is above the dotted line and will not be detected by the program. $\theta_i = 22° BTDC$, $r_c = 11$.

of these are treated as if they don't knock. An example of this is the cycle in figure 5.3 with the least amount of burned n-heptane. As can be seen in figure 5.4 the knock in the cycle is small and the oscillations barely noticeable.

Even though the method for detecting knock is not perfect, it has a high level of reliability. Most of the undetected cycles are on the limit of being knock and are therefore hard to detect with any method. The difference between these cycles and the ones where the only oscillations are interference from the sensors or other things is very small. Therefore this limitation does not affect the general system all that much and can be accepted as a part of the model.

## 5.2 Time of knock

To determine the time of knock is rather difficult using this model. The best way is to look at the concentration of n-heptane. When knock occurs, the n-heptane will start to burn faster. The derivate of the n-heptane concentration therefore decreases at the same time as the knock starts. This decrease should be easy to find if the knock was obvious, but in this model it is harder. It is found by looking for the biggest difference between two samples of the derivate of the concentration of n-heptane. In MatLab it looks like this:

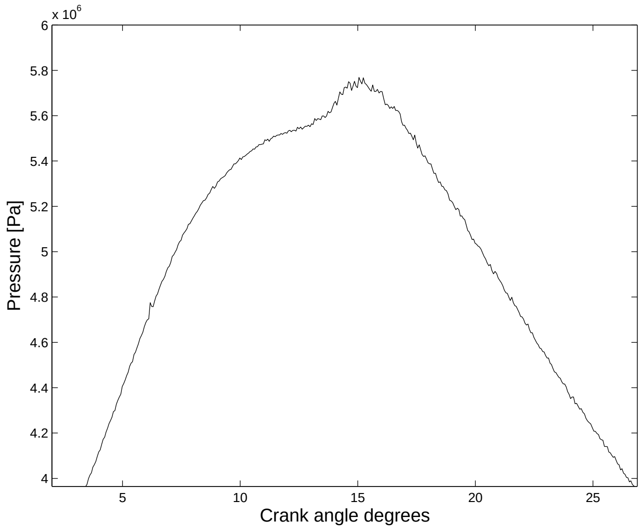

Figure 5.4: A zoom of the pressure curve for a cycle with knock that is not detected by the model.

`min(diff(diff(C)/diff(t)))`

where C is the concentration of n-heptane. As stated previously, this should be easy to find if the knock is obvious, but in this model the knock is quite vague and therefore also this point. However, for most cases the model works with only a difference of less than 2 crank angle degrees. In many of these cases the error is less then 1°. Here consideration must be taken as to when knock really occurs. The model is validated against a function that isolates the oscillations of the pressure curve to determine knock. This method is not exact either, and throughout the process of developing this program the method has in some cases been wrong with more than 1°. In appendix B tables showing the validation series are presented, along with a comparison of this model with knock index, as presented in section 5.3.

There is one big disadvantage with this process. On some occasions the biggest difference is not at the time of knock, but far from it. This is most common in cycles with very little knock. In these cases the program can place the time of knock almost anywhere on the cycle. This is because the biggest difference in the derivate will not be because of the knock, but rather due to some measurement error or disturbance in the data. This can only be verified by looking at the pressure curve itself. Some of these curves will not appear as knocking though. This is explained in the previous section. This will reduce the number of cycles where the knock time is hard to define. The other cycles often

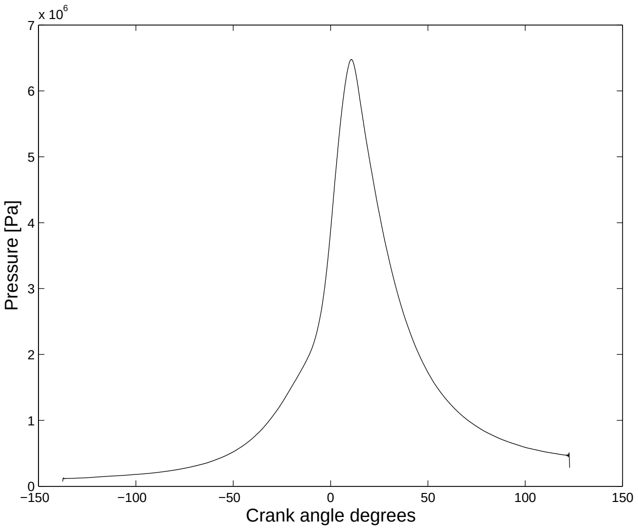

Figure 5.5: A simulated pressure curve.

give results that are very improbable and can therefore easy be found.

The disadvantage when using this method is that it cannot detect the correct knock time without using a real pressure curve as in signal. If using a simulated curve, as figure 5.5, the time of the knock will be much harder to predict. The curve in figure 5.5 is a filtered version of one of the curves used to test the model. The filtering has been done to keep the amplitude of the curve, but to remove the oscillations that appear due to knock. The model should be able to predict the time of knock even from this curve, but instead of giving the correct value, 9.4242 degrees ATDC, it returns the time of knock as 3.2367 degrees ATDC. Since the model is tested with the the non-filtered version of this curve this should be the best result a simulated curve can give, and it is more than 6 degrees wrong.

## 5.3 Knock index

When developing a new method, it is very interesting to compare this to older methods to see if the new method is an improvement of the older ones. One method used to determine the time of knock is known as knock index [6]. Knock index is calculated with the integral:

$$\mathcal{K}(t_i) = \int_{t=0}^{t_i} \frac{dt}{\tau} \tag{5.1}$$

where

$$\tau = Ap^{-n}e^{(B/T)} \tag{5.2}$$

Knock is expected to occur when $\mathcal{K}(t_i) = 1$. As can be seen the expression for calculation of $\tau$ is very like the modified Arrhenius expression used in section 3.1.1.

Sometimes $\mathcal{K}(t_i) = 1$ very late in the cycle, when it is not very likely that it will knock, since it is not enough fuel left. According to Soltic [12], there is an upper limit to how much of the fuel can be burnt and still cause knock. This is because the temperature of the outer layers of the fuel never can rise so high as to cause knock since the cooling effect of the cylinder prevents this. Soltic sets this limit to 75% of the fuel. In appendix B several series of validation data can be found. The data compares the knock index with the model used in this report and verifies both models against the observed time of knock.

# Chapter 6

# Conclusions

The method studied in this report has proven to be fairly reliable when detecting knock. It has, however, difficulties detecting the time of the knock, especially when running the model with a simulated pressure curve. Even when running the program with a real pressure curve, some of the estimations for the knock time is very wrong, sometimes as much as 8 or 10 degrees. The results can be summed up as follows:

+ Predicts if knock occurs with good reliability
+ Can predict time fairly well when using a real pressure curve
- Can not predict time of knock when using a simulated pressure curve
- Some estimations of knock time are very wrong, up to 8 or 10 degrees
- Hard to detect knock in the border between knock and no knock

Of these, the last point is not that serious. The border between knock and no knock is very vague and there can be no expectations on a model of this kind to be able to simulate that with good accuracy. The real big errors fall into this category too. Since there is no clear knock on the pressure curve, there will be no clear knock time either. This normally occurs when the knock is very small.

The other two negative factors are, however, a big disadvantage to the model. The simulation time is much longer then when running a knock index simulation. This could be made faster, but not without reducing the accuracy of the model. The big danger by doing this is that there is a risk of getting negative concentrations, and if this occurs the model will give a really bad result. Compared to knock index the biggest disadvantage is that you cannot use a simulated pressure curve as input to the model. It will be able to detect if knock occurs, but not when, at least not with any accuracy.

On the total, this model is not an improvement over knock index.

The only thing that it might do better is to determine whether knock has occurred or not, but even this is not clear. The small advantages with this model is not enough to use it instead of knock index, since the disadvantages with the model are too great.

## 6.1 Future work

As shown, the model used here was not sufficient to model knock in iso-octane combustion. This does not mean that the model is unusable. Further evaluation of the model when using n-heptane, or diesel, fuel could be tried. As shown above, this will probably give a more satisfying result.

To be able to model iso-octane combustion, a more thorough model might have to be used. At least, the model should be based on iso-octane, and not, as in this case, an adaption of an n-heptane model. It could be used to adapt the existing model, by adding other substances and reactions. If using the same temperature model, this is easy to do. The program in its current state is however not very usable

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# Notation

Symbols used in the report.

## Variables and parameters

| | |
|---|---|
| $t$ | Time |
| $T$ | Temperature |
| $p$ | Pressure |
| $A$ | Constant of the Ahrenius function |
| $n$ | Exponent of the Ahrenius function |
| $E$ | Energy barrier of the Ahrenius function |
| $R$ | Rydbergs constant |
| $k_f$ | Transfer rate |
| $K$ | Chemical equilibrium concentration |
| $M$ | Molemass |
| $c_p$ | Specific heat |
| $h$ | Enthalpy |
| $x$ | Fraction |
| $\omega$ | Total reaction rate |
| $c_p$ | Specific heat |
| $\nu$ | Number of reacting molecules |
| $A_w$ | Wall area of cylinder |
| $V$ | Volume |
| $r_c$ | Compression ratio |

## Abbreviations

| | |
|---|---|
| BDC | Bottom Dead Center |
| TDC | Top Dead Center |
| CN | Cetane Number |

## Operators

| | |
|---|---|
| $[A]$ | Concentration of A |
| $\tilde{A}$ | Mole fraction of A |

## Subscripts

| | |
|---|---|
| $u$ | Unburned |
| $w$ | Wall of cylinder |

# Appendix A

# Manual for the program

The program consists of four files:

```
KnockPrediction.m
CalcCombReac.m
Init_Reac.m
solve_conc.m
```

The first of these `KnockPrediction.m` is the file that is called in a MatLab command window, to run the program. This is done with the command:

```
[t,C,T,T_e,th,t_k]=KnockPrediction(tp_vector,rc,samplerate);
```

There are three inputs to the program, `tp_vector`, `rc` and `samplerate`. `tp_vector` is a two-column matrix, with angles in the first column and pressure in the second. `rc` is the compression rate of the engine for the cycle and `samplerate` is the sample frequency in kHz (a sample frequency of 192000 Hz will thus have an input to the program of 192). The outputs of the system are `t, C, T, T_e, th` and `t_k`. `t` is the time at each sample, with the first sample having time 0. `C` is a matrix with the concentrations for the nine substances at all times in `t`. `T` is a vector of the temperatures during the cycle, and `T_e` is the affect of the chemical reactions on the derivate $\frac{dT}{dt}$. `th` is the crank angles, and should be the same vector as the first column of the input `tp_vector`. Finally, `t_k` is the time of knock in the cycle. `t_k` will be `NaN` if there is no knock.
A summarize of the inputs and outputs in tabular form follows below

| Input | Explanation |
|---|---|
| `tp_vector` | Input data of the system, crank angle and pressure. |
| `rc` | Compression rate |
| `samplerate` | Sample frequency of input data (in kHz). |

| Output | Explanation |
|---|---|
| `t` | Time |
| `C` | Concentrations of the reacting substances |
| `T` | Temperature. |
| `T_e` | Affect of chemical reactions on the temperature. |
| `th` | Crank angle |
| `t_k` | Time of knock (`Nan` if no knock) |

When running the program, an external window will open for Chepp. This will be done in the lowest available figure number of MatLab. It is necessary to have a Chepp version that can handle all the substances in the reactions, or the program will not work. The substances specifically added for this program is $C_7H_{16}$ and $HO_2C_7H_{13}O$.

# Appendix B

# Validation data

The results from the validation of the program is shown below. The first column, observed, is the observed time of knock from a pressure curve. The second column, model, is the result from the model described in this report and the third column, index, is the result when using knock index as described in section 5.3. All values are crank angle degrees an NaN (Not a Number) means no knock has been detected. NaN will never appear in the knock index column since knock index can not decide whether knock has occurred or not, only when it has occurred.

$\mathbf{r_c = 10}$

| Observed | model | Index |
|---|---|---|
| 0.8617 | 3.1117 | 1.6117 |
| -1.8836 | -0.2633 | -1.2008 |
| 1.3617 | NaN | 1.7992 |
| 1.0492 | NaN | 0.5492 |
| NaN | NaN | 0.6117 |
| NaN | NaN | 2.5492 |
| -1.0133 | NaN | -1.1383 |
| 2.5492 | NaN | 3.1117 |
| NaN | NaN | 1.9242 |
| NaN | NaN | 0.7992 |
| NaN | NaN | 2.3617 |
| 5.7992 | NaN | 4.6117 |
| -2.0758 | -1.9508 | -2.4508 |
| NaN | NaN | -0.7008 |
| NaN | NaN | 2.1117 |
| NaN | NaN | -0.1383 |
| 0.3617 | NaN | 0.6117 |
| -0.0758 | NaN | -0.3883 |
| NaN | NaN | 2.1117 |
| 1.1742 | NaN | 0.2367 |

$\mathbf{r_c = 11}$

| Observed | model | Index |
|---|---|---|
| Nan | NaN | 13.6325 |
| 6.9200 | NaN | 5.4825 |
| NaN | NaN | 9.8325 |
| 4.6700 | 5.9200 | 4.8575 |
| NaN | NaN | 10.4200 |
| NaN | NaN | 8.2325 |
| 12.6700 | NaN | 11.0450 |
| NaN | NaN | 9.6325 |
| 9.4325 | NaN | 7.1700 |
| NaN | NaN | 10.6700 |
| 4.8575 | NaN | 4.1658 |
| NaN | NaN | 5.9825 |
| NaN | 15.4825 | 7.4200 |
| NaN | 4.8575 | 11.7950 |
| NaN | NaN | 7.5450 |
| NaN | NaN | 6.6700 |
| NaN | NaN | 13.9658 |
| NaN | NaN | 7.4200 |
| NaN | NaN | 6.6700 |

$\mathbf{r_c = 12}$

| Observed | model | Index |
|---|---|---|
| NaN | NaN | 15.6742 |
| 10.2846 | 5.9868 | 9.4867 |
| 10.8616 | 11.1119 | 9.9867 |
| NaN | NaN | 17.7367 |
| NaN | NaN | 16.5033 |
| 11.4867 | 12.4240 | 10.3617 |
| 8.5697 | 12.4240 | 10.3617 |
| 9.6744 | 10.4868 | 9.1033 |
| NaN | NaN | 12.9867 |
| 13.3700 | 7.1740 | 11.2992 |
| NaN | NaN | 16.0492 |
| 12.0493 | 4.5492 | 9.5700 |
| NaN | NaN | 14.9242 |
| NaN | 8.9868 | 12.1117 |
| 10.6742 | 11.6740 | 10.9867 |
| 13.7699 | 6.9866 | 12.5492 |

$\mathbf{r_c = 13}$

| Observed | model | Index |
|---|---|---|
| NaN | NaN | 22.3700 |
| NaN | 19.3700 | 22.7700 |
| NaN | NaN | 22.9700 |
| NaN | NaN | 20.5492 |
| NaN | NaN | 19.4367 |
| NaN | NaN | 30.6117 |
| NaN | NaN | 20.3617 |
| NaN | NaN | 18.7367 |
| NaN | NaN | 32.7037 |
| NaN | NaN | 21.5492 |
| NaN | NaN | 28.6742 |
| NaN | NaN | 16.2367 |
| NaN | NaN | 20.3617 |
| NaN | NaN | 20.7367 |
| NaN | NaN | 29.1742 |
| NaN | NaN | 19.9033 |
| NaN | NaN | 19.7700 |
| NaN | NaN | 17.6117 |
| NaN | 15.7033 | 22.0492 |