

Numerical simulation of laminar flames  
relevant for a Jet-in-Hot-Coflow burner  
**Bachelor Eind Project**

Naam:	Mike van der Houwen		
Studentnummer:	1321242		
Opleiding:	Technische Natuurkunde		
Begeleider:	Prof. D. Roekaerts	Sectie:	MSP
2de beoordelaar:	Dr. L. Portela		
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# Numerical simulation of laminar flames relevant for a Jet-in-Hot-Coflow burner

Mike van der Houwen — 1321242

Bachelor Thesis,  
Multi-Scale Physics Department

Supervisor: Prof. dr. D. Roekaerts  
Dr. P. Sathiah

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TU Delft

## Abstract

This report investigates the laminar flame speed of a one-dimensional freely propagating Dutch natural gas/coflow flame. This flame is relevant for research on a Jet-in-Hot-Coflow burner, which is created to research a more efficient and less polluting combustion process.

First the laminar flame speed of a methane/air flame has been calculated with two different combustion programs, Chemkin and Cosilab, to validate these programs with experimental results. Secondly the laminar flame speed of a Dutch natural gas/air flame has been investigated to compare different compositions of Dutch natural gas. The main results contain the laminar flame speeds of a Dutch natural gas/coflow flame for two different coflow compositions.

According to the calculated laminar flame speeds the flame in the Jet-in-Hot-Coflow burner would be able to come below the lift-off height, which is where the flame stabilizes. A possible explanation is that in a one-dimensional calculation some factors like strain, curvature and spatial variation of the equivalence ratio are not taken into account. The calculated flame speeds seem to be higher than the axial velocities. More research should be conducted to relate the calculated laminar flame speeds to the experiments.

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# Chapter 1

## Introduction

Combustion has a very important role in our world. The largest part of our worldwide energy support is provided by combustion. Researchers are trying to develop new combustion techniques, which produce more energy, use less fuel, and produce less by-products.

One of the new combustion techniques is Excess Enthalpy Combustion. The products of a combustion process are lead back to the oxidizer to create a new gas mixture. This gas mixture will be used as an oxidizer for the fuel. This technique is more efficient than the regular technique, it also produces less  $NO_x$ . Excess Enthalpy Combustion is used in the Delft Jet-in-Hot-Coflow Burner.

Lots of properties of the Delft Jet-in-Hot-Coflow burner have to be studied. This thesis involves laminar flame speed calculations relevant for the burner. First two computational programs, Chemkin and Cosilab, will be used to calculate the laminar flame speed of a methane/air flame. These results can be validated with experimental and other computational results. Then the laminar flame speed of a Dutch natural gas/air flame will be studied. After that the main results will be shown, the laminar flame speeds of two different coflows with Dutch natural gas.

This bachelor thesis has been done as a part of the Applied Physics Bachelor programme for students of Applied Physics at the TU Delft.

# Chapter 2

## Theory

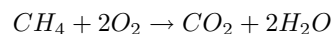
This chapter contains the theory. The chapter starts with parts of combustion theory being discussed. After that flameless combustion and the Delft Jet-in-Hot-Coflow burner will be explained, followed by an introduction to some relevant dimensionless numbers. Next is an explanation of a combustion mechanism. This chapter also contains the governing equations and a broad explanation of the numerical methods and algorithms behind Cosilab and Chemkin.

### 2.1 Combustion

Combustion is a chemical process in which a fuel and an oxidizer react producing new products and heat. This section contains parts of theory about combustion.

#### 2.1.1 Chemical reaction

Together, the fuel and oxidizer are called reactants. In a combustion process the reactants react to create products which differ from the reactants. In a combustion process atoms are not destroyed, however molecules are destroyed and created. The rearrangement of atoms between colliding molecules is called chemical reaction. An example of a chemical reaction is the combustion process of methane ( $CH_4$ ) and oxygen ( $O_2$ ):



The numbers of C, H and O atoms remain the same, but the number of different molecules are not conserved. From the chemical reaction it can be seen that one mole ( $=6.023 \cdot 10^{23}$  particles) of methane reacts with two moles of oxygen to produce one mole of carbon dioxide and two moles of water.

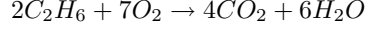
#### 2.1.2 Equivalence ratio

A stoichiometric combustion means that no reactants remain after the combustion process. A combustion is called a lean combustion if any oxidizer remains after the combustion process. In the same way a combustion is called a rich combustion if any fuel remains after the combustion process.

Premixed gases containing fuel and oxidizer are characterized by the equivalence ratio. The equivalence ratio is defined as:

$$\begin{aligned}\phi &= \frac{\text{fuel-to-oxidizer ratio}}{(\text{fuel-to-oxidizer ratio})_{st}} \\ &= \frac{n_{fuel}/n_{oxidizer}}{(n_{fuel}/n_{oxidizer})_{st}}\end{aligned}$$

where  $n_{fuel}/n_{oxidizer}$  is the fuel-to-oxidizer ratio and  $st$  is short for the stoichiometric condition. The stoichiometric fuel-to-oxidizer ratio can be taken from the chemical reaction. As an example the reaction between ethane ( $C_2H_6$ ) and air, which consists of 79% nitrogen ( $N_2$ ) and 21% oxygen ( $O_2$ ). The chemical reaction is:



This means that there should be 7 moles of oxygen for every 2 moles of ethane, which equals to a stoichiometric ratio of  $0.21 \cdot 7/2 = 0.735$  moles of fuel (ethane) for every mole of air.

If the equivalence ratio is lower than 1 the process is a lean combustion and if the equivalence ratio is higher than 1 the process is a rich combustion. Appendix A.1 contains the derivation of a mixture composition from the equivalence ratio.

### 2.1.3 Adiabatic flame temperature

The adiabatic flame temperature is the final temperature after a combustion process takes place in a box with constant pressure, no heat transfer and no changes in kinetic or potential energy. The volume of this box is allowed to change. The adiabatic flame temperature is a good indication of the right boundary (burnt side) temperature of the flame front of a premixed flame.

Since there is no heat loss to the surrounding environment and the box is at constant pressure it follows from the first law of thermodynamics that there is no change in the specific enthalpy. Which means:

$$h^l = \sum_i Y_i^l h_i^l = \sum_i Y_i^r h_i^r = h^r \quad (2.1)$$

where  $h$  is the specific enthalpy in [ $Jkg^{-1}$ ],  $Y_i$  is the mass fractions of species  $i$ ,  $h_i$  the specific enthalpy of species  $i$  in [ $Jkg^{-1}$ ] and  $r$  and  $l$  indicate the right (hot) and left (cold) boundary respectively. At a constant pressure the specific enthalpy of species  $i$  can be written in terms of the specific heat capacity of species  $i$ :

$$h_i^r = h_i^l + \int_{T_l}^{T_{ad}} c_{p,i} dT \quad (2.2)$$

where  $T_{ad}$  is the adiabatic flame temperature in [ $K$ ],  $T_l$  the temperature of the left (cold) boundary in [ $K$ ] and  $c_{p,i}$  is the specific heat capacity of species  $i$  in [ $Jkg^{-1}K^{-1}$ ]. Using 2.1 and 2.2 the adiabatic flame temperature can be determined, if the reactants and products are known.

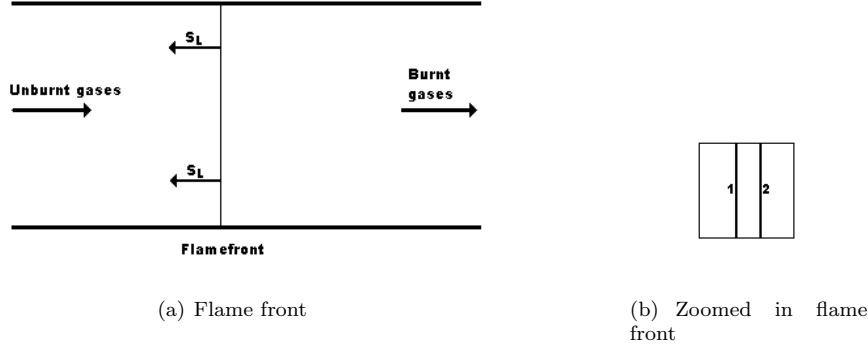
### 2.1.4 Laminar, 1D, premixed, freely propagating flames

In a laminar premixed flame, fuel and oxidizer have already been mixed before the combustion takes place. The laminar part indicates that the flow is laminar, which will be the case at sufficiently low Reynolds number. More information about Reynold's number is in the dimensionless numbers section. An example of a laminar freely propagating flame is a laminar flat flame shown in figure 2.1. This flame can be approached as a one-dimensional flame, because the flame only moves in the x-direction. When the velocity profile of the flame front is computed, the laminar flame speed can be obtained because it is the velocity of the mixture at the cold boundary.

### 2.1.5 Laminar Flame speed

The expansion of the flame front of a flat flame into the unburnt mixture is characterized by the laminar burning velocity or laminar flame speed. The laminar flame speed mainly depends on pressure, the mixture composition and the temperature of the initial premixed gas. The higher the initial temperature, the lower the characteristic time of reaction. This means the reactions will happen faster, increasing the laminar flame speed. How the laminar flame speeds changes with pressure depends on the reaction order. Also it is expected that the laminar flame speed is the highest in stoichiometric conditions, because that is the point





**Figure 2.1** – The left figure illustrates a laminar flat flame. On the left side the unburnt gases are flowing till they reach the cold (left) boundary (1), the region between (1) and (2) is called the flame front and after the flame front the gases flow from the hot (right) boundary (2).  $S_L$  is the flame speed of the flame front. The right figure illustrates a zoomed in version of the left figure on the flame front.

where the most chemical reactions happen. For fuel-rich or fuel-lean conditions less chemical reaction will happen, decreasing the laminar flame speed.

If the laminar flame speed is lower than the velocity of the unburnt gases the flame will blow off. Right before the flame blows off the laminar flame speed is equal to the velocity of the unburnt gases. So the velocity of the unburnt gases at the blow off is a good measurement of the laminar flame speed. The flame speed has also been added in figure 2.1.

### 2.1.6 Soret effect

Species transport happens due to convection, but also due to concentration and temperature gradients. Concentration gradients lead to diffusion and temperature gradients lead to heat conduction. Heat conduction due to temperature gradients is described by the law of Fourier:

$$j_q = -\lambda \frac{\partial T}{\partial x} \quad (2.3)$$

where  $j_q$  is the heat flux in [ $Jm^{-2}s^{-1}$ ],  $\lambda$  the heat conductivity in [ $JK^{-1}m^{-1}s^{-1}$ ],  $T$  the temperature in [ $K$ ] and  $x$  the spatial coordinate in [ $m$ ]. Mass transport due to concentration gradients are described by the law of Fick:

$$j_i = -D_i \rho \frac{Y_i}{X_i} \frac{\partial X_i}{\partial x} - \frac{D_i^T}{T} \frac{\partial T}{\partial x} \quad (2.4)$$

where  $j_i$  is the mass flux in [ $kgm^{-2}s^{-1}$ ],  $D_i$  the diffusion coefficient of species  $i$  in [ $m^2s^{-1}$ ],  $\rho$  the density in [ $kgm^{-3}$ ],  $Y_i$  the mass fraction of species  $i$ ,  $X_i$  the mole fraction of species  $i$ ,  $x$  the spatial coordinate in [ $m$ ],  $D_i^T$  the thermal diffusion coefficient in [ $kgm^{-1}s^{-1}$ ] and  $T$  the temperature in [ $K$ ].

Species transport due to a temperature gradient is also called the Soret effect. The Soret effect is only relevant for species with a low weight (H, He) or at low temperature. For higher weight species and higher temperatures the first term in equation 2.4 will be much higher than the second term, making the Soret effect (second term) not relevant.

## 2.2 Delft Jet-in-Hot-Coflow burner

In this section a brief explanation will be given on flameless combustion and the Delft Jet-in-Hot-Coflow (DJHC) burner.

### 2.2.1 Flameless combustion

A flame loses heat to the environment. Also, there is NO<sub>x</sub> formation which increases with higher flame temperatures. A way to use some of the lost heat is to capture it and use it to preheat the unburnt gases. As a result there will be a higher efficiency. The downside to this increase in efficiency is that the temperature of the flame will be higher. And with a higher flame temperature the NO<sub>x</sub> formation will also increase. This means that the solution is creating more pollution, which is bad for the environment.

Another way to increase efficiency is to recycle the burnt gases. Instead of using air as an oxidizer, the burnt gases will be lead back and combined with air. The new mixture will be the oxidizer. Since the burnt gases carry the heat back, the efficiency will increase. The burnt gases will be lead back, but also carrying a deficit in enthalpy. A deficit in enthalpy will lead to a lower flame temperature, decreasing the NO<sub>x</sub> formation. In this method the NO<sub>x</sub> and soot formation is lower leading to a flame with no red/orange glow. The method is called 'Excess Enthalpy Combustion' because of the deficit in enthalpy or 'Flameless combustion' because you cannot see the flame. Figure 2.2 contains a normal and a flameless flame. The mixture of air and burnt gases that is used as an oxidizer is called coflow.

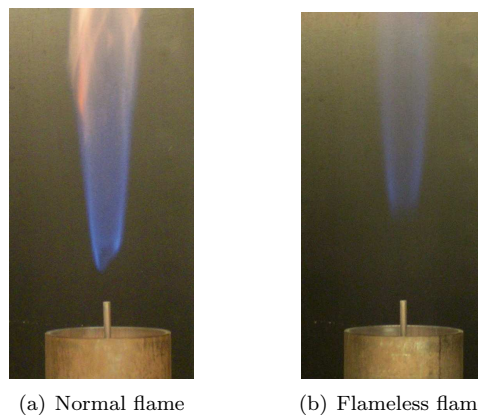


Figure 2.2 – In this figure a normal and a flameless flame are shown.

### 2.2.2 Delft Jet-in-Hot-Coflow Burner

The Delft Jet-in-Hot-Coflow burner has been designed to conduct research on flameless combustion. [7] The DJHC burner has been designed to mimic the burnt gases being lead back into the system. To mimic this situation the DJHC burner consist of two burners. One burner where air is used as an oxidizer and one where coflow is used as an oxidizer. The burnt gases of the first burner have the same composition as the coflow if the gases would be lead back, so the burnt gases from the first burner are lead to the second burner right away. The DJHC burner can be used to measure velocity, temperature and composition of the burnt and unburnt gases.

## 2.3 Mixture fraction

A definition that is used a lot in non-premixed combustion studies is the mixture fraction. The mixture fraction is defined as the fraction of the mixture that originates from the fuel inlets:

$$f = \frac{m_{fuel}}{m_{fuel} + m_{oxidizer}} \quad (2.5)$$

where  $f$  is the mixture fraction and  $m$  is the mass of fuel or oxidizer in the mixture in [kg].

The Dutch natural gas/coflow flame that has been calculated with Fluent uses a mixture fraction based on a Dutch natural gas/air flame. Since the equivalence ratio will be used in the laminar flame speed calculations the right corresponding equivalence ratio to the mixture fraction based on a Dutch natural gas/air flame must be calculated. This is done in two steps. The first step is to calculate the right mixture fraction based on a Dutch natural gas/coflow flame. The second step is to convert the mixture fraction based on a Dutch natural gas/coflow flame to the correct equivalence ratio. The mixture fraction based on a Dutch natural gas/air flame can be rewritten to the mixture fraction based on a Dutch natural gas/coflow flame using:

$$f_{coflow} = \frac{f - fc}{1 - fc}$$

where  $f$  is the mixture fraction based on a Dutch natural gas/air flame,  $f_{coflow}$  is the mixture fraction based on a Dutch natural gas/coflow mixture and  $fc$  the value of the mass fraction  $f$  in the coflow. For DJHC-I-S coflow,  $fc = 0.044$ . A derivation of this formula is found in appendix A.2.

In appendix A.3 it is shown that equation 2.5 can be written in terms of the equivalence ratio:

$$f = \frac{\phi}{\phi + r}$$

where  $\phi$  is the equivalence ratio and  $r$  is the stoichiometric oxidizer-to-fuel mass ratio. This formula will be used to convert the mixture fraction based on a Dutch natural gas/coflow flame to the equivalence ratio based on a Dutch natural gas/coflow flame.

## 2.4 Dimensionless numbers

When doing calculations on transport phenomena it useful to work with dimensionless numbers. Dimensionless numbers usually are a ratio between two fluxes. They are called dimensionless, because they don't have a dimension. This section explains four dimensionless numbers, of which three are used as a measurement of how much diffusion is relevant for a calculation and one is used to check if the flow is laminar.

### 2.4.1 Prandtl number

The Prandtl number is defined as the ratio between momentum and energy transport coefficients in flow systems. The Prandtl number can be written as:

$$Pr = \frac{\nu}{\alpha}$$

where  $\nu$  is the kinematic viscosity in [ $m^2s^{-1}$ ] and  $\alpha$  the thermal diffusivity in [ $m^2s^{-1}$ ]. Since the kinematic viscosity is defined as  $\mu/\rho$  and thermal diffusivity as  $k/\rho c_p$ , the Prandtl number can also be written as:

$$Pr = \frac{\mu}{\rho} \frac{\rho c_p}{k} = \frac{\mu c_p}{k}$$

where  $k$  is the thermal conductivity in [ $Wm^{-1}K^{-1}$ ],  $\mu$  the viscosity in [ $kgm^{-1}s^{-1}$ ] and  $c_p$  the specific heat capacity in [ $Jkg^{-1}K^{-1}$ ]. For gas mixtures the Prandtl number is usually around 0.7 [2] and for an ideal gas the Prandtl number is around 1.

### 2.4.2 Schmidt number

The Schmidt number is defined as the ratio between momentum and mass transport coefficients in flow systems. The Schmidt number can be written as:

$$Sc = \frac{\nu}{D}$$

where  $\nu$  is the kinematic viscosity in  $[m^2s^{-1}]$  and  $D$  the diffusion coefficient in  $[m^2s^{-1}]$ . Since the kinematic viscosity is defined as  $\mu/\rho$  the Schmidt number can also be written as:

$$Sc = \frac{\mu}{D\rho}$$

where  $\mu$  is the viscosity in  $[kgm^{-1}s^{-1}]$  and  $\rho$  the density in  $[kgm^{-3}]$ . For gas mixtures the Schmidt number is usually between 0.2 and 3 [2].

### 2.4.3 Lewis number

The Lewis Number is defined as the ratio between energy and mass transport coefficients in flow systems. The Lewis number is therefore defined as:

$$Le = \frac{\alpha}{D} = \frac{k}{\rho c_p D} = \frac{Sc}{Pr}$$

When the Lewis number is equal to one, the thermal diffusivity and diffusion coefficient are equal. If thermal diffusivity and diffusion coefficient are of the same order, the Soret effect will be relevant for species with low weight (H, He) and at low temperatures. [3]

### 2.4.4 Reynold's number

The Reynold's number is defined as the ratio between inertia and friction of the flow. The Reynold's number is therefore defined as:

$$Re = \frac{\rho v D}{\mu} = \frac{\rho v D}{\mu}$$

where  $v$  is the velocity of the flow in  $[ms^{-1}]$ ,  $\rho$  the density in  $[kgm^{-3}]$ ,  $D$  the characteristic length in  $[m]$  and  $\mu$  the viscosity in  $[kgm^{-1}s^{-1}]$ . A flow is laminar if the Reynold's number is lower than a certain threshold value. A flow is turbulent if the Reynold's number is higher than the threshold. For pipe flow the threshold value is about 2000. [1] Turbulent flow is characterized by stochastic fluctuations, whereas laminar flow is regular.

## 2.5 GRI-Mechanism

A combustion mechanism contains elementary chemical reactions and associated rate coefficient expressions and thermo chemical parameters for species involved in them. A correct mechanism is very important for a calculation. Combustion mechanisms are optimized with experimental results.

The GRI-3.0 mechanism [4] has been optimized for methane and natural gas as a fuel. The conditions for which GRI-Mech 3.0 has been optimized are roughly 1000-2500 K, 10 Torr to 10 atm, and equivalence ratio from 0.1 to 5 for premixed systems.

## 2.6 Governing equations

Modeling of a flame is based on several governing equations. These equations are the continuity equation, species-mass conservation equations, energy equation and ideal-gas equation of state. This section contains an introduction to conservation equations and an explanation of the governing equations. Also assumptions that will simplify the governing equations for a laminar, one-dimensional, freely propagating flame will be made before explaining the governing equations. More insight on the derivations of the governing equations is given in appendix B

### 2.6.1 Conservation equations

A conservation equation contains a variable that is conserved. There are three terms in a conservation equation. The first term is the change of the density of the conserved variable in time, the second term is the change of flux in space and the third term is the source (for example: production) of the conserved variable.

In one dimension a conservation equation for a conserved variable  $X$  looks like:

$$\frac{\partial A}{\partial t} + \frac{\partial B}{\partial x} = C$$

where  $A$  is the density of the conserved variable in  $[[X]/m^3]$ ,  $B$  the flux density of the conserved variable  $[[X]/m^2s]$ ,  $C$  the source in  $[[X]/m^3s]$ ,  $x$  the spatial coordinate in  $[m]$  and  $t$  the time in  $[s]$ .

### 2.6.2 Assumptions

Several assumptions can be made to simplify the governing equations [3]. The assumptions will be made for a laminar, one-dimensional, freely propagating flame.

- External forces like radiation and gravity will be neglected.
- The pressure remains constant through the flame.
- The kinetic energy of the gas flow is negligible compared to other terms in the energy conservation equation.
- The system is continuous, which means that the mean free path of the molecules is small compared to the flame thickness.
- The Dufour effect (Energy flux due to a concentration gradient) is negligible.
- The flame is stationary, which means that there are no temporal changes.
- No heat loss to a wall or other solid objects.

### 2.6.3 Continuity equation

The continuity equation is also called the mass conservation equation. The conserved variable in the continuity equation is the total mass of the gas mixture. Because mass cannot be destroyed or created in combustion, the source is equal to zero. The density of mass is of course the mass density and the density flux is defined by the movement of mass, which is defined as the product of density and mean mass velocity. The continuity equation can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = 0$$

where  $\rho$  is the density in  $[kgm^{-3}]$ ,  $t$  time in  $[s]$ ,  $x$  the spatial coordinate in  $[m]$  and  $v$  the flow velocity in  $[ms^{-1}]$ .

### 2.6.4 Species-mass conservation equation

Another conserved variable is the mass of the species. The density of the mass of a species is given by the partial density of species  $i$ . The flux is given by the product of the partial density and the mass velocity of species  $i$ . Since species can be destroyed or created in a reaction, there is also a term source term. The species-mass conservation equation can be written as:

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial (\rho Y_i v_i)}{\partial x} = r_i$$

where  $\rho$  is the density in  $[kgm^{-3}]$ ,  $Y_i$  the mass fraction,  $t$  the time in  $[s]$ ,  $v_i$  the mass velocity of species  $i$  in  $[ms^{-1}]$ ,  $x$  the spatial coordinate in  $[m]$  and  $r_i$  the chemical rate of production in  $[kgm^{-3}s^{-1}]$ .

In appendix B.2 it is shown that the equation can be rewritten to:

$$\rho \left( \frac{\partial Y_i}{\partial t} + v \frac{\partial Y_i}{\partial x} \right) = - \frac{\partial}{\partial x} (j_i) + r_i, \quad i = 1, \dots, I$$

where  $v$  is the mean mass velocity in  $[ms^{-1}]$  and  $j_i$  the diffusion flux of species  $i$  in  $[kgm^{-2}s^{-1}]$ , which is given in equation 2.4.

### 2.6.5 Energy equation

The energy equation is based on the conservation of enthalpy of the mixture. The density of enthalpy is given by the sum of the products of specific enthalpy and partial density of the species. The enthalpy flux is given by the movement of the density of enthalpy and a heat flux caused by transport of energy due to temperature gradients. [3] Since energy is conserved the source term is zero. The conservation of enthalpy equation is written as:

$$\sum_i \frac{\partial}{\partial t} (\rho Y_i h_i) + \sum_i \frac{\partial}{\partial z} (\rho v_i Y_i h_i) + \frac{\partial j_q}{\partial z} = 0$$

where  $t$  is time in  $[s]$ ,  $\rho$  the density in  $[kgm^{-3}]$ ,  $Y_i$  the mass fraction,  $h_i$  the specific enthalpy of species  $i$  in  $[Jkg^{-1}]$ ,  $x$  the spatial coordinate in  $[m]$ ,  $v_i$  the mass velocity in  $[ms^{-1}]$  and  $j_q$  the heat flux in  $[Jm^{-2}s^{-1}]$ . In appendix it is shown that the equation can be rewritten to:

$$\rho c_p \left( \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) - \frac{dT}{dx} \sum j_i c_{p,i} - \sum_{i=1}^I h_i Y_i$$

where  $c_p$  is the specific heat capacity at constant pressure in  $[Jkg^{-1}K^{-1}]$ ,  $c_{p,i}$  the specific heat capacity of species  $i$  at constant pressure in  $[Jkg^{-1}K^{-1}]$ ,  $T$  the temperature in  $[K]$ ,  $\lambda$  the heat conductivity of the mixture in  $[JK^{-1}m^{-1}s^{-1}]$  and  $j_i$  the diffusion flux of species  $i$  in  $[kgm^{-2}s^{-1}]$ .

### 2.6.6 Ideal-gas equation of state

The ideal-gas equation of state is simply the ideal gas equation:

$$p = \rho \bar{R} T \sum_{i=1}^I \left( \frac{Y_i}{W_i} \right)$$

where  $p$  is the pressure in  $[Pa]$ ,  $\rho$  the density in  $[kgm^{-3}]$ ,  $R$  the gas constant in  $[Jmol^{-1}K^{-1}]$ ,  $Y_i$  the mass fraction and  $W_i$  the molecular weight of species  $i$  in  $[kgmol^{-1}]$ .

## 2.7 Boundary conditions

To solve the governing equations boundary conditions have to be used. Boundary conditions have to be imposed to the mixture density, temperature and mass or molar compositions of all species relevant in the combustion process. First the computational region has to be defined. The calculation will be done in the flame front, the width of the flame front is in the order of millimeters. The computational region is illustrated in figure 2.1, where the computational region is the region between the left and right boundary, (1) and (2).

Boundary conditions have to be imposed on the hot and cold boundary. The cold boundary is on the left side, it is the where the unburnt gases are coming in the computational region. The hot boundary is on the right side, it is where the burnt gases leave the computational region. If there is no heat loss a change of temperature only occurs in the computational region, therefore the temperature gradient should be zero

at the hot and cold boundary. This also holds for the mass or molar fractions of the different species. Most of the time it suffices to make sure that the temperature, mixture density and mass or molar fractions are constant on the cold boundary. The boundary conditions become:

$$T = T_{unburnt}, Y_i = Y_{i,unburnt} \text{ at } x = x_{left}$$

$$\frac{\partial T}{\partial x} = \frac{\partial Y_i}{\partial x} = 0 \text{ at } x = x_{right}$$

To make sure that the profiles are fixed in the computational domain a fixed temperature at a fixed position should be added. A temperature  $T_0$  is given to a position  $x_0$ , at approximately one third of the computational domain. The temperature  $T_0$  is usually about 100 degrees Kelvin higher than the temperature of the unburnt gases.

$$T = T_0 \approx T_{unburnt} + 100 \text{ at } x = x_0$$

There is no boundary condition needed for the velocity. The velocity at the cold boundary is equal to the flame speed and is obtained as a result from the calculation.

## 2.8 Solution method for 1D laminar flames

The relevant solution method for 1D laminar flames is to first impose the boundary value problem by discretizing by finite difference approximations, by yielding an algebraic set of equations. The system of algebraic equations can be solved by the damped modified Newton algorithm. The modified damped Newton algorithm is explained in 'Numerical modeling of turbulent natural-gas diffusion flames' by Peeters [12].

### 2.8.1 Chemkin/Cosilab differences

The difference between Chemkin and Cosilab is that Cosilab tries to solve the solution directly. Chemkin uses a two-step procedure [5]. The first solution uses the initial temperature profile as given and fixed. It only solves for the species composition and velocity profile. The second solution adds the energy equation to go to the final solution. The two-step procedure is usually more efficient than solving directly.

Another big difference of Chemkin and Cosilab is the number of input values. Chemkin doesn't need the species profiles, only needs an estimated peak of intermediate species, unreacted mole-fractions and product mole fractions. Cosilab requires an input of all species profiles, which takes a lot of time to create.

# Chapter 3

## Validation

In this chapter the results from calculations with Cosilab and Chemkin will be validated. First the flame speed of the well-known methane/air flame with an initial premixed gas temperature of 298K will be calculated and validated with experimental results. Secondly the flame speed of the Dutch natural gas/air flame will be calculated to see if the results are the same for Cosilab and Chemkin, and to check if there are any differences between the two different Dutch natural gas compositions.

### 3.1 Methane/Air Flame 298K

In this section the laminar, one-dimensional, premixed, freely propagating methane/air flame will be studied. First the adiabatic flame temperatures will be calculated to get a good guess for the hot boundary temperature. After that the flame speed of the methane/air flame at 1 atmosphere and with a cold boundary of 298K will be calculated with Cosilab and Chemkin. The results will be validated with experimental and other computational results. Also a study is done on whether diffusion does, or doesn't affect the laminar flame speed. The fuel used in a methane/air flame is of course methane  $CH_4$ . The oxidizer that is used is air, which is composed of 21% oxygen  $O_2$  and 79% nitrogen  $N_2$ .

#### 3.1.1 Adiabatic flame temperature

The adiabatic flame temperature can be used as a good guess for the hot boundary temperature. The adiabatic flame temperature has therefore been computed for a methane/air premixed gas with pressure at one atmosphere and the temperature of unburnt mixture at 298 degrees Kelvin. The flame temperatures have been computed for different equivalence ratio's, ranging from 0.7 to 1.3 in steps of 0.1. The results are given in table 3.1.

#### 3.1.2 Flame speed calculation with Cosilab

The laminar flame speed has been computed with Cosilab. The first step was to create a good input profile for an equivalence ratio of 1, using the adiabatic flame temperature as a guess for the right boundary. The left boundary temperature was set at 298 degrees Kelvin and the composition of the left boundary was set at the composition of methane/air for an equivalence ratio of 1.

After getting a solution for  $\phi = 1$ , the laminar flame speed for other equivalence ratio's were found by setting up a batch process. In this batch process the output profile of a  $\phi = 1$  solution was used as an input profile for a  $\phi = 1.1$  calculation. Afterwards the output profile of a  $\phi = 1.1$  solution could be used as an input profile for a  $\phi = 1.2$  calculation and so on. The results are given in table 3.2

The laminar flame speed could not be computed for  $\phi < 0.6$  and  $\phi > 1.3$ . Part of this can be explained by the flammability limits. The flammability limits of methane are 5-15 volume % [8] which matches an



Equivalence ratio [-]	Adiabatic flame temperature [K]
0.7	1837
0.8	1995
0.9	2133
1.0	2225
1.1	2210
1.2	2136
1.3	2056

**Table 3.1** – This table contains the adiabatic flame temperatures of different methane-air compositions. The adiabatic flame temperatures are given in [K].

Equivalence ratio [-]	Laminar flame speed [ $ms^{-1}$ ]
0.6	0.1243
0.7	0.2061
0.8	0.2778
0.9	0.3386
1.0	0.3769
1.1	0.3812
1.2	0.3404
1.3	0.2497

**Table 3.2** – This table contains the laminar flame speed of different methane-air compositions computed with Cosilab, for a left boundary temperature of 298 Kelvin and at a pressure of 1 atmosphere. The laminar flame speed is given in [ $ms^{-1}$ ].

equivalence ratio of  $\phi = 0.5 - 1.7$ . Outside the flammability limits it is not possible to create a flame at standard conditions. It seems like Cosilab is not able to solve the problem for an equivalence ratio of  $0.5 < \phi < 0.6$  and  $1.3 < \phi < 1.7$ .

### 3.1.3 Flame speed calculation with Chemkin

The laminar flame speed has also been computed with Chemkin. An example of a Chemkin input file can be found in appendix D. The same steps as in the Cosilab calculation were followed. First the stoichiometric solution was found ( $\phi = 1$ ) and afterwards the lean and rich mixtures were solved in a batch process starting from the stoichiometric solution. The results are given in table 3.3

The laminar flame speed could not be computed for  $\phi < 0.6$  and  $\phi > 1.4$ . Part of this can be explained by the flammability limits. The flammability limits of methane are 5-15 volume % [8] which matches an equivalence ratio of  $\phi = 0.5 - 1.7$ . Outside the flammability limits it is not possible to create a flame at standard conditions. It seems like Chemkin is not able to solve the problem for an equivalence ratio of  $0.5 < \phi < 0.6$  and  $1.4 < \phi < 1.7$ . Chemkin is able to solve a greater range of  $\phi$  than Cosilab.

In figure 3.1 the temperature profile of methane air flame in stoichiometric conditions is shown. The figure also contains the molar fraction profiles of species  $CH_4$ ,  $O_2$ ,  $CO_2$  and  $H_2O$ .

### 3.1.4 Flame speed comparison

The laminar flame speed computed with Cosilab and Chemkin can be compared to the experimental data from Egolfopoulos et al. [10] In figure 3.2 the laminar flame speed is plotted against the equivalence ratio.

Equivalence ratio [-]	Laminar flame speed [ $ms^{-1}$ ]
0.6	0.1018
0.7	0.1895
0.8	0.2776
0.9	0.3504
1.0	0.3952
1.1	0.4027
1.2	0.3560
1.3	0.2533
1.4	0.1355

**Table 3.3** – This table contains the laminar flame speed of different methane-air compositions computed with Chemkin, for a left boundary temperature of 298 Kelvin and at a pressure of 1 atmosphere. The laminar flame speed is given in [ $ms^{-1}$ ].

The results of Chemkin and Cosilab have been added to the figure. The figure also contains the results from Egolfopolous et al, vanMaaren et al, GRI Mech 3 optimalization and of a base mechanism.

It can be concluded that both Chemkin and Cosilab are sufficient to calculate the flame speed of a laminar methane/air flame. The results are within a 10% range of the GRI Mech 3 optimalization line. This is as expected, because the GRI 3.0 Mechanism has been used for the calculations in Chemkin and Cosilab. It must be noted that Chemkin is able to solve a greater range of equivalence ratio than Cosilab.

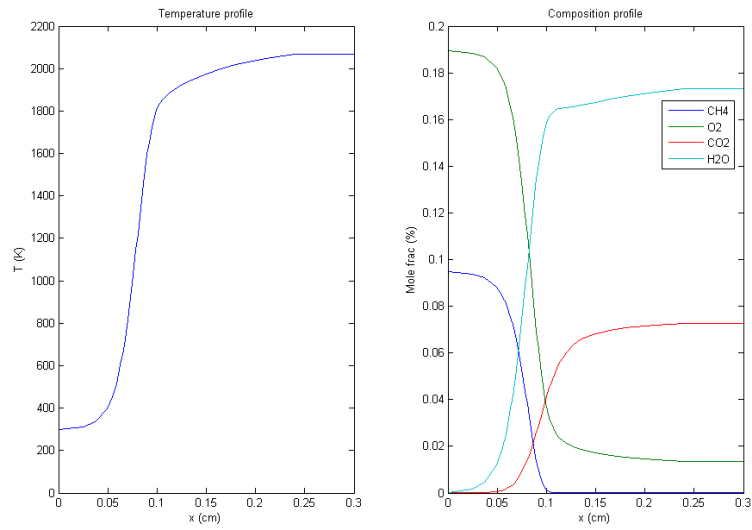
### 3.1.5 Soret effect

The results in the paragraphs above are calculated with the Soret effect not being neglected. In this section the laminar flame speed calculated with and without neglecting species mass diffusion due to a temperature gradient will be compared. These calculations have been done in Cosilab. Table 3.4 is an extended version of table 3.2. It contains the equivalence ratio and laminar flame speed of methane/air at 298K and 1 atm, with and without the Soret effect.

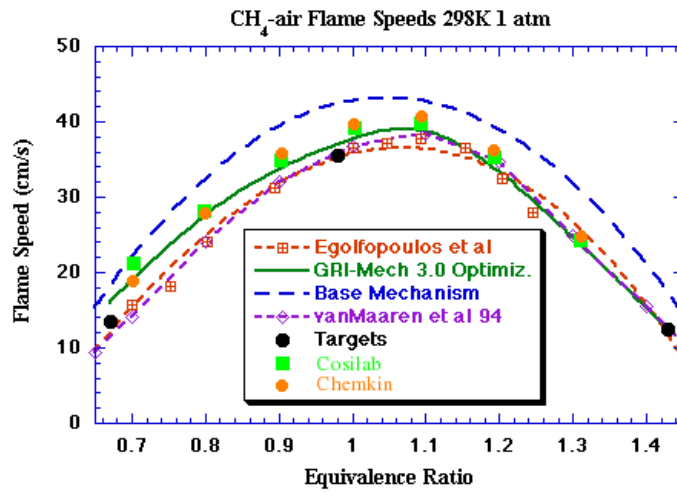
Equivalence ratio [-]	Laminar flame speed [ $ms^{-1}$ ]		Difference [%]
	Soret effect	No Soret effect	
0.7	0.2061	0.2066	0.24
0.8	0.2778	0.2804	0.93
0.9	0.3386	0.3426	1.17
1.0	0.3769	0.3819	1.31
1.1	0.3812	0.3858	1.19
1.2	0.3404	0.3443	1.16
1.3	0.2497	0.2555	2.27

**Table 3.4** – This table contains the laminar flame speed of different methane-air compositions computed with Cosilab, for a left boundary temperature of 298 Kelvin and at a pressure of 1 atmosphere, with and without neglecting the Soret effect. The laminar flame speed is given in [ $ms^{-1}$ ].

As expected from the theory the Soret effect doesn't have a great impact on the results. The relevant molecules in the methane/air combustion process are heavy, making the Soret effect not relevant. The biggest difference is smaller than 2.5%, hence the Soret effect will be neglected in the other calculations.



**Figure 3.1** – The left figure contains the temperature profile of a methane/air flame in stoichiometric conditions. The right figure contains the molar fraction profiles of species  $CH_4$ ,  $O_2$ ,  $CO_2$  and  $H_2O$ .



**Figure 3.2** – This figure contains the laminar flame speed calculated with Cosilab and Chemkin. The results are compared with experimental data from Egolfopoulos et al.

## 3.2 Dutch Natural Gas

In this section the laminar, one-dimensional, freely propagating Dutch natural gas/air flame will be studied. Two different compositions of Dutch natural gas will be used. First the adiabatic flame temperatures will be calculated for both compositions. After that the flame speed will be calculated with Chemkin and Cosilab. Results will be compared with each other, but because of a lack of data the results will not be validated with experimental results.

### 3.2.1 Different compositions

Dutch natural gas is composed of mainly methane and nitrogen. But also higher alkanes, like ethane and propane are present in Dutch natural gas. In this thesis two simplified compositions of Dutch natural gas will be used. One is the most used simplified composition, which consists only of methane and nitrogen. The other composition is more complicated and also consists of ethane and has a small fraction of oxygen and carbon dioxide. The compositions are shown in table 3.5.

Component [-]	NG-C2 [mol%]	NG-C1 [mol%]
CH4	81.29	85.3
C2H6	3.89	-
N2	14.26	14.7
O2	0.01	-
CO2	0.89	-

**Table 3.5** – This table contains two different Dutch natural gas compositions called NG-C2 and NG-C1.

### 3.2.2 Adiabatic flame temperature

The adiabatic flame temperature has been calculated for several mixtures of Dutch natural gas and air using the two different compositions introduced in the previous subsection. The calculations have been done with Cosilab for different equivalence ratio's [0.6-1.3] and also different values of the unburnt gases [300-1000K]. The results are shown in figure 3.3. In the appendix there also tables available containing the adiabatic flame temperatures.

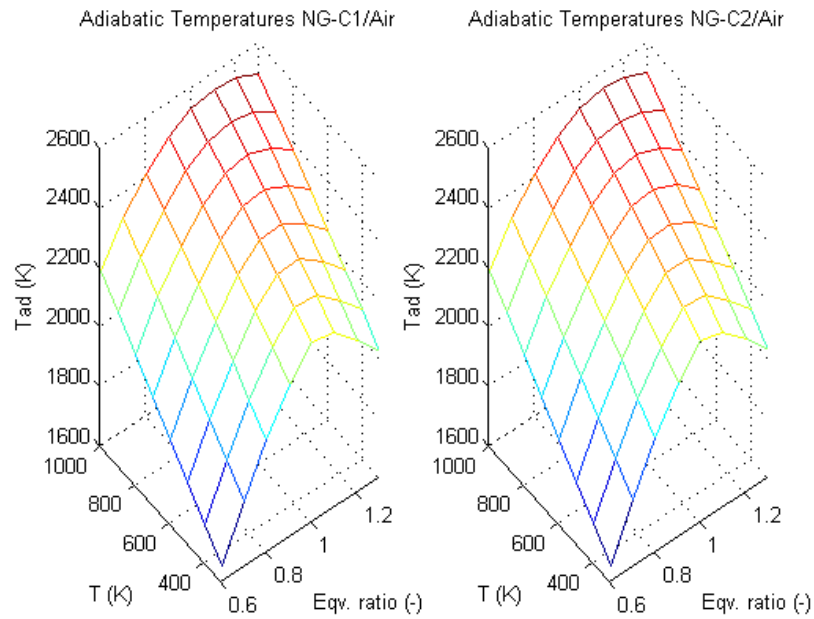
The adiabatic flame temperatures of both compositions are almost the same. The adiabatic flame temperatures of the NG-C2 composition are only 1-3 Kelvin higher than the NG-C1 composition. The highest difference is 3 Kelvin or 0.15 %, the absolute difference (and therefore the difference in percentages) tend to decrease with a higher temperature of the unburnt gases. This is as expected, because the two Dutch natural gas compositions were chosen to meet these adiabatic flame temperature criterion.

The results show that the highest adiabatic flame temperature as a function of the equivalence ratio is found around the stoichiometric composition for the lower initial temperatures of the unburnt gases. For higher initial temperatures of the unburnt gases the highest adiabatic flame temperature is found in the fuel-rich regions.

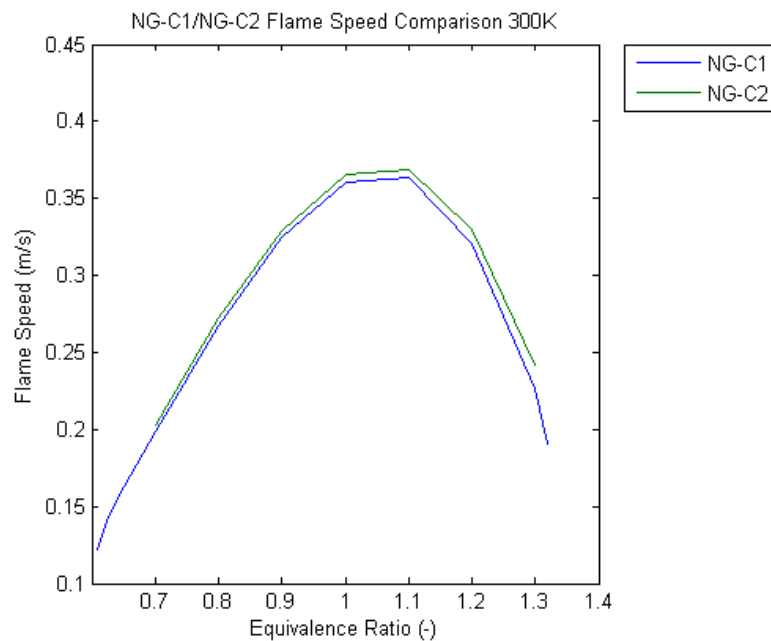
### 3.2.3 Flame speed calculation with Cosilab

The flame speed has been calculated with Cosilab for different compositions of Dutch natural gas and air. The first calculation has been done for an equivalence ratio of  $\phi = [0.7 - 1.3]$  with the premixed gas (unburnt gases) at 300 Kelvin. For an equivalence ratio of 0.7, 1.0 and 1.3 the flame speed has also been calculated with the temperature of the premixed gas at 400-1000 Kelvin. The results are shown in figure 3.4 and 3.5.

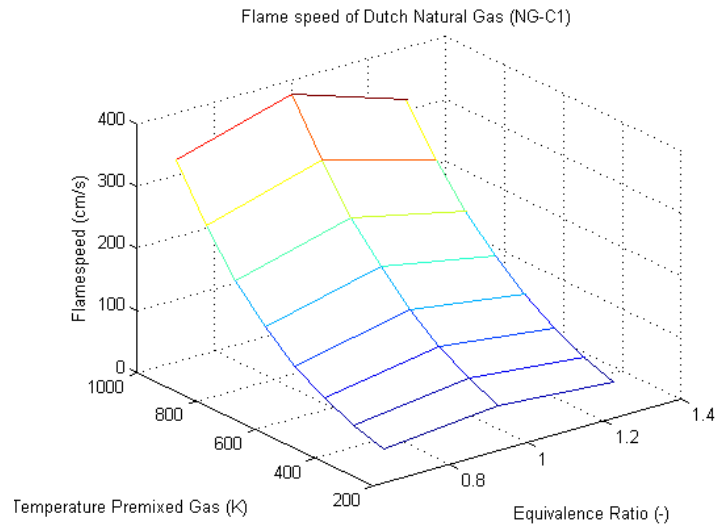
There are no big differences between the two different compositions of Dutch natural gas, NG-C1 and NG-C2. The differences tend to decrease with a higher initial temperature of the premixed gas. The differences



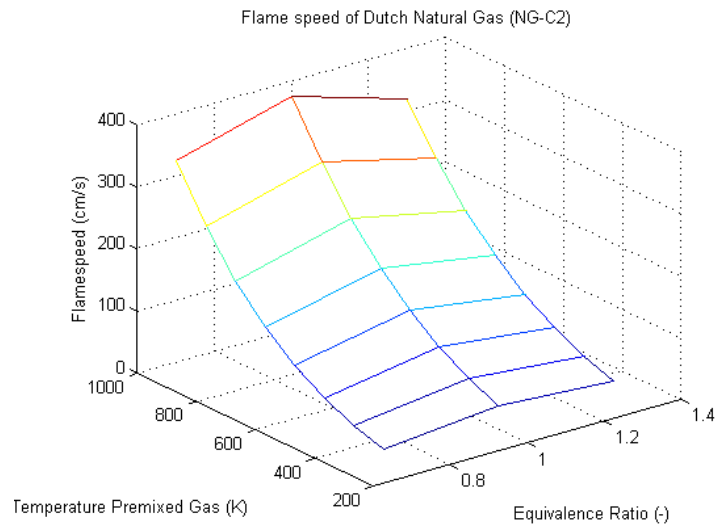
**Figure 3.3** – This figure contains the adiabatic flame temperatures of several mixtures of Dutch natural gas and air. The adiabatic flame temperature calculations have been done for two different compositions of Dutch natural gas. In this figure  $T$  is the initial temperature of the unburnt gases and  $T_{adb}$  the adiabatic temperature.



**Figure 3.4** – This figure contains the laminar flame speed of a Dutch natural gas/air flame with an initial temperature of 300K for two different Dutch natural gas compositions.



(a)



(b)

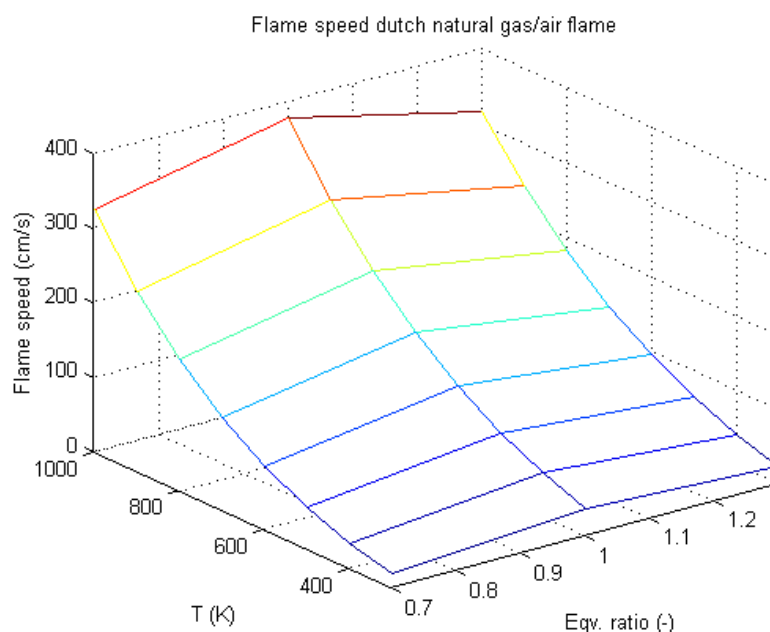
**Figure 3.5** – This figure contains the laminar flame speed of a Dutch natural gas/air flame at different initial temperatures and different equivalence ratio's.

are also higher at the fuel-rich side than at the fuel-lean side. This is because the fuel has more influence on the fuel-rich side.

The differences range from -1 to +4 cm/s. The highest difference in percentages is 6% for an equivalence ratio of 1.3 and a initial temperature of 300 Kelvin. The differences in percentages tend to decrease with a higher initial temperature of the premixed gas. The absolute difference tend to increase a bit a the fuel-rich side. The adiabatic flame temperature and flame speed of the NG-C1 and NG-C2 compositions are roughly equal, therefore from hereon the simpler NG-C1 composition will be used for all calculations.

### 3.2.4 Flame speed calculation with Chemkin

The flame speed of different Dutch natural gas/air flames has also been calculated with Chemkin. This has only been done with the NG-C1 composition. The calculation has been done for an equivalence ratio of 0.7, 1.0 and 1.3 and with the premixed gas at 300-1000 Kelvin. The results are shown in figure 3.6.



**Figure 3.6** – This figure contains the laminar flame speed of a Dutch natural gas/air flame computed with Chemkin for several mixtures and initial temperatures.

From the figure one can conclude that the flame speed increases with the temperature of the premixed gases. Also the flame speed is higher for a stoichiometric flame than a fuel-lean or fuel-rich flame.

### 3.2.5 Flame speed comparison

The flame speed of a Dutch natural gas/air flame calculated with Cosilab and Chemkin are not identical. The difference in percentages remains within 12%. The difference does increase with temperature, which means that for coflow/Dutch natural gas calculations the differences will be higher between Chemkin and Cosilab. This is because these calculations are done with the premixed gas at a temperature higher than 1000 Kelvin.

The difference in flame speed calculated by Cosilab and Chemkin can be explained by the different way these two programs obtain a solution. The differences between this two programs are explained in section 2.8.1.

# Chapter 4

## Main results

This chapter contains the results the main results of the thesis. Two different coflow compositions will be introduced. The laminar flame speed will be calculated for these two compositions and then compared. In the last section a flame speed profile will be created starting from a dataset containing a temperature and a mixture fraction profile. The flame speed calculation of the coflow and Dutch natural gas has only been done with Chemkin. Troubles were encountered when trying to do the calculation in Cosilab (see appendix C).

### 4.1 Coflow compositions

The flame speed will be calculated for two different coflow compositions with Dutch natural gas. The simplified NG-C1 composition will be used for Dutch natural gas. The coflow compositions DJHC-I-S and DJHC-X-S are given in table E.2.

Component [–]	DJHC-X-S [mol%]	DJHC-I-S [mol%]
CO2	04.788	05.934
H2O	09.576	11.863
N2	75.520	74.665
O2	10.116	07.539

**Table 4.1** – This table contains two different coflow compositions called DJHC-I-S and DJHC-X-S.

### 4.2 Coflow / Dutch natural gas calculation method

The solution of a premixed coflow/Dutch natural gas flame has to be reached in small steps. The first step is to find a solution of a stoichiometric methane/air flame for the appropriate initial temperature. The next step is to slowly add some carbon dioxide and remove some methane. This is done until the appropriate methane and carbon dioxide fraction are reached for a stoichiometric coflow/Dutch natural gas flame. The last step is to remove some oxygen and add some water until the right fractions are reached. The nitrogen fraction also has to be changed to the right value. After doing these steps the stoichiometric coflow/Dutch natural gas solution has been reached. The fuel-lean and fuel-rich solutions can now be found starting from the stoichiometric coflow/Dutch natural gas flame.

The appropriate stoichiometric species fractions are calculated using the same method as in A.1. The stoichiometric species fractions of a coflow/Dutch natural gas mixture for the two different coflow compositions are given in table 4.2

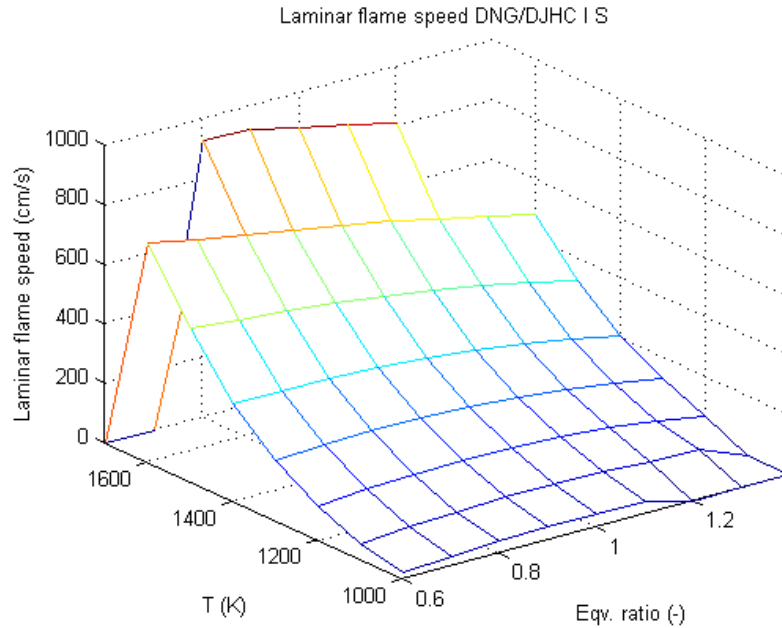


Component [-]	DJHC-X-S/DNG [mol%]	DJHC-I-S/DNG [mol%]
CO2	04.520	0.5683
H2O	09.040	11.361
N2	72.116	72.127
O2	09.550	07.220
CH4	04.775	03.601

**Table 4.2** – This table contains the stoichiometric species fractions for a coflow/Dutch natural gas mixture for two different coflow compositions.

### 4.3 Flame speed composition I-S

Using the method described in the previous subsection the flame speed of a laminar, one-dimensional, premixed freely propagating Dutch natural gas/coflow (DJHC-I-S) flame has been calculated with Chemkin. A solution was only found for a temperature between 1000 and 1700 Kelvin and an equivalence ratio of 0.6-1.4 for most of these temperatures. In figure 4.1 the laminar flame speed is shown for the solutions that were found.

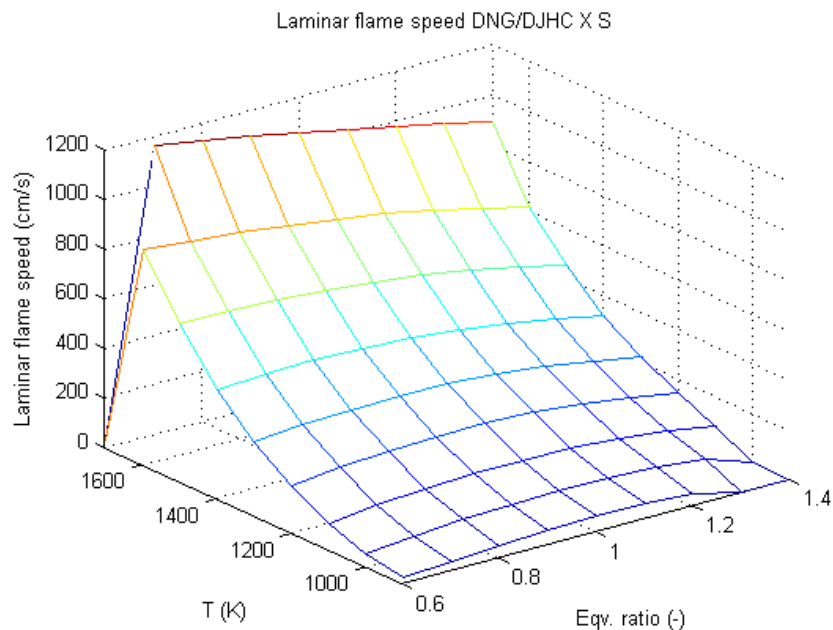


**Figure 4.1** – This figure contains the laminar flame speed of a Dutch natural gas/coflow (DJHC-I-S) computed with Chemkin for several mixtures and initial temperatures. A laminar flame speed of zero means that Chemkin wasn't able to compute the laminar flame speed for that point.

It was not possible to calculate the laminar flame speed for temperatures higher than 1700 Kelvin. A possible explanation is that the flame cannot stabilize at higher temperatures. The reactants are instantly converted to the products, because of the high temperature. This process happens so fast that the flame cannot stabilize.

## 4.4 Flame speed composition X-S

The flame speed of a Dutch natural gas/coflow flame with a DJHC-X-S composition has also been calculated with Chemkin. A solution was only found for a temperature between 900 and 1700 Kelvin and an equivalence ratio of 0.6-1.4 for most of these temperatures. In figure 4.2 the laminar flame speed is shown for the solutions that were found.



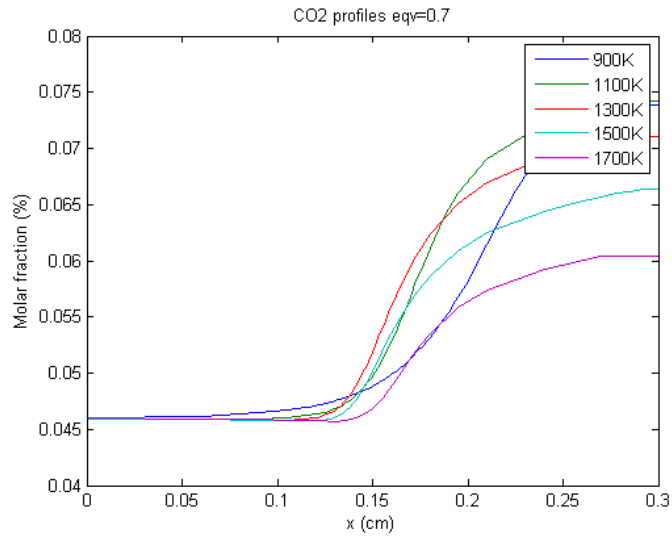
**Figure 4.2** – This figure contains the laminar flame speed of a Dutch natural gas/coflow (DJHC-X-S) computed with Chemkin for several mixtures and initial temperatures. A laminar flame speed of zero means that Chemkin wasn't able to compute the laminar flame speed for that point.

It can be seen that at lower temperatures (1000-1200 Kelvin) the flame speed is at its maximum when the flame is in stoichiometric conditions. For higher temperatures the maximum shifts to the lean side of the flame. At the highest temperatures the maximum isn't even visible in the calculated regions. An explanation for this occurrence is that a second fuel becomes relevant at higher temperatures. This second fuel, carbon monoxide is created from the carbon dioxide at higher temperatures. It can be seen in figure 4.3 that the CO<sub>2</sub> molar fraction is a lot lower at higher temperatures, which means that less CO<sub>2</sub> is created in the combustion process. This indicates that part of the CO<sub>2</sub> is split into CO and oxygen. This will increase the laminar flame speed.

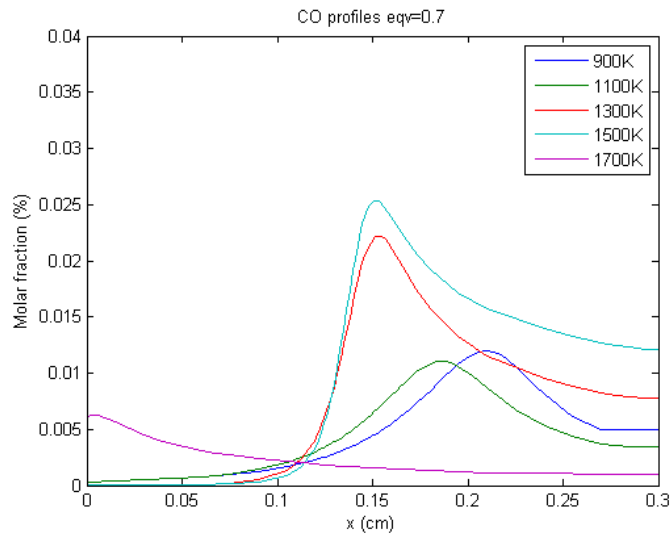
## 4.5 Flame speed profile

A Matlab script has been written that is able to read a temperature profile and mixture fraction profile of a flame region (2D) and then convert it to a laminar flame speed profile. As an input profile computational results computed with Fluent were used [11]. The Matlab script is given in appendix F. The results are given in figure 4.4. The laminar flame speed profile can be compared to a axial velocity profile gotten from the same computational results from Fluent.

It is expected that the laminar flame speed profile values are lower than the axial velocity profile values. This is because the axial velocity profile is obtained from a computation which also takes turbulence into

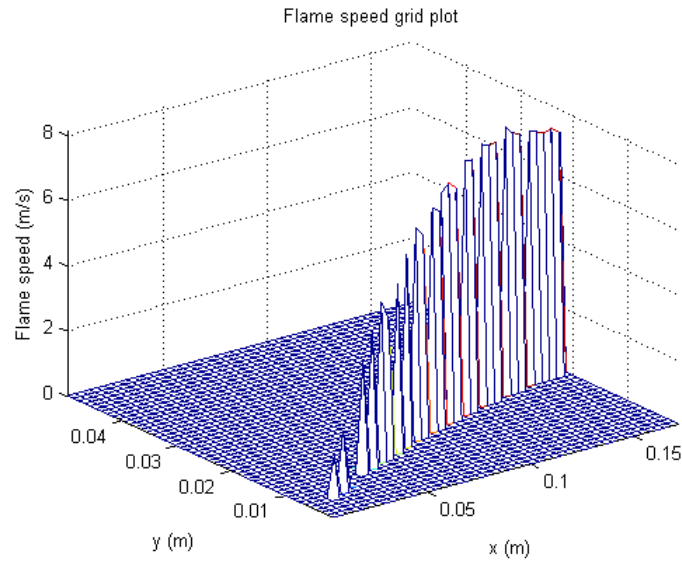


(a) CO2 profiles

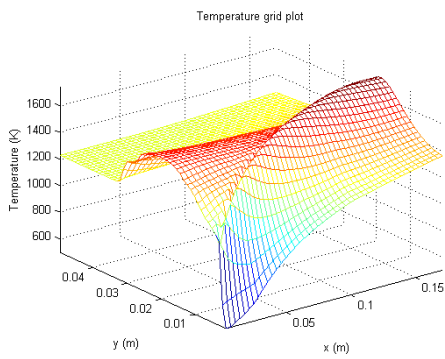


(b) CO profiles

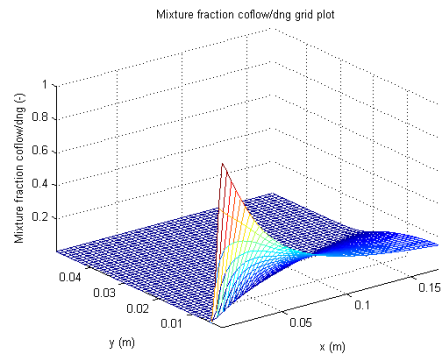
**Figure 4.3** – This figure contains the CO<sub>2</sub> and CO profiles of a Dutch natural gas / coflow (XS) flame with an equivalence ratio of 0.7 . It shows that the higher the initial temperature, the lower the CO<sub>2</sub> molar fraction of the burnt gases. It also shows that for higher initial temperatures the CO peak is a lot earlier, which means that the role of CO is more relevant in these flame.



(a) Flame speed profile



(b) Temperature profile



(c) Mixture fraction profile

**Figure 4.4** – This figure contains the flame speed, temperature and mixture fraction grid plots of a Dutch natural gas / coflow flame. In the flame speed grid plot a value of zero means that the flame speed for this point couldn't be computed with Chemkin.

account. For all calculated points, the axial velocities and calculated laminar flame speeds are given in appendix E.3. According to the results the laminar flame speeds are not always lower than the axial velocities. They're actually higher most of the time. If the two highest differences are removed, all differences are within 50%.

A reason for the higher laminar flame speed is that the temperature picked from the temperature profile isn't equal to the initial temperature. In the regions where there has been combustion the temperature from the fluent data is equal to the initial temperature of the mixture plus a temperature increase from chemical reactions that have taken place. Because the temperature from the fluent data is higher than the initial temperature, the flame speed will also be higher when the temperature from the fluent data is used.

Another reason for the higher laminar flame speed could be that the laminar flame speeds are calculated in one dimension. In an experiment the flame is able to move in more than one direction, the flame expands and becomes wider. In the calculations the flame can only move in one dimension, which means that everything is concentrated on one line. Therefore it is a possibility that the laminar flame speed calculated in one dimension is higher than the laminar flame speed obtained from experimental results.

Experimental results show that the lift-off height where this flame stabilizes is between 80 and 100 mm. In the results it can be seen that a laminar flame speed could be calculated even below the 80-100 mm line, while in the experiment there is no laminar flame below this line. An explanation of there being no flame, while according to the calculations there could be a flame is that in a one-dimensional calculation some factors like strain, curvature and spatial variation of equivalence ratio aren't taken into account.

Experimental results also show that there is auto-ignition. After the auto-ignition has taken place the pocket will expand with a flame speed of around 2 m/s. The corresponding initial temperature to a laminar flame speed of 2 m/s of a stoichiometric flame is approximately 1300 Kelvin. A speed of 2 m/s is also found at the fuel-rich (equivalence ratio = 1.4) side at about 1400 Kelvin. Since experimental results show that the temperature should be around 1500 Kelvin, the calculated laminar flame speeds corresponding to 1500 Kelvin are too high. More research will have to be conducted to relate the calculated laminar flame speeds to the experiments.

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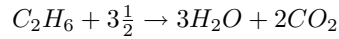
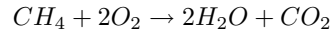
# Appendix A

## Mixture composition and mixture fraction

### A.1 Mixture composition

This section contains an example of the mixture composition being derived from the equivalence ratio. The example is based on a combustion process between Dutch natural gas (NG-C2 composition) and air.

The two important chemical equations in the calculation are:



The equivalence ratio is defined as:

$$\phi = \frac{\text{fuel-to-oxidizer ratio}}{\text{stoichiometric fuel to oxidizer ratio}} = \frac{fto}{fto_{st}}$$

Dutch natural gas consists of five components:

80.95%  $CH_4$

03.89%  $C_2H_6$

14.26%  $N_2$

00.01%  $O_2$  ← will be neglected

00.89%  $CO_2$

Air consist of two components:

21.00%  $O_2$

79.00%  $N_2$

Using the two chemical equations the stoichiometric fuel-to-oxidizer ratio can be calculated:

$$fta_{st} = \frac{\text{moles of fuel}}{\text{moles of oxidizer}} = \frac{1\text{mole}CH_4 + x\text{moles}C_2H_6}{2\text{moles}O_2 + 3\frac{1}{2}x\text{moles}O_2} = \frac{1+x}{2+3\frac{1}{2}x} \quad (\text{A.1})$$

In equation A.1  $x$  is a constant defined as the ratio between methane and ethane in Dutch natural gas. With the help of the definition of the equivalence ratio the fuel to oxidizer ratio  $fto$  can be calculated:

$$fto = \phi fto_{st} = \phi \frac{1+x}{2+3\frac{1}{2}x}$$

With the help of the fuel to oxidizer ratio the Dutch natural gas to air ratio  $dta$  can be calculated:

$$fto = \frac{\text{moles}CH_4 + \text{moles}C_2H_6}{\text{moles}O_2}$$

$$dta = \frac{n_{dng}}{n_{air}} = \frac{\frac{100}{80.95+3.89}}{\frac{100}{21}} fto$$

$$dta = \frac{21}{80.95 + 3.89} fto = \frac{21}{80.95 + 3.89} \phi \frac{1 + x}{2 + 3\frac{1}{2}x}$$

The composition of the premixed gas can now be calculated using the Dutch natural gas to air ratio and normalization:

$$\%CH_4 = \frac{n_{CH_4,DNG}dta + n_{CH_4,air}}{dta + 1}$$

$$\%C_2H_6 = \frac{n_{C_2H_6,DNG}dta + n_{C_2H_6,air}}{dta + 1}$$

$$\%N_2 = \frac{n_{N_2,DNG}dta + n_{N_2,air}}{dta + 1}$$

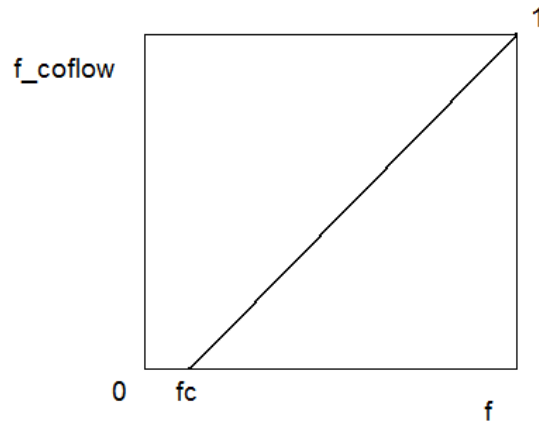
$$\%CO_2 = \frac{n_{CO_2,DNG}dta + n_{CO_2,air}}{dta + 1}$$

$$\%O_2 = \frac{n_{O_2,DNG}dta + n_{O_2,air}}{dta + 1}$$

The results have been validated with a program called GASEQ which can calculate mixture compositions for different equivalence ratios.[9]

## A.2 Mixture fraction to coflow mixture fraction

In this section a short derivation will be given of the formula that is used to convert the mixture fraction based on Dutch natural gas/air to the mixture fraction based on Dutch natural gas/coflow. The mixture fractions have a linear connection, as is seen in figure A.1.



**Figure A.1** – This figure illustrates the linear connection between the mixture fraction based on a Dutch natural gas/air mixture and a dutch natural gas/coflow mixture.

As seen in figure A.1 there are two points known. Both  $f_{coflow}$  and  $f$  are 1 when the mixture is fully composed of dutch natural gas. Also  $f_{coflow}$  is equal to zero when the mixture is fully composed of coflow,



but since the coflow comes from a lean Dutch natural gas/air combustion process the mixture fraction  $f$  is not equal to zero. In coflow the mixture fraction based on Dutch natural gas/air is a constant:  $fc$ .

Using two points the linear formula can be derived:

$$\begin{aligned}
 f_{coflow} &= af + b \\
 a &= \frac{\Delta f_{coflow}}{\Delta f} \\
 &= \frac{1}{1 - fc} \\
 b &= f_{coflow} - a \cdot f \\
 &= 0 - a \cdot fc \\
 &= -\frac{fc}{1 - fc} \\
 f_{coflow} &= \frac{f - fc}{1 - fc}
 \end{aligned}$$

### A.3 Mixture fraction

In this section the derivation of the mixture fraction in terms of the equivalence ratio will be shown. The mixture fraction is defined as:

$$f = \frac{m_f}{m_f + m_o} \quad (\text{A.2})$$

If both the numerator and denominator are divided by the oxidizer mass  $m_o$ , equation A.2 will become:

$$f = \frac{\frac{m_f}{m_o}}{\frac{m_f}{m_o} + 1} \quad (\text{A.3})$$

The next step is to divide both numerator and denominator by the stoichiometric fuel-to-air mass ratio. Equation A.3 becomes:

$$f = \frac{\frac{m_f}{m_o} \left( \frac{m_o}{m_f} \right)_{st}}{\frac{m_f}{m_o} \left( \frac{m_o}{m_f} \right)_{st} + \left( \frac{m_o}{m_f} \right)_{st}} \quad (\text{A.4})$$

In equation A.4 the equivalence ratio  $\phi$  can now be recognized. Also the stoichiometric air-to-fuel mass ratio will be defined as  $r$ . Equation A.4 is therefore written as:

$$f = \frac{\phi}{\phi + r}$$

# Appendix B

## Derivation governing equations

In this chapter the governing equation will be derived starting from the conservation equation:

$$\frac{\partial A}{\partial t} + \frac{\partial B}{\partial x} = C$$

### B.1 Continuity equation

The density, flux density and source for total mass as a conserved variable are defined as:

$$\begin{aligned} A &= \rho \\ B &= \rho v \\ C &= 0 \end{aligned}$$

This leads to the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = 0 \tag{B.1}$$

For a computational model it is useful to rewrite the equation in terms of the mass flux  $m = \rho v$ . Another form of equation B.1 is:

$$\frac{\partial \rho}{\partial t} = - \frac{\partial m}{\partial x}$$

### B.2 Species-mass conservation equation

The density, flux density and source for the mass of species  $i$  as a conserved variable are defined as:

$$\begin{aligned} A &= \rho_i = \rho Y_i \\ B &= \rho_i v_i = \rho Y_i v_i \\ C &= r_i \end{aligned}$$

This leads to the species-mass conservation equation:

$$\frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho Y_i v_i)}{\partial x} = r_i \tag{B.2}$$

The mass velocity  $v_i$  of a species  $i$  is composed of two components. The first component being the mean mass velocity of the whole mixture  $v$  and the second component being the diffusion velocity  $V_i$  due to a concentration gradient of species  $i$ . Equation B.2 can therefore be rewritten to:

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho Y_i v)}{\partial x} + \frac{\partial(\rho Y_i V_i)}{\partial x} = r_i \quad (\text{B.3})$$

With the help of the product rule equation B.3 can be rewritten to:

$$Y_i \frac{\partial \rho Y_i}{\partial t} + \rho \frac{\partial Y_i}{\partial t} + Y_i \frac{\partial(\rho v)}{\partial x} + \rho v \frac{\partial Y_i}{\partial x} + \frac{\partial(\rho Y_i V_i)}{\partial x} = r_i \quad (\text{B.4})$$

Using the continuity equation and the fact that the diffusion flux  $j_i$  is defined as  $Y_i V_i \rho$  equation B.4 can be reduced to:

$$\rho \frac{\partial Y_i}{\partial t} + \rho v \frac{\partial Y_i}{\partial x} + \frac{\partial j_i}{\partial x} = r_i \quad (\text{B.5})$$

For a computational model it is useful to rewrite the equation in terms of the mass flux  $m = \rho v$ . Another form of equation B.5 is:

$$\frac{\partial Y_i}{\partial t} = -\frac{m}{\rho} \frac{\partial Y_i}{\partial x} - \frac{1}{\rho} \frac{\partial j_i}{\partial x} + \frac{r_i}{\rho}$$

### B.3 Energy equation

The density, flux density and source for total enthalpy conserved variable are defined as:

$$\begin{aligned} A &= \sum_i \rho_i h_i = \sum_i \rho Y_i h_i \\ B &= j_q + \sum_i \rho_i v_i h_i = j_q + \sum_i \rho Y_i v_i h_i \\ C &= 0 \end{aligned}$$

This leads to the enthalpy conservation equation:

$$\sum_i \frac{\partial}{\partial t} (\rho Y_i h_i) + \frac{\partial j_q}{\partial z} + \sum_i \frac{\partial}{\partial z} (\rho v_i Y_i h_i) = 0 \quad (\text{B.6})$$

Since the mass velocity  $v_i$  is composed of the mean mass velocity of the whole mixture and the diffusion velocity of species  $i$   $V_i$  equation B.6 can be written as:

$$\sum_i \frac{\partial}{\partial t} (\rho Y_i h_i) + \frac{\partial j_q}{\partial z} + \sum_i \frac{\partial}{\partial z} (\rho v Y_i h_i) + \sum_i \frac{\partial}{\partial z} (\rho V_i Y_i h_i) = 0 \quad (\text{B.7})$$

Using the product rule equation B.7 can be written to:

$$\sum_i \left[ \rho Y_i \frac{\partial h_i}{\partial t} + h_i \frac{\partial(\rho Y_i)}{\partial t} \right] + \frac{\partial j_q}{\partial z} + \sum_i \left[ \rho v Y_i \frac{\partial h_i}{\partial z} + h_i \frac{\partial(\rho v Y_i)}{\partial z} \right] + \sum_i \left[ \rho Y_i V_i \frac{\partial h_i}{\partial z} + h_i \frac{\partial(\rho Y_i V_i)}{\partial z} \right] = 0$$

Using equation B.3 the second and fifth term in the above equation can be rewritten, leading to:

$$\sum_i \rho Y_i \frac{\partial h_i}{\partial t} + \frac{\partial j_q}{\partial z} + \sum_i \rho v Y_i \frac{\partial h_i}{\partial z} + \sum_i \rho Y_i V_i \frac{\partial h_i}{\partial z} + \sum_i h_i \frac{\partial(\rho Y_i V_i)}{\partial z} + \sum_i h_i r_i - \sum_i h_i \frac{\partial j_i}{\partial z} = 0 \quad (\text{B.8})$$

Since  $j_i$  is defined as  $\rho Y_i V_i$  the fifth and last term are equal. They disappear because of the minus and plus sign. Equation B.8 is therefore written as:

$$\sum_i \rho Y_i \frac{\partial h_i}{\partial t} + \frac{\partial j_q}{\partial x} + \sum_i \rho v Y_i \frac{\partial h_i}{\partial z} + \sum_i j_i \frac{\partial h_i}{\partial z} + \sum_i h_i r_i = 0 \quad (\text{B.9})$$

Under a constant pressure the change in specific enthalpy is given by:

$$d(h_i) = c_{p,i} d(T) \quad (\text{B.10})$$

Combining equations B.9 and B.10 leads to:

$$\rho \sum_i Y_i c_{p,i} \frac{\partial T}{\partial t} + \frac{\partial j_q}{\partial x} + \rho v \sum_i Y_i c_{p,i} \frac{\partial T}{\partial x} + \sum_i j_i c_{p,i} \frac{\partial T}{\partial x} + \sum_i h_i r_i = 0 \quad (\text{B.11})$$

Using equation 2.3 and the property that the total specific heat capacity of a mixture is defined as the sum of products of specific heat capacity and mass fraction of species  $i$  equation B.11 can be reduced to:

$$\rho c_p \left( \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) - \frac{\partial T}{\partial x} \sum_i j_i c_{p,i} - \sum_{i=1}^I h_i r_i \quad (\text{B.12})$$

For a computational model it is useful to rewrite the equation in terms of the mass flux  $m = \rho v$ . Another form of equation B.12 is:

$$\frac{\partial T}{\partial t} = -\frac{m}{\rho} \frac{\partial T}{\partial x} + \frac{1}{\rho c_p} \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) - \frac{1}{\rho} \frac{\partial T}{\partial x} \sum_{i=1}^I \left( \frac{c_{p,i}}{c_p} \right) j_i - \sum_{i=1}^I \frac{h_i}{\rho c_p} r_i$$

## B.4 Ideal-gas equation of state

The formula of the ideal gas equation of state is:

$$pV = nRT$$

The molar density is defined as:

$$c = \frac{n}{V} = \frac{\rho}{\bar{M}} \quad (\text{B.13})$$

where  $\bar{M}$  is the mean molar mass which is defined as:

$$\bar{M} = \frac{1}{\sum_i \frac{Y_i}{W_i}} \quad (\text{B.14})$$

Using equation B.13 and B.14, the ideal gas equation of state can be written as:

$$p = \rho RT \sum_i \frac{Y_i}{W_i}$$

# Appendix C

## Problems

### C.1 Cosilab coflow

Using the same procedures as in Chemkin, Cosilab wasn't able to find any solution for a Dutch natural gas/coflow problem. Cosilab has no problem with exchanging some  $CH_4$  with  $CO_2$ , but it does give errors when exchanging  $O_2$  for  $H_2O$ . At a certain point in the process Cosilab isn't able to find a solution for the problem. Different lengths of the computational region have been tried. This could also not solve the problem.

### C.2 x-end

The length of the computational region has an impact on the laminar flame speed. If the length of the computation region is increased or decreased, there is a huge change another solution is found. This solution will look like it sufficient, but the laminar flame speed may differ up to 50%. It is difficult to say which solution is the correct solution, and therefore there is quite an insecurity in the results.

It would be useful to create a program which also increases or decreases the length of the computational region to the most correct solution. This way the laminar flame speeds obtained from all the calculation can be compared in a better way, because the solution are always gotten using the same procedure. This especially relevant for comparing calculations with different initial temperatures. The x-end and x-start differ a lot for different initial temperatures.

### C.3 Input profile in Cosilab

When working with Cosilab a input profile should be created for all species and temperature. When an input profile isn't sufficient Cosilab is not able to find a solution. Since it takes a lot of time to find the right input profile Cosilab isn't always that nice to use.

Chemkin only needs a temperature profile estimation, molar fractions of the unreacted fuel-oxidizer set up, an estimation of the products and an estimation of the intermediate products. This takes a lot less time than building a profile for 20 different species and the temperature.

### C.4 Low temperature coflow

For temperatures lower than 1000 Kelvin the laminar flame speed of a Dutch natural gas/coflow flame couldn't be calculated. This is partially explained by the fact that there is a lot less  $CH_4$  in the mixture. Since there is a lot less methane in the mixture the lower flammability limit will be reached. The higher

the temperature, the lower the flammability limit, therefore the laminar flame speed could be calculated for higher temperatures.

At temperatures higher than 1700 the laminar flame speed couldn't be calculated either. An explanation could be similar to the low temperature explanation, but this time it involves the higher flammability limit.

## Appendix D

# Chemkin input file

This chapter contains an example of a Chemkin input file.

```
/ freely propagating flame
FREE
ENRG
/ initial flow-rate estimate
FLRT .05 ! gm/cm**2-sec
/ atmospheric pressure
PRES 1.0 ! atmospheres
/ initial grid and profile specifications
NPTS 6
XEND 0.3 ! cm
XCEN 0.1 ! cm
WMIX 1.0 ! cm
/ temperature T0, which is fixed for the flame
TFIX 398.
/ mesh adaptation criteria
GRAD 0.5
CURV 0.5
/ unreacted fuel-oxidizer makeup
MOLE
REAC CH4 0.095023
REAC N2 0.714932
REAC O2 0.190045
/ estimated product mole fractions
PROD H2O 0.190
PROD CO2 0.095
PROD N2 0.715
/ estimated peak intermediate mole fractions
INTM CO 0.08
INTM HCO 0.00001
INTM HO2 0.0001
INTM O 0.0001
INTM H2O2 0.0001
INTM H 0.02
INTM H2 0.01
INTM OH 0.001
```

```
INTM  CH2 0.0001
INTM  CH  0.00001
INTM  CH20 0.001
INTM  CH3 0.0005
/  convergence tolerance for Newton
ATOL 1.E-9
RTOL 1.E-4
/  convergence tolerance for time stepping
ATIM 1.E-5
RTIM 1.E-5
/  how much information is printed
PRNT  1
/  time step control
TIME  100  5.0E-7 ! sec
TIM2  200  1.0E-6 ! sec
/  estimated temperature profile
TEMP  0.0  298.
TEMP  0.03  300.
TEMP  0.05  400.
TEMP  0.06  766.
TEMP  0.07 1512.
TEMP  0.08 1892.
TEMP  0.09 2000.
TEMP  0.1  2030.
TEMP  0.2  2111.
TEMP  0.35 2190.
TEMP 10.0  2190.
CNTN
/ CNTN indicates that a continuation
/ (batch process) can be created
END
```



# Appendix E

## Data

### E.1 Laminar flame speed Coflow-I-S/DNG

T(K)	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4
1000	22.41	31.79	39.82	44.63	46.39	43.41	-	-	-
1100	54.32	65.44	73.93	79.11	80.14	75.50	64.8500	64.99	-
1200	115.80	127.60	135.70	139.30	137.70	129.90	116.6000	94.99	65.80
1300	201.60	210.30	214.60	214.10	208.50	197.60	179.2000	156.70	125.90
1400	327.00	328.60	326.10	319.10	307.10	289.90	267.3000	238.00	206.40
1500	515.80	501.80	487.10	469.90	449.30	424.50	396.2000	363.30	325.40
1600	734.60	704.60	677.40	650.00	621.00	589.60	555.3000	518.40	481.10
1700	-	-	927.30	921.10	884.00	847.30	810.5000	-	-

**Table E.1** – This table contains the flame speed of Dutch natural gas with DJHC-I-S in [*cm/s*].

### E.2 Laminar flame speed Coflow-X-S/DNG

T(K)	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4
900	0.287	0.409	0.514	0.589	0.626	0.612	0.519	-	-
1000	0.582	0.740	0.869	0.957	0.993	0.966	0.853	0.670	-
1100	1.083	1.275	1.419	1.506	1.529	1.480	1.350	1.115	0.813
1200	1.914	2.118	2.256	2.323	2.314	2.227	2.061	1.770	1.420
1300	2.977	3.146	3.244	3.267	3.212	3.076	2.866	2.568	2.189
1400	4.415	4.513	4.542	4.500	4.383	4.191	3.922	3.577	3.164
1500	6.396	6.361	6.283	6.151	5.957	5.698	5.370	4.977	4.531
1600	8.668	8.493	8.302	8.076	7.802	7.476	7.096	6.664	6.191
1700	-	11.660	11.310	10.960	10.600	10.210	9.804	9.380	8.952

**Table E.2** – This table contains the flame speed of Dutch natural gas with DJHC-X-S in [*m/s*].

### E.3 Laminar flame Speed profile data

In this section all the calculated points from the Fluent 2D grid are given. In this table,  $SL$  means flame speed in  $[ms^{-1}]$ ,  $T$  means temperature in thousands of Kelvin,  $v$  means axial velocity in  $[ms^{-1}]$  and  $dif$  means the relative difference  $(v-SL)/SL$  in hundreds of percentages.

x(nr)	y(nr)	T *1000K	eqv	SL	v	dif *100%
6.0000	5.0000	1.1966	0.6131	1.2518	2.7991	-1.2360
7.0000	7.0000	1.2748	1.0622	1.8125	3.1195	-0.7211
10.0000	12.0000	1.4070	0.6505	3.3994	3.6941	-0.0867
11.0000	14.0000	1.4555	0.7105	4.1650	3.8727	0.0702
12.0000	16.0000	1.4886	0.6688	4.8196	4.0032	0.1694
12.0000	17.0000	1.5313	1.2553	4.2188	4.0941	0.0295
13.0000	19.0000	1.5478	1.0634	5.0819	4.1601	0.1814
14.0000	21.0000	1.5594	0.8696	5.7897	4.2044	0.2738
15.0000	23.0000	1.5678	0.6870	6.3995	4.2330	0.3385
15.0000	24.0000	1.6034	1.0515	6.1301	4.2836	0.3012
16.0000	26.0000	1.6018	0.8214	6.7597	4.2839	0.3663
16.0000	27.0000	1.6339	1.1248	6.5894	4.3320	0.3426
17.0000	28.0000	1.5979	0.6146	7.0058	4.2814	0.3889
17.0000	29.0000	1.6260	0.8756	7.2533	4.3126	0.4054
17.0000	30.0000	1.6548	1.1305	7.0586	4.3532	0.3833
18.0000	32.0000	1.6412	0.8724	7.6625	4.3190	0.4364
18.0000	33.0000	1.6675	1.0862	7.6487	4.3512	0.4311
19.0000	35.0000	1.6486	0.8308	7.9160	4.3094	0.4556
19.0000	36.0000	1.6715	1.0102	7.8194	4.3379	0.4452
19.0000	37.0000	1.6905	1.1706	7.8709	4.3711	0.4446
20.0000	39.0000	1.6595	0.8890	8.1251	4.3062	0.4700
20.0000	40.0000	1.6743	1.0162	7.8781	4.3284	0.4506
20.0000	41.0000	1.6862	1.1286	7.7869	4.3520	0.4411
21.0000	43.0000	1.6390	0.8379	7.6599	4.2323	0.4475
21.0000	44.0000	1.6488	0.9283	7.5989	4.2449	0.4414
21.0000	45.0000	1.6572	1.0093	7.4927	4.2588	0.4316
21.0000	46.0000	1.6647	1.0848	7.5803	4.2758	0.4359
21.0000	47.0000	1.6702	1.1483	7.3964	4.2899	0.4200
22.0000	45.0000	1.5971	0.6414	6.9893	4.0887	0.4150
22.0000	47.0000	1.6171	0.8016	7.1867	4.1030	0.4291
22.0000	48.0000	1.6261	0.8707	7.2658	4.1182	0.4332
23.0000	48.0000	1.5791	0.6069	6.6495	3.9459	0.4066

# Appendix F

## Matlab script

### F.1 Flame speed calculation from flame speed data set

This section contains the mat lab scrip that is used to read and interpolate the flame speed for a defined temperature and equivalence ratio.

```
function s=flamespeed(eqv,t)
% Round equivalence ratio to the nearest 1/10th
eqv1=floor(10*eqv)/10;
eqv2=ceil(10*eqv)/10;
% Round temperature to the nearest 100.
t1=floor(t/100)*100;
t2=ceil(t/100)*100;
% Load flamedata. Flamedata is a dataset containing
% the flame speeds from 100 to 1900 Kelvin and
% an equivalence ratio of 0.1 to 1.5.

flamedata=load('flamedata.txt')

% Script to make sure flame speed is zero if
% the flame speed isn't within the limits of the calculated
% flame speeds.
if eqv < 0.1
    s=0;
elseif eqv > 1.5
    s=0;
elseif t > 1900
    s=0;
elseif t < 200
    s=0;
elseif flamedata(t1/100,eqv1*10)==0
    s=0;
elseif flamedata(t1/100,eqv2*10)==0
    s=0;
elseif flamedata(t2/100,eqv1*10)==0
    s=0;
elseif flamedata(t2/100,eqv2*10)==0
    s=0;
```

```

% Interpolation script.
elseif eqv2==eqv1
    if t1==t2
        s=flamedata((t2/100),(eqv2*10));
    else
        s=((t2-t)*flamedata(t1/100,eqv*10)+(t-t1)
            *flamedata(t2/100,(eqv*10)))/(t2-t1);
    end
else
    if t1==t2
        s=((eqv2-eqv)*flamedata(t/100,eqv1*10)+(eqv-eqv1)
            *flamedata(t/100,eqv2*10))/(eqv2-eqv1);
    else
        eqvT1=((eqv2-eqv)*flamedata((t1/100),(eqv1*10))
            + (eqv-eqv1)*flamedata((t1/100),(eqv2*10)))/(eqv2-eqv1);
        eqvT2=((eqv2-eqv)*flamedata((t2/100),(eqv2*10))
            + (eqv-eqv1)*flamedata((t2/100),(eqv2*10)))/(eqv2-eqv1);
        s=((t2-t)*eqvT1+(t-t1)*eqvT2)/(t2-t1);
    end
end
end
end

```

## F.2 Flame speed profile from temperature and mixture fraction profile

This section contains the Matlab script that is used to convert a data file DJHC containing temperature and mixture fraction to a flame speed profile.

```

clear
A=load('DJHC');
A=A(:,2:6);

% Creates a x times y grid profile.
xmin=min(A(:,1));
xmax=max(A(:,1));
ymin=min(A(:,2));
ymax=max(A(:,2));
gridnumber=50;
xstep=(xmax-xmin)/(gridnumber);
ystep=(ymax-ymin)/(gridnumber);
xi=[xmin:xstep:xmax]; % Define x-vector
yi=[ymin:ystep:ymax]'; % Define y-vector

% Reads the temperature and mixture fraciton profile.
T=griddata(A(:,1),A(:,2),A(:,4),xi,yi);
T=T(2:(gridnumber-1),2:(gridnumber-1));
f=griddata(A(:,1),A(:,2),A(:,5),xi,yi);
f=f(2:(gridnumber-1),2:(gridnumber-1));

% Calculation of equivalence ratio from mixture fraction
mcf=0.07539*32+0.74665*28.02+0.05934*44+0.11863*18;

```

```

mdng=0.853*16.042+0.147*28.02;
r=22.6297*mcf/mdng;
fc=0.044;
fco=(f-fc)/(1-fc);
eqv=(fco.*r)/(1-fco);

% Calculates flame speed for every grid point.
% flamespeed is a script which converts temperature and
% equivalence ratio to flame speed.
gridjes=size(T);
s=zeros(gridjes(1),gridjes(2));
for k=1:gridjes(1)
    for l=1:gridjes(2)
        s(k,l)=flamespeed(eqv(k,l),T(k,l));
    end
end

% Creates a mesh plot of the flame speed.
mesh(xi,yi,s);
xlabel('x (m)');
ylabel('y (m)');
zlabel('Flame speed (m/s)');
title('Flame speed grid plot');
axis([min(xi) max(xi) min(yi) max(yi) min(min(s)) max(max(s))]);

```