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Work Package 3
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Sub Package 3.6
Modelling of Minimum Ignition Energy

Deliverable No. 20
Model, software development for calculation of Markstein numbers and minimum ignition energies (MIE)

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1 Introduction

This deliverable describes a method to simulate minimum ignition energies (MIE) of combustible gaseous hydrocarbon fuel-oxidiser mixtures and Markstein lengths of (incipient) stretching flames. Both minimum ignition energies and Markstein lengths can be simulated with a one-dimensional model for spherical expanding flames and therefore are described together in this deliverable. The software used for the simulations is called INSFLA, the post processing software that is needed for the calculation of the flame front radius, flame front speed, burning velocity, stretch rate and other parameters has been developed in the last few months within work package 3.6 of the SAFEKINEX project. As the program INSFLA can not directly be used to calculate minimum ignition energies, a second software package has been developed which uses INSFLA for the simulations and automatically finds the minimum ignition energy of a given mixture.

As ignition, one describes the time dependent process in which starting from reactants a chemical reaction takes place until a steadily burning flame is formed or until the system has completely reacted to products. Ignition processes are always unsteady. Examples are induced ignition processes (spark ignition in Otto engine) or auto ignitions (Diesel engine). In safety engineering the value of the minimal ignition energy (MIE) is of utmost importance, as it gives an evidence of the maximum energy (e.g. in form of an electrical spark) an ignitable mixture can be exposed to without causing uncontrolled explosively flame propagation, which may hold a high risk.

An exact simulation of such unsteady ignition processes in consideration of all occurring processes (diffusion, chemical reaction and flow) is very complex and only possible by using numerical methods. A qualitative declaration is also given by dealing with highly simplified systems. In this connection the theory of Seminov [1], in which a spatial homogeneous system is treated, and the thermal theory of explosion by Frank Kamenetskii [2], in which an inhomogeneous system with ideal heat transfer to the surrounding area is treated, are mentioned. Within the bounds of this work the ignition process ought to be analyzed in detail and the simplified theories will not be applied. Hereunto the problem of ignition will be analyzed by using a one-dimensional numerical solving method in consideration of a detailed chemical mechanism and physical transport mechanism.

The objective of this work is to deepen the understanding of ignition processes and to describe a method to analyze the ignition mechanism with simulations. Additionally, Markstein lengths will be simulated with the same method. With the Markstein lengths the influence of flame stretch at the early stages of ignition process can be understood. As flame stretch has an influence on the ignition process, it is necessary to understand and simulate both parameters. This deliverable gives several results of the simulations for minimum ignition energies and Markstein lengths. The influence of the Markstein numbers on the minimum ignition energy will be described in more detail in deliverable no. 21, as more simulations for minimum ignition energies are needed. Some other simulations of Markstein lengths were already presented in deliverable no. 6.
2 Theory

2.1 Definition of ignition

It is possible to pass small electric sparks through an explosive gas without producing ignition. When the spark energy is increased a threshold energy is eventually obtained at which a spark becomes incendiary, in the sense that a combustion wave propagates from the spark through the volume of gas. This minimum ignition energy is a function of several parameters such as cold gas mixture composition, ambient pressure and temperature, configuration of the spark gap (electrode form, material and distance) and energy deposition parameters (spatial and temporal energy deposition profile).

Ignition by a hot kernel may be characterized by three different processes which appear in dependence of the ignition parameters successively or superposed. These different processes are energy deposition, induction phase and laminar flame front propagation.

Energy deposition is mainly characterized by the energy deposition time, source width and power. During the induction phase the increased temperature in the hot spot causes the formation of a radical pool. This phase is mainly controlled by the formation of radicals due to the energy deposition leading to the following exothermic reaction of fuel and oxygen to carbon dioxide and water. After induction phase the flame front starts propagating and the chemical reaction is self-preserving, leading to a laminar flame front propagation.

2.2 Effect of flame stretch on the laminar burning velocity

The flame stretch rate $\alpha$ is defined by the fraction of change of the flame surface $A$ normalized by the flame surface itself:

$$\alpha = \frac{1}{A} \frac{dA}{dt}. \quad (2-1)$$

For spherical symmetrical flames, the flame surface area $A$ is determined by the flame front radius $r_f$. In this case the total stretch rate can be calculated with the stretched flame front velocity $S_n$ and the flame front radius $r_f$:

$$\alpha = \frac{1}{A} \frac{dA}{dt} = \frac{1}{4\pi r_f^2} \frac{d(4\pi r_f^2)}{dt} = \frac{2}{r_f} S_n, \quad \text{with} \quad S_n = \frac{dr_f}{dt}. \quad (2-2)$$

Flame front propagation in a non-uniform flow is subject to strain and curvature effects, which lead to changes in flame area [3]. In this work solely the total stretch rate $\alpha$ is considered. A universally valid relationship between the change in the laminar flame front velocity and flame stretch rate $\alpha$, that embodies all kinds of stretch effects, has been derived theoretically in [4] and [5]. For the case of a constant pressure and single adiabatic reaction controlled by the concentration of the deficient reactant, a relationship has been introduced and can be written as

$$S_s - S_n = L_b \alpha - O(\varepsilon^2 S_s), \quad (2-3)$$

where $S_s$ and $S_n$ are the unstretched and stretched laminar flame front velocity, respectively, $L_b$ is the burned gas Markstein length, while $O$ designates a function. It is supposed, that $\varepsilon$,
the ratio of laminar flame thickness $\delta_l$ and the length scale of disturbance $\Lambda$, is much smaller than unity and the change of the laminar flame front velocity due to stretch is of first order.

### 2.3 Burned gas Markstein length and Markstein number

Markstein lengths characterize the variation in the local burning velocity or flame speed due to the influence of stretching. There exist linear relationships between stretch rates and the changes in flame speed or burning velocity. Apparently, there exist different Markstein lengths for strain rate and curvature. This work concentrates on the determination of the burned gas Markstein length $L_b$, which characterizes the linear relationship between the total stretch rate $\alpha$ and the change in the flame speed as

$$S_\delta - S_n = L_b \alpha.$$  \hfill (2-4)

The dimensionless Markstein number $Ma$ can be derived from the Markstein length $L_b$, normalized by the characteristic laminar flame thickness $\delta_l$:

$$Ma = \frac{L_b}{\delta_l}.$$  \hfill (2-5)

The flame thickness $\delta_l$ is normally calculated with the kinematic viscosity $\nu$ and the unstretched laminar burning velocity $u_l$:

$$\delta_l = \frac{\nu}{u_l}.$$  \hfill (2-6)
3 General procedure and data analysis

3.1 Ignition model and simulation of spherically expanding flames

A simplified model as shown in Fig. 3-1 is used for numerical simulation of the ignition process.

![Fig. 3-1: Schematic of ignition geometry with the energy deposition radius \( r_d \) and the flame front at three different time steps \((t_d, t_1, t_2)\)](image)

It is assumed that the ignition by a spark can be modelled with a spherical geometry, which means that the energy deposition kernel and the adjacent flame front propagation are spherical.

The energy source can be characterized by a deposition radius \( r_d \), deposition time \( t_d \) and deposited energy whereat the energy source term has a nearly rectangular shape described by the following equation:

\[
q = \frac{e}{t_d} \exp \left( - \left( \frac{r}{r_d} \right)^4 \right) \text{ for } 0 < t < t_d, \quad (3-1)
\]

\[
q = 0 \text{ for } t > t_d. \quad (3-2)
\]

Before energy deposition the unburned gas is in quiescent state. After energy deposition the adjacent flame front propagation is laminar.

For the numerical simulation of the ignition process and the adjacent flame front propagation the program INSLFA [6, 7], which can be used to simulate one-dimensional geometries, is used. This program solves the conservation equations of continuity, species mass, momentum and energy of the corresponding system, which may universally be written as [8]:

Continuity:

\[
\frac{\partial p}{\partial t} + \text{div}(pv) = 0 \quad (3-3)
\]

Specie mass:
\[ \frac{\partial \vec{w}_i}{\partial t} + \rho \vec{v} \cdot \nabla \left( \frac{w_i}{2} \right) + \text{div} \left( \frac{w_i}{2} \right) = w_i, M_i \]  \hspace{1cm} (3-4)

Momentum:

\[ \frac{\partial (\rho \vec{v})}{\partial t} + \text{grad}(P) + \text{div} \left( \frac{\rho \vec{v} \cdot \vec{v}}{2} \right) = 0 \]  \hspace{1cm} (3-5)

Energy:

\[ \frac{\partial (\rho h)}{\partial t} - \frac{\partial P}{\partial t} + \text{div} (\rho h) - \vec{v} \cdot \nabla \left( \frac{h}{2} \right) + \text{div} \left( \frac{h}{2} \right) + \text{div} (\rho \vec{v} \cdot \vec{v}) = q \]  \hspace{1cm} (3-6)

The equation systems used in INSFLA can be obtained by using the following simplifications and empirical laws:

Assumptions:

- Negligence of radiation, thus limiting heat loss from the flame
- Negligence of gravitation, hence no buoyancy and flame shape distortion
- Using of the Curtis-Hirschfeld-Assumption for the mass diffusion in a multicomponent mixture
- Negligence of the Dufour-Effect, thus mass diffusion has no influence on heat transport

Empirical Laws:

- Newton’s shearing stress law to account for viscosity effects
- Fourier’s law of thermal diffusion (conduction): rate of heat transfer proportional to the temperature gradient
- Fick’s law of diffusion in which the rate of mass diffusion is proportional to the concentration gradient
- Ideal gas law

After transformation into Lagrange coordinates, which leads to elimination of the convective terms, restriction to one-dimensional geometries (infinite slab, infinite cylinder and sphere), assumption of uniform pressure and usage of the ideal gas law, the following equation system for a spherical geometry results:

\[ \frac{\partial T}{\partial t} - \frac{1}{\rho r^2} = 0 \]  \hspace{1cm} (3-7)

\[ \frac{\partial P}{\partial T} = 0 \]  \hspace{1cm} (3-8)

\[ \frac{\partial T}{\partial t} - \frac{1}{\rho C_p} \frac{\partial P}{\partial t} - \frac{1}{\rho C_p} \frac{\partial}{\partial T} \left( \rho r^2 \frac{\partial T}{\partial T} \right) + \frac{1}{\rho C_p} \sum_{i=1}^{n} w_i h_i M_i - \frac{r^2}{C_p} \sum_{i=1}^{n} \rho D_i \left( \frac{w_i}{x_i} \frac{\partial x_i}{\partial T} + \frac{D_i}{T} \frac{\partial T}{\partial T} \right) C_i p \frac{\partial T}{\partial T} = \frac{q}{\partial T} \]  \hspace{1cm} (3-9)

\[ \frac{\partial \vec{w}_i}{\partial t} - \frac{\partial}{\partial T} \left( \rho D_i \left( \frac{w_i}{x_i} \frac{\partial x_i}{\partial T} + \frac{D_i}{T} \frac{\partial T}{\partial T} \right) \right) \frac{w_i M_i}{\rho} = 0 \]  \hspace{1cm} (3-10)
Spatial discretization using finite differences leads to a system of coupled differential and algebraic equations that are solved numerically. After each time step a new grid point system is calculated and the mesh is automatically adapted to the flame front in order to have a higher density of grid points in the reaction zone.

In the present computations spherical geometry is calculated with usually 130 grid points. Isobar pressure is assumed. Symmetry conditions are used as the boundary conditions at $\psi = 0$, the centre of the reaction vessel:

$$ \begin{align*}
  r = 0, \quad \frac{\partial T}{\partial \psi} &= 0, \quad \frac{\partial w_i}{\partial \psi} = 0. 
\end{align*} \quad (3-11) $$

At $\psi = \psi_0$, the outer boundary, conditions are simplified by assuming zero gradients of temperature and mass fraction:

$$ \begin{align*}
  r &= R_0, \quad \frac{\partial T}{\partial \psi} = 0, \quad \frac{\partial w_i}{\partial \psi} = 0. 
\end{align*} \quad (3-12) $$

The spherically expanding methane-air flames were computed up to a radius of 5 cm.

A full kinetic scheme for C1 with 56 species and 311 reactions used by Prof. Mass (Institute of Technical Thermodynamics, University of Karlsruhe, Germany) was adopted for the simulations demonstrated in the present study.
3.2 Approach to determine the minimum ignition energy

Fig. 3-2: Procedure to determine the minimum ignition energy $E_{i,\text{min}}$

Fig. 3-2 shows the general procedure used to determine the minimum ignition energy (MIE). The calculations are performed for a given set of ignition parameters deposition time $t_d$, deposition radius $r_d$ and equivalence ratio $\Phi$, while the energy input $E_i$ is varied. Starting from an energy value below the estimated MIE the energy input is increased stepwise till successful ignition and adjacent flame front propagation take place. For automation a software is used starting INSFLA calculations (see Chapter 3.1) and subsequently checking, whether it comes to self-preservative flame front propagation or energy is not high enough for successful ignition. In the latter case the energy is increased with a predefined amount and subsequently the calculation is restarted. The energy, at which a self-preservative flame front propagation occurs, is defined as the minimum ignition energy (MIE).

3.3 Simulation post-processing for extracting characteristic parameters to determine Markstein lengths and ignition properties

A post-processing of the simulations is necessary to get the parameters, which are necessary to characterize the ignition process and to get the burned gas Markstein length. The procedures to get those parameters are described in this chapter.
Flame front radius $r_{ff}$

Fig. 3-3: Temperature and mole fraction of HO$_2$ versus radius at a given time step

Fig. 3-3 shows the temperature pattern and the mole fraction of HO$_2$ of a spherical propagating laminar flame calculated with INSFLA. The flame front radius $r_{ff}$ describes the instantaneous distance between spherical flame front and centre of energy deposition. As the temperature profile in above figure shows, the temperature is increasing by leaps and bounds from the cold unburned fresh mixture’s temperature to the burned gas temperature within the flame front. At this point the mole fraction of HO$_2$ has a maximum, indicating the centre of the reaction zone. In this work the position marked through this maximum is defined as the flame front radius $r_{ff}$ and serves for calculating the stretched flame front velocity $S_n$ and the total stretch rate $\alpha$. 
Stretched laminar flame front velocity $S_n$ and stretch rate $\alpha$

![Graph showing flame front radius $r_{ff}$ versus time $t$.](image)

Fig. 3-4: Flame front radius $r_{ff}$ versus time of a successful ignition

Fig. 3-4 shows a typical course of the flame front radius versus time at successful ignition and adjacent self-preservative flame front propagation. The laminar flame front velocity $S_n$ is calculated as shown in above figure via the gradient at each point of the graph. This is done by numerical time derivation of the fitted radius-time curve. The flame stretch rate can then be calculated with the flame front radius: $\alpha = 2 \cdot S_n / r_{ff}$. The slope of $S_n$ plotted against $\alpha$ gives the burned gas Markstein length $L_b$. 
**Induction time** $t_i$

![Graph showing the stretched flame front speed versus time for a stoichiometric propane-air mixture within induction controlled region ($t_d = 600 \mu s$, $r_d = 6 \text{ mm}$)](image)

During the induction phase, the increased temperature in the hot spot causes the formation of a radical pool, leading to ignition. This phase is mainly controlled by the chemical kinetics and (if the induction time is sufficiently long) by diffusion and heat conduction. During the induction time the flame is not propagating. After induction time (i.e. after radical pool has grown) ignition of the hot spot follows and the flame starts propagating.

The flame front velocity versus time of a successful ignition in the induction controlled ignition region of a propane-air mixture is shown in Fig. 3-5. It is obvious that an erratic rising of the flame front velocity takes place right after induction phase. At this point the flame starts propagating. This point of time is defined as ignition time $t_z$. The induction time $t_i$ is determined by the difference of ignition time $t_z$ and energy deposition time $t_d$: $t_i = t_z - t_d$.

In the case of induction controlled ignition energy deposition time is much shorter than ignition time and induction time, and ignition are approximately the same.
It has been shown that a criterion for successful ignition is the hot gas kernel to reach a minimum size called the critical radius [9]. Ignition occurs because thermal diffusion from the hot kernel to the surrounding gas mixture is in equilibrium with the heat release by the chemical reaction. For flame radii smaller than the critical radius thermal diffusion from the hot kernel cools the kernel and leads to a reduction of the chemical reaction rate (decreasing flame front velocity). If the flame does not reach the critical radius at a sufficient high temperature due to affection by thermal diffusion for a self-preserving of the chemical reaction the thermal energy is not high enough and the flame extinguishes.

Therefore, the critical radius $r_c$ can be detected by the minimum of the laminar flame front velocity as shown in Fig. 3-6 at the minimum ignition energy.
4 Results

4.1 Markstein lengths

4.1.1 Markstein lengths for methane- and propane-air mixtures

4.1.1.1 Markstein lengths in comparison to values from literature and experimental results of deliverable no. 6

Methane-air Markstein lengths in comparison to experiments

Fig. 4-1 shows the computed Markstein lengths for methane-air mixtures in comparison to experimental ones of deliverable no. 6. Both computed and measured values show that the Markstein lengths increase with an increasing equivalence ratio and the tendencies - increasing Markstein length with increasing equivalence ratio - are in good agreement. Therefore, measured and computed results are comparable and can together be used for the interpretation of stretch effects on the laminar flame speed.

![Fig. 4-1: Simulated Markstein lengths for methane-air in comparison to experimentally determined Markstein lengths of deliverable no. 6](image-url)

Propane-air Markstein lengths in comparison to experiments

In Fig. 4-2 computed Markstein lengths for propane-air mixtures are shown in comparison to the experimental determined Markstein lengths of deliverable no. 6. The measured Markstein lengths are systematically higher than the computed Markstein length. Nevertheless, the
tendencies - decreasing Markstein length with increasing equivalence ratio - are reflected by the computations quite well.

Fig. 4-2: Simulated Markstein lengths for propane-air in comparison to experimentally determined Markstein lengths of deliverable no. 6
Methane-air Markstein lengths in comparison to values from literature

In Fig. 4-3 computed Markstein lengths for methane-air mixtures are shown in comparison to values from literature [10, 11, 12]. The values from Tseng et al. [11] and Aung et al. [12] at $\Phi=0.6$ are negative and different to the values calculated with INSFLA and the values of Bradley et al. [10]. This can not be explained here. Nevertheless, all other values are in good agreement with the computations of INSFLA.

![Graph showing simulated Markstein lengths for methane-air in comparison to values from literature](image)

Propane-air Markstein lengths in comparison to values from literature

In Fig. 4-4 computed Markstein lengths for propane-air mixtures are shown in comparison to values from literature [11]. The computed values are in good agreement to the experimentally determined Markstein lengths from Tseng et al. [11] though the experimental results of deliverable no. 6 are systematically higher than the computations (see Fig. 4-2). Assumingly the experimentally determined Markstein lengths of deliverable no. 6 have a systematic error whereas the computed values give good results. This error may be caused by influences of the electrodes on the spherical flame propagation, whereas the simulated flame is ideal spherical.
Fig. 4-4: Simulated Markstein lengths for propane-air in comparison to values from literature
4.1.1.2 Markstein lengths at elevated pressure

Methane-air

Fig. 4-5 shows the computed Markstein lengths for methane-air mixtures at different pressures and stoichiometries. It can be seen that independent of the stoichiometry the Markstein lengths becomes smaller with an increasing pressure. This means that the influence of stretch on the laminar flame front velocity is decreased for an increasing pressure. This is consistent with the result of Gu et al. [13].

![Graph showing Markstein lengths for methane-air at different pressures](image-url)
Propane-air

Fig. 4-6 shows the computed Markstein lengths for propane-air mixtures at different pressures and stoichiometries. As already observed in Fig. 4-5, the absolute values of the Markstein lengths become smaller with an increasing pressure independent of the stoichiometry. It is important to mention, that the negative Markstein length at $\Phi=1.666$ is increased and the positive Markstein lengths for $\Phi=1$ and $\Phi=0.666$ are decreased by an increasing pressure. This means, that the influence of stretch on the laminar flame is decreased by an increasing pressure.

![Graph showing simulated Markstein lengths for propane-air at different pressures](image-url)
4.1.2 The influence of fuel gas diffusion properties on the Markstein length

This chapter demonstrates the influence of the fuel gas diffusion coefficient on the Markstein length. Therefore, spherically expanding methane-air flames at equivalence ratios of 0.8, 1.0 and 1.25 have been carried out with the binary diffusion coefficient of N₂-CH₄ changed to a nonnatural value. Fig. 4-7 shows several Markstein lengths calculated with INSFLA. The abscissa of Fig. 4-7 shows the ratio of the binary diffusion coefficient N₂-CH₄ (indicated with a star ⊕, as changed to a nonnatural value for some simulations) to the binary coefficient of N₂-O₂ (kept constant to the natural value for all simulations). In nature the diffusion of methane is slightly higher than the diffusion of oxygen. The natural Markstein lengths of methane-air mixtures for the three different stoichiometries are therefore plotted on the black solid vertical line. To investigate the influence of the diffusion on the Markstein length, the binary diffusion coefficient of N₂-CH₄ has been set to the value of the binary diffusion coefficient of other fuels (C₃H₈, C₂H₆, H₂) as well as oxygen to nitrogen. Those results are plotted on the dotted lines. It can be seen, that this strongly influences the Markstein length.

Naturally, the Markstein length of methane-air mixtures increase with an increasing equivalence ratio, this can be seen on the values on the solid black line but also in Fig. 4-3. Setting the binary diffusion coefficient of N₂-CH₄ to the value of the binary diffusion coefficient of N₂-C₃H₈ turns around this behaviour. This can be seen on three values on the dotted line on the far left of the diagram. Though always the fuel gas methane is burned in these simulations, the Markstein lengths seem to show a dependency on the equivalence ratio as also observed for propane-air mixtures (see Fig. 4-4). For the diffusion coefficient of N₂-CH₄ set to a value of the diffusion coefficient of N₂-C₃H₈, the Markstein length decreases with an increasing equivalence ratio. Increasing the value of the binary diffusion coefficient of N₂-CH₄ to a value of the diffusion coefficient of N₂-H₂, leads even to a negative Markstein length for the lean mixture and to a not ignitable mixture for the rich methane-air composition.

![Fig. 4-7: Markstein lengths for methane-air mixtures at atmospheric conditions with the diffusion coefficient of methane-oxygen changed to nonnatural values](image-url)
Fig. 4-8 shows the corresponding simulated flame front speeds (taken at a radius of 5 cm of the spherically expanding flame) to the calculated Markstein lengths of Fig. 4-7. Though the Markstein length are strongly dependent on the diffusion coefficient of the fuel gas, the flame front speeds are hardly influenced.

This numerical experiment shows that the Markstein length is a parameter strongly influenced by the diffusion properties of fuel gas and oxygen. Not the chemical kinetics but the diffusion is the main parameter influencing the Markstein length. The effect of "preferential diffusion" has already been explained in deliverable no. 6. These calculations assert the theory and show the importance of simulations to understand the theory.
4.2 Minimum ignition energies

4.2.1 The influence of energy deposition time and radius on minimum ignition energy

In Fig. 4-9 the calculated minimum ignition energies and densities for stoichiometric propane-air mixtures and different deposition times are plotted against deposition radius.

For small deposition radii the minimum ignition energy is largely dependent on the deposition time and seems to tend to a constant value with decreasing energy deposition radius and constant deposition time. With longer deposition times the amount of energy for a successful ignition increases. This effect is stronger the smaller the deposition radius. This ignition region is called the \textit{diffusion controlled region}. In this region the heat loss, which is mainly due to the thermal diffusion, is the determining process of the ignition. The diffusion controlled region will be explained in Chapter 4.2.1.2.

For radii larger than about 1 mm the minimum ignition energy density reaches nearly a constant value for all deposition radii and times. The minimum ignition energy shows an asymptotic and deposition time independent behaviour. The minimum ignition energy increases proportional to the energy deposition volume ($\sim r_d^3$). This region is called the \textit{induction controlled region}. In this region the ignition process is mainly controlled by the formation of a radical pool within the induction time. This region will be explained in Chapter 4.2.1.1.
4.2.1.1 Induction controlled ignition

**Criterion for successful ignition**

For large deposition radii \((\text{induction controlled region})\) the ratio of surface of the deposition volume to deposition volume is smaller than for small radii \((\text{diffusion controlled region})\). As the heat of reaction is proportional to the volume:

\[
Q_{\text{comb}} = w_{\text{fuel}} h_{\text{cal}} V
\]  \hspace{1cm} (4-1)

and the heat flux is proportional to the area:

\[
Q_{\text{flux}} = \lambda A \frac{\partial T}{\partial r}
\]  \hspace{1cm} (4-2)

heat loss by diffusion in comparison to heat production by the exothermic chemical reaction is much smaller than in the diffusion controlled region \((Q_{\text{flux}} / Q_{\text{comb}} \propto 1/r)\). In the induction controlled region the thermal diffusion is almost negligible, compared to the diffusion controlled region, so that the MIE approximately depends only on the deposition radius and is independent from the deposition time. Thus the energy density is nearly constant. As one can see in Fig. 4-9 the energy density tends for a radius larger than 1 mm toward a constant value and is not depending on the deposition time.
Time flow of ignition

Fig. 4-11: Induction controlled ignition ($E_i=144.4$ mJ, $t_d=600$ µs, $r_d=4$ mm) of stoichiometric propane-air at atmospheric conditions: temperature (left) and mole fraction CH$_3$ (right) versus radius and time.

Fig. 4-11 shows the spatial temperature and CH$_3$ mole fraction profiles in time. As one can see the temperature profile remains almost unchanged between deposition time and induction time, which is much longer than the deposition time ($t_i=4.5$ ms, $t_d=600$ µs). This demonstrates that the heat loss by thermal diffusion is very small for an induction controlled ignition. After the induction phase the temperature arises erratically to the burning temperature and the flame front, indicated by the rise in temperature within the reaction zone, starts to propagate. Beholding the CH$_3$ mole fraction profile one can see a first slow than faster increase of the CH$_3$ mole fraction in the centre of the ignition kernel within the induction phase. A radical pool is formed during the induction phase, which decomposes suddenly in the consecutive reaction at the time of ignition. It is then reaching a constant peak value while the flame front propagates. Looking at the CH$_3$ mole fraction profile one can see that there is a sharp peak in position of the flame front due to the main reaction is taking place there. The CH$_3$ radical is just an intermediate of the reaction mechanism. Therefore the flame front is well indicated by the CH$_3$ mole fraction.
4.2.1.2 Diffusion controlled ignition

Criterion for successful ignition

Fig. 4-12: Diffusion controlled ignition ($t_d=600 \mu s$, $r_d=0.2 \text{ mm}$) of stoichiometric propane-air at atmospheric conditions: temperature profiles at three different points in time; unsuccessful ignition at $E_i=542.1 \ \mu \text{J}$ (left), successful ignition at $E_i=542.2 \ \mu \text{J}$ (right)

Fig. 4-12 shows three temperature profiles at different points in time in case of successful and unsuccessful ignition. Looking at these graphs one can see that the temperature after energy deposition is much higher in comparison to the temperature in the induction controlled region, even if the energy amount is not high enough for a successful ignition with adjacent flame front propagation. Further one can notice a local raise of the temperature profile starting in the centre of the energy deposition volume. This is a sign of an already starting exothermic chemical reaction, meaning that the exothermic reaction can start in the diffusion controlled region even if the energy input is lower than the MIE. Because of the small energy deposition radius the heat diffusion is high and the temperature is then decreasing rapidly in case of an energy value smaller than the MIE. If the minimum ignition energy is reached, the temperature is first decreasing after energy deposition. After passing a critical radius the temperature is increasing and reaches the burned gas temperature. This is shown in Fig. 4-13. This figure shows the temperature in the centre of the ignition kernel ($r=0 \text{ mm}$) versus time of a diffusion controlled ignition.

Beside the thermal diffusion, the gas expansion due to the decreasing density in the kernel during energy deposition leads to a flattening of the temperature profile. This has surely no influence for the induction controlled ignition as ignition time is much longer than deposition time and the deposition radius does not significantly influence the minimum ignition energy density. In the diffusion controlled region it could have an influence, but on the other hand, the critical radius is always larger than the deposition radius. For the ignition in Fig. 4-12 and 4-13 the critical radius is about 0.6 mm. It is difficult to understand the impact of the gas expansion on the ignition. In the next deliverable the critical radius will be investigated for ignitions at different stoichiometries and more information will be available to understand the influence of different parameters on the critical radius.
In comparison to the induction controlled ignition, in the diffusion controlled region the ratio of energy deposition surface to volume is larger while energy deposition takes place. Therefore the thermal diffusion is high. So the power input has to be high enough to conserve the chemical reaction as far as a radius is reached at which the heat loss due to thermal diffusion is at least equal to the heat production by the exothermic chemical reaction. This equilibrium is reached at the so called critical radius $r_c$. In the diffusion controlled region the criterion for a successful ignition is to reach this critical radius. Due to the strong influence of the thermal diffusion in the first ignition phases the minimum ignition energy is highly depending on the deposition time and hence on power.

**Time flow of ignition**

Fig. 4-14: Diffusion controlled ignition $(E_i=542.2 \, \mu J, \, t_d=600 \, \mu s, \, r_d=0.2 \, \text{mm})$ of stoichiometric propane-air at atmospheric conditions: temperature (left) and mole fraction CH$_3$ (right) versus radius and time
The right plot of Fig. 4-14 shows the spatial CH\textsubscript{3} mole fraction profiles in time. During deposition phase the CH\textsubscript{3} mole fraction rises rapidly to a high level due to power input and increasing temperature. The reaction starts already during energy deposition phase. After the energy deposition the mole fraction is decreasing fast to a minimum, as the temperature decreases and the reaction is slowed. This can also be seen in the left plot of Fig. 4-14, in which the spatial temperature profiles are plotted against time. After the temperature rise in the deposition phase a rapid decay of the temperature occurs. The reason is the higher thermal diffusion in comparison to the heat produced by the exothermic chemical reaction. Due to the strong dependency of the CH\textsubscript{3} formation on the temperature the CH\textsubscript{3} mole fraction decreases too. After passing the critical radius the thermal diffusion is decreasing to a level lower than the heat release of the exothermic reaction and the flame becomes self-preservative. Temperature as well as CH\textsubscript{3} mole fraction and laminar flame front velocity increase again till they reach a nearly constant level. The temperature approximates the combustion temperature and the flame front velocity approximates the planar laminar flame front velocity.

### 4.2.2 Ignition process of stoichiometric propane-air in comparison to methane-air mixture

![Graph showing minimum ignition energies](image)

Fig. 4-15: Minimum ignition energies of stoichiometric methane-air (left) and propane-air (right) mixtures versus deposition radius at various deposition times and atmospheric conditions

In this work calculations for stoichiometric propane-air and methane-air mixtures have been carried out. All calculated minimum ignition energies are shown in Fig. 4-15. The ignitions of both fuels - those of the methane-air mixtures and those of the propane-air mixtures - are showing the same typical behaviour for large and small deposition radii and long and short deposition times. For both fuel-air mixtures one can see the two different ignition regions: the diffusion controlled and the induction controlled region. A difference is that the minimum ignition energy for propane-air mixtures is at the same set of ignition parameters lower than the minimum ignition energy of methane-air mixtures. This arises from the more stable methane molecule and is consistent with values form literature. More energy is needed to break up the methane molecule than the propane molecule.
5 Conclusion

The present report documents the modelling of Markstein lengths and minimum ignition energies. The method and software have been described and it has been shown, that Markstein lengths and minimum ignition energies can be calculated.

Markstein lengths

Post-processing software to analyze the calculations and to get Markstein lengths from the simulations of spherically expanding flames has been developed. Subsequently, Markstein lengths for methane- and propane-air mixtures for different stoichiometries and pressures up to 9 bars have been calculated. The results have been compared with the experimental results of deliverable no. 6 and validated with values from literature. The good agreement with the values from literature show, that the model works and it can be used to get Markstein lengths for mixtures where there are no experimental results.

Minimum ignition energies

Software that accelerates the modelling of minimum ignition energies has been developed. Consecutively, minimum ignition energies for stoichiometric methane- and propane-air mixtures have been calculated. The influence of the energy deposition radius and energy deposition time on the MIE has been investigated. It has been shown, that there are two ignition regions, the induction controlled ignition for larger radii and the diffusion controlled ignition for smaller radii. It has been shown that spatial and temporal profiles of temperature and species mole fraction give important information. With the data of the simulations the mechanisms of the induction and diffusion controlled ignition could be explained and understood.
## Listings

### Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
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<tr>
<td>$A$</td>
<td>m$^2$</td>
<td>Surface</td>
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<tr>
<td>$C_p$</td>
<td>kJ/K</td>
<td>Heat capacity</td>
</tr>
<tr>
<td>$E_{\text{min}}$</td>
<td>J</td>
<td>Minimum ignition energy (MIE)</td>
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<tr>
<td>$E_i$</td>
<td>J</td>
<td>Energy Input</td>
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<td>Diffusion flux of species i</td>
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<td>Burned gas Markstein length</td>
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<tr>
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</tr>
<tr>
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</tr>
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<td>Energy deposition radius</td>
</tr>
<tr>
<td>$r_{ff}$</td>
<td>m</td>
<td>Flame front radius</td>
</tr>
<tr>
<td>$r_{HO_2}$</td>
<td>m</td>
<td>Flame front radius by maximum of HO$_2$ mole fraction</td>
</tr>
<tr>
<td>$S_n$</td>
<td>m/s</td>
<td>Stretched laminar flame front velocity</td>
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<td>$t_z$</td>
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</tr>
<tr>
<td>$\vec{v}$</td>
<td>m/s</td>
<td>Velocity vector</td>
</tr>
</tbody>
</table>
\[ w_i \text{ mol m}^{-3}\text{s} \]

Molar scale rate of formation of species \( i \)

**Greek**

- \( \alpha \) \( \frac{1}{\text{s}} \) Flame stretch rate
- \( \delta_i \) \( \text{m} \) Laminar flame thickness
- \( \varepsilon \) - Air factor
- \( \lambda \) - Length scale of disturbance
- \( \Lambda \) \( \text{m} \) Length scale of disturbance
- \( \rho \) \( \frac{\text{kg}}{\text{m}^3} \) Density
- \( \Pi \) Stretch tensor
- \( \Psi \) Lagrange Coordinate
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