

### UNIVERSIDADE ESTADUAL DE CAMPINAS Faculdade de Engenharia Química

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## COMPUTATIONAL MODELLING OF LAMINAR BURNING VELOCITY OF GASES VENTED BY LI-ION BATTERIES

### MODELAGEM COMPUTACIONAL DA VELOCIDADE DA CHAMA LAMINAR DE GASES EXPELIDOS POR BATERIAS DE LÍTIO

CAMPINAS - SP 2023

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Supervisor: Prof. Dr. Sávio Souza Venâncio Vianna

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## Resumo

Devido aos efeitos das mudanças climáticas, a implementação de fontes alternativas e renováveis de energia tem crescido na última década. A energia solar e eólica tornaram-se opções notáveis devido à falta de resíduos sólidos. No entanto, atualmente, o mercado é liderado pelas baterias de íons de lítio (LIBs) devido à sua alta densidade de energia, baixo peso e ciclos de descarga mais baixos em comparação com outras baterias. No entanto, o uso dessas baterias também revelou problemas associados a condições de superaquecimento e abuso térmico. O aumento da temperatura interna da bateria nos cenários mencionados acima pode ser a causa de um processo chamado de fuga térmica (TR), no qual a bateria, quando exposta a operações ou ambientes com alta temperatura, começa a sofrer reações de decomposição de eletrólitos, gerando gases tóxicos e inflamáveis. Isso aumenta a pressão dentro da célula até que seja atingido um ponto em que a bateria tenta reduzir sua temperatura interna e expelir esses gases, criando um risco de explosão se entrar em contato com uma fonte de calor próxima. O objetivo desta pesquisa é obter uma equação para a velocidade de queima de chama laminar (LBV) para esses gases. Portanto, é pertinente desenvolver uma correlação matemática que descreva a velocidade laminar da chama em explosões causadas por baterias de lítio. Para isso, serão utilizadas simulações por meio de fluidodinâmica computacional (CFD), usando o software de código aberto STOKES.

Palavras-chave: explosões, baterías de litio, thermal runaway, abuso térmico, simulações, superaquecimento.

# Abstract

Due to the effects of climate change, the implementation of alternative and renewable sources of energy has grown over the last decade. Solar and eolic energy have been strong contenders for the number one spot for their lack of solid waste. However, in this present time the market is lead by lithium-ion batteries (LIBs) for their high energy density, low weight and lower discharge cycles compared to other batteries. In the last few years LIBs have been associated to explosion incidents, this is due to a process called thermal runaway that can be triggered by a plethora of technical factors associated with overheating. During this process, exothermical decomposition reactions start to occur inside the solid electrolyte interphase (SEI) adding to the highly volatile nature of lithium and rising the pressure and temperature even more. It reaches a certain point that the battery releases all of the heat that has been building up inside, ejecting toxic and flammable gases that have been the cause of the aforementioned incidents. The objective of this research is to obtain a new correlation for the laminar burning velocity of the vented gases by failed LIBs to further understand the propagation of this flames through the use of computational fluid dynamics and open-source code STOKES.

**Keywords**: explosion, lithium batteries, thermal runaway, computational fluid dynamics, thermal abuse, simulations, overheating.

## Resumen

En la última década la implementación de energías renovables ha sido notable a raíz de la emergencia causada por por el cambio climático y gases de efectos invernaderos. Dentro de estas nuevas alternativas, se encuentran las baterías de litio (LIBs) que ya eran usadas en aplicaciones de dispositivos electrónicos, su uso se ha expandido a otras áreas tales como en la industria automotriz y almacenamiento de energía en operaciones industriales por medio de estaciones de almacenamiento de energía (BESS). Sin embargo, con su uso también se han descubierto defectos asociados a condiciones de sobrecalentamiento, abuso térmico. El aumento de temperatura interna dentro de la batería en los escenarios anteriormente mencionados puede ser la causa detonante de un proceso llamado fuga térmica (TR) en el cual la batería cuando es expuesta a operaciones o ambientes de con alta temperatura comienza a sufrir reacciones de descomposición de electrolito generado gases tóxicos e inflamables, aumentando la presión dentro de la celda de energía, hasta que que se llega a un punto que la batería intenta disminuir su temperatura interna y expulsa estos gases, creando un riesgo de explosión si entra en contacto con una fuente de calor en las cercanías. El objetivo de esta investigación es obtener una ecuación para la velocidad de quema de llama laminar (LBV) para estos gases ya que considerando los últimos incidentes de explosiones accidentales causadas por LIBs es pertinente desarrollar una correlación matemática que describa la velocidad de la llama en explosiones causadas por baterías de litio. Para esto se utilizarán simulaciones por medio de dinámica computacional de fluidos (CFD), utilizado el software de código abierto STOKES.

**Keywords**: explosion, baterias de litio, fuga térmica, dinámica computacional de fluidos, abuso térmico, simulaciones, sobrecalentamiento

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# Chapter 1

# Introduction

Computational fluid dynamics (CFD) has simplified the study of accidental explosions in the process industries. Premixed combustion can occur when the flammable cloud or fuel is mixed with an oxidant agent. Besides typical petrochemical scenarios, explosion incidents can also happen when using renewable energy sources. For this study, explosions caused by vented gasses of Lithium-ion batteries will be the sole focus.

Empirical studies have been conducted for studying the cause of explosions by LIBs. Thermal runaway is the reason for this. It is caused by overheating or thermal abuse conditions that can be provoked by a plethora of technical factors, all associated with the rise in internal temperature of the LIB(Wang et al., 2017). When li-ion batteries are exposed to high temperatures, decomposition reactions start to occur inside the battery cell generating flammable and toxic gases, such reactions are exothermic and rise the temperature even more while also inner pressure starts to build up (Golubkov et al., 2013).

By implementing CFD simulations, thermal runaway can be studied to understand subsequent explosion incidents. Thus, by using empirical data it is possible to obtain a mathematical correlation to analyze and predict flame velocity in explosions caused by flammable gasses vented by LIBs.

In the last few years, several numerical models have been developed to understand the propagation of thermal runaway dispersion and combustion of the flammable cloud ejected by these batteries. So far, the developed models have been able to represent accurately the evolution of electrothermal and kinetic parameters during thermal runaway. Also, CFD simulations have successfully represented the propagation of thermal runaway from one battery to another as well as temperature distribution profiles during venting(Wang et al., 2021). Dispersion CFD studies regarding lithium batteries have very prominent in the last few years. However, explosion modeling of LIBs is an area in which knowledge can be deepened. Thus, this work aims to push the boundaries in the modeling of accidental explosions caused by lithium-ion batteries and overpressure effects. Taking this into consideration, simulations of premixed combustion will be conducted by using the open-source code tool STOKES developed by Ferreira and Vianna (2021), designed to carry out premixed explosion simulations in complex geometries. For this study, the considered geometry is a rectangular channel of 1 meter in length. Parameters such as flame temperature, speed, and pressure will be studied by running several CFD cases.

This work introduces the modelling of explosions caused by vented gasses of LIBs using CFD simulations, for the composition of Lithium iron Phosphate batteries (LFP), studied by Henriksen et al. (2021).

The application of transport phenomena concepts in a programming language allows understanding of how some simulators might work such as FLACS and ANSYS. Moreover, some of these simulators require an additional high cost for acquiring their license, and their frameworks are usually complicated to be comprehended by researchers. Thus, by modifying the source code of STOKES, the proposed laminar burning correlation will be used to calculate flame speed and propagation. Moreover, future studies can be easily analyzed in different explosion scenarios.

The contribution of this work will be to further improve STOKES development process for the sake of simulating scenarios of accidental explosions besides that conventional petrochemical incidents.

### 1.1 Objectives

#### 1.1.1 General Objective

The general objective of this study is to develop a mathematical correlation for the laminar burning velocity (LBV) of gases vented by lithium-ion batteries by executing premixed explosions simulations in a semi-confined geometry, to predict overpressure in accidental explosions.

### 1.1.2 Specific Objectives

The specific objectives of this study are:

- Estimate and predict velocity and propagation of the flame in accidental explosions caused by failed LIBs;
- Validate the obtained correlation with pre-existing experimental data from the literature;
- To compare and analyze the obtained results of the simulated cases with compositions of gases ejected by batteries with cases carried out with flammable clouds of one component.

### **1.2** Organization of this Dissertation

This dissertation is intended to fill part of the gap regarding explosion modeling of accidental explosions caused by LIBs and to create a discussion about other LBV correlations that could be presented by using different compositions of vented gases. Chapter 1 is intended to introduce the reader to CFD, and thermal runaway in LIBs along with the main objectives of this research. Chapter 2 will present the fundamental concepts of an explosion caused by lithium batteries and empirical and numerical research that has been done on this topic. Chapter 3 will elaborate on the concepts of premixed combustion and the main equations that are used by STOKES and CFD's software in general to run explosion cases. In Chapter 4 the reader is going to find the proposal of this project and the respective methodology of all the computational tools that will be applied. Finally, chapter 5 will display the obtained results for the proposed study and will discuss the numerical findings and compare them to the experimental data.

# Chapter 2

# **Fundamental Concepts**

### 2.1 Accidental gas explosions

The possibility of catastrophic scenarios in industrial processes is amplified when a flammable cloud is released into the atmosphere. The outcome of such scenarios relies on whether the ignition happens right away after finding a heat source or after an undetermined period. Accidental gas explosions are the repercussion of delayed ignition, in this scenario oxidizer and fuel combine each other to form a flammable cloud before ignition takes place(Jerketvedt et al., 1997).

The flammability of the cloud is highly dependent on the composition of the volatile compounds within it. The combustion process of the mixture of air and fuel is only feasible if they are at a specific interval of composition. Upper and lower flammability limit. The blast generated by the explosion itself is defined by turbulence while parameters such as rate of combustion, dictate the degree of destruction caused by the explosion(Li et al., 2018).

The main repercussions of accidental gas explosions are associated with the effects of overpressure during combustion, which can be the cause of other accidental events, causing a chain reaction of incidents(Eckhoff, 2016).

Usually, accidental explosion incidents are detonated by a series of different events that ultimately lead to the ignition of the flammable cloud. A leakage, being the point of conception of this kind of accident is the consequence of a loss of containment that can be caused by multiple factors in industrial operations. Loss of containment in operations where lithium-ion batteries are used is caused by thermal runaway. The following section will elaborate on the fundamental concepts of this phenomenon and how it has been studied throughout the last few years.

## 2.2 Thermal Runaway and Experimental studies

Lithium-ion battery applications have expanded in recent years, their use ranging from implementation in electronic devices to transport applications. In addition to being an alternative energy source which is very necessary considering the effects of climate change due to anthropogenic activities, this type of battery has more capacity than other types of conventional batteries and also has a longer life cycle. However, they also have disadvantages. When exposed to high-temperature environments, a process called thermal runaway occurs in which, due to the abrupt increase in temperature, the solid electrolyte interphase (SEI) faces a decomposition process, generating toxic and flammable gases, at the same time high pressures begin to be generated inside the battery until reaching a point where the gases are released and if ignited they can be the cause of an explosion.

Accidents in which lithium-ion batteries were the cause of explosions have been reported in the past decade, as was the case in 2019 when there was a battery energy storage system (BESS) explosion in Arizona caused by the spread of thermal runaway from one set of batteries to another (DNV.GL, 2020). It is for this reason that is justified the relevance of research in which the process of thermal runaway is studied as well as the variables and conditions that facilitate this process. In this section, the reader will find the most relevant information found in the literature from li-ion batteries, regarding thermal runaway and collaborating factors that can cause an explosion.

A commonly studied variable in lithium battery research is the influence of battery state of charge (SOC%) on accidental explosions, Wang et al. (2017) Analyzed through experiments the behavior of lithium battery explosions in different SOCs. It was found that explosions, where the SOC of the battery is close to 100% or under overcharge conditions, tend to be more violent compared to explosions with lower states of charge. Key parameters such as total heat release (THR) and heat release rate (HRR) were also studied, these two are key in the study of fires caused by accidental explosions since they are an indicator of the amount of energy that is being released in such fires. For this, new safety regulations have been implemented for the use of LIBs in industrial operations, for example, in South Korea, a limit of 90% SOC has been established in energy storage stations in urban settings.

TR has been studied in a variety of ways, Li et al. (2019) studied the effect of the space between the heat source and a battery in different states of charge, to analyze this process under different side heating conditions. it was established that higher spacing and lower heating power contribute to mitigating or avoiding thermal runaway.

The amount of energy required to reach TR decreases with higher SOCs Zang et al. (2016) evaluated the behavior of thermal runaway in LIBs under different heating conditions and calculated the amount of heat required to reach thermal runaway in different SOCs, from 30% to 50% only small amount of gases were vented, however from 70% to 100 % sparks and burning was observed, with jet fires only occurring at 100% SOC. Battery cells with lower states of charge required more heat to reach thermal abuse conditions. Also, it is important to clarify that thermal abuse and thermal runaway are not the same thing. Overheating conditions caused by thermal abuse can give way to thermal runaway that can ultimately lead to an explosion incident.

As mentioned, when the battery cell reaches certain peaks of temperature and pressure it begins to eject toxic and flammable gases, the composition of such gases is going to vary depending on the employed electrolyte. The components of this mixture of gases have been studied in the past by Golubkov et al. (2013), who managed to determine the flammable species in the gases vented by commercial Nickel-Cobalt-Aluminum (NCA), lithium Ferro phosphate batteries (LFP), and lithium cobalt oxide (LCO) under thermal abuse conditions. Table 2.1 illustrates the detected compounds and elements in the flammable mixture expelled by these batteries.

Table 2.1: Detected components in experiments in mole percentage. (Golubkov et al.,2013)

Type of Battery	$H_2(\%)$	$\operatorname{CH}_4(\%)$	$\operatorname{CO}_2(\%)$	CO(%)	$C_2H_4(\%)$	$C_2H_6(\%)$
NCA	30.8	6.8	41.2	13.0	8.2	-
LCO	30.8	7.7	24.9	27.6	7.7	1.2
LFP	30.9	4.1	53.0	4.8	6.8	-

Once studied the correlation of employed electrolyte and the composition of

the vented flammable gases, it was pertinent to further analyze the influence of other parameters in the concentration of volatile and flammable components in the gaseous mixture. Which is why, the author carried a similar study in later years, by carrying out experiments with NMC, LFP and lithium titanate (LTO) batteries with a SOCs ranging from 0% to 100%sGolubkov et al. (2015). The content of the flammable species within the flammable cloud is going to rise in batteries at higher states of charge. It is for this reason that failed LIBs with a SOC near 100 % are associated with explosion incidents of higher magnitude.

Table 2.2: Detected components in experiments in mole percentage.(Golubkov et al., 2015)

Type of Battery	%SOC	$H_2(\%)$	$CH_4(\%)$	$\operatorname{CO}_2(\%)$	CO(%)	$C_2H_4(\%)$	$C_2H_6(\%)$
NCA	25	15	8.7	62.7	2.5	7.5	1.2
NCA	100	28.5	5.9	17.5	41.5	1.3	0.03
LFP	25	7.1	1.2	85.3	3.1	3.1	0.2
LFP	100	29.4	5.4	48.3	9.1	7.2	0.5

Table 2.2 shows the variation of the most prominent flammable components and species that were detected by recreating thermal abuse conditions in LIBs at different SOCs. Please examine the LFP battery in the aforementioned table, it can be observed that the amount of hydrogen is larger in flammable clouds expelled at higher states of charge. This is a more detailed argument of why more violent and higher magnitude explosions are often caused by fully or overcharged battery cells.

The study of parameters such as upper and lower flammability limits are important as well since they determine the maximum and minimum concentration of a compound that will result in a flammable reaction if a heat source is provided. Chen et al. (2020) presented an experimental method in order to establish the lower explosion limit (LEL) of gases vented by lithium batteries in different states of charge at different heating temperatures. However, the implemented method has problems regarding the consistency of the results, since the tests to calculate The LEL had to be carried out more than once with more than two batteries in each group, affecting the gas collection process and the precision of the obtained results.

Despite their valuable contributions, experimental and/or empirical investigations of LIBs have a limiting factor. Some research centers lack this type of specialized equipment and its purchasing cost is high. Likewise the amounts of energy that must be produced must be very high and in some cases for very long periods of time, as is the case of the study presented in the works of Yuan et al. (2016) that carried out test by accelerated rate calorimetry (ARC) to study the composition of LFP, NMC, and LTO battery cells and other kinetic parameters such as self-heat rate and information related to pressure parameters are studied. Also, experimental projects that study explosion on BESS on a 1:1 scale are too expensive, considering the cost of the sensors and containers to simulate explosions in energy storage operations.

The generation of flammable and toxic fumes during TR are the result of decomposition reactions in the solid electrolyte interphase. Researchers have also managed to study TR by surveying the materials that compose the SEI and their chemical stability, due to the high volatility of lithium. The knowledge of reaction kinetics during the decomposition process of the electrolyte has not been fully grasped, consequently restricting computational scientists that seek to comprehend ion conducting mechanisms of the SEI in order to mitigate the chances of reaching TR and optimizing future designs of the solid intherphase.

Taking into consideration all the aforementioned limitations, new alternatives have been proposed in order to study thermal runaway and explosions caused by LIBs. In recent years works cited above, have worked as a benchmark for the elaboration of numerical models and simulation through CFD simulations in order to analyze, predict thermal runaway, optimize future designs of LIBs and to further understand LBV and propagation of the flame in accidental explosions.

### 2.3 Numerical Modeling and CFD Simulations

As stated in the introduction of this project, researchers around the globe have used the data obtained in experiments on thermal runaway to elaborate numerical models and CFD simulations from them. By doing this the budget of projects of this kind could be much lower in comparison to the purchase of specific equipment. Nevertheless, the computers that run simulations of this kind must be able to process and execute the calculations to solve the governing equations in each control volume.Voigt et al. (2022) simulated thermal abuse conditions by using the sensible enthalpy rise approach (SERA). This technique consists of balancing the heat flows inside the testing facility/geometry, quite similar to ARC tests, obtaining quite accurate results after comparing them to experimental data similar to the ones obtained by experimental projects. Yuan et al. (2016).

$$HRR = \dot{m}C_{\rm p,air} \cdot (T_{\rm out} - T_{\rm amb}) + C_1 \cdot (T_{\rm w} - T_{\rm amb}) + C_2 \cdot \frac{dT_{\rm w}}{dt}$$
(2.1)

Equation 2.1, shows the expression that (Voigt et al., 2022) used to calculate HRR. Other variables such as  $C_1$  and  $C_2$  constants are calculated according to the setting of the calorimeter apparatus.

Researchers have been driven to study thermal runaway through numerical methods and simulation using computational fluid dynamics methods. Projects of this type usually have information compiled from previously published articles or display results of experiments carried out by themselves for the subsequent validation of the elaborated model. However, one of the disadvantages of building numerical models and simulating them is the precision of the obtained results, since there are in some cases discrepancies between experimental results and results from simulations.

Wang et al. (2021) carried out experiments to analyze the propagation of thermal runaway in an NMC battery module in different SOCs, later using the experimental information to perform the validation of a one-dimensional model and a 3D electrothermal model elaborated to establish a correlation between battery charging process and abusive operation conditions, respectively. These models were applied for further examination by using CFD simulation methods.

$$\rho C_{\rm p} \frac{dT}{dt} = \lambda \nabla^2 T + q_{\rm rea} + q_{\rm act} + q_{\rm ohm} + q_{\rm abu}$$
(2.2)

Equation 2.2, is the corresponding expression for the 3D electrothermal model. According to this, the generation of heat that is produced in abuse conditions is divided into four different stages that can parallel one another. The terms regarding heat generation (q) are yielded from the heating due to chemical decomposition reactions, polarization, electrical resistance, and thermal abuse respectively. Valuable kinetic parameters were determined in this paper, such information can be used for the elaboration of a model of reaction kinetics during TR. Propagation speed and time interval were successfully modeled and simulated. In investigations of this type, it would be pertinent to study the behavior of the gases vented by each of the batteries in the module, the average pressure at which the batteries eject the gases generated by the decomposition of the electrolyte, and the variation in the composition of the gases while considering the number of batteries in the module, it would be important to establish whether the composition varies linearly or in some other way, as well as its behavior through dispersion simulations.

Kim et al. (2021) presented a numerical model to study the internal pressure of the cell venting during thermal runaway. This model considered reaction parameters studied in previous literature to be able to study the kinetics during the decomposition of the SEI to accurately predict vapor generation during thermal runaway. Additionally, the developed model was used to simulate the distribution of the temperature and pressure profiles during venting by using CFD. Equations 2.3 and 2.4 are the expressions for the volumetric rate of gas generation and rate of reaction progress during thermal runaway. The xW term represents the global composition of volatile gas. Ostanek et al. (2020) Managed to introduce a similar model based on Dalton's law and heat flow balances to represent pressure venting and heat generation during thermal runaway. Their most recent study presented by Li et al. (2021) presented a set of dispersion simulations that were the result of the analysis of different cap designs for LIBS, accurately calculating a representing velocity of the gas current coming out the cell and their mass flow.

$$\dot{S}_{\rm m,ab} = xW\frac{d\alpha}{dt} \tag{2.3}$$

$$\frac{d\alpha}{dt} = -A_{\rm ab}(\alpha)^m (1-\alpha)^n exp(-\frac{E_{\rm a,ab}}{RT}) exp(-B_{\rm ab}\alpha)$$
(2.4)

Most of the models that have been introduced in the literature on lithium-ion batteries are predominately for gas/heat generation and the spread of thermal runaway in single cells or battery modules. Nonetheless, at the beginning of this decade, researchers started to study the behavior of the ignition of the vented gases by LIBs while also studying onset temperature and venting pressure. Kong et al. (2022) presented a conjugated model that consisted of a pressure and gas accumulation model built to represent venting during thermal runway and an electro-thermal sub-model based on the kinetics of the reaction of decomposition, it is indeed similar to the models shown previously in this section, but this study was notable because of the CFD simulations that were subsequently made, managing to simulate the propagation of thermal runaway through the cell, jet fires, and flame height. These parameters were studied with SOCs ranging from 25% to 100%. The compared model managed to predict the onset temperature with small differences from the temperature obtained through empirical means. However, simulated flame height results presented bigger discrepancies when compared to the experiments.

$$\rho C_{\rm p} \frac{dT}{dt} = \nabla \cdot (k \nabla T) + \Sigma \dot{Q}_{\rm i}$$
(2.5)

$$\frac{dP_{\text{cell}}}{dt} = \frac{dP_{\text{DMC}}}{dt} + \frac{dP_{\text{gas}}}{dt}$$
(2.6)

Although the previously presented models represent a valuable contribution toward understanding and avoiding thermal runaway, explosion modeling has not been fully explored yet. Henriksen et al. (2021) paved the way for this topic by studying through experiments and CFD simulations premixed combustion using the composition of gases vented by LFP batteries, by using the equation presented by Gulder (1984) (see eq 2.7) and finding the corresponding coefficients through the use of the solver Mech2foam elaborated by themselves. Projects such as these can be the benchmark of future papers for the elaboration of other LBV equations, which is the main focus of this study.

$$u_{\rm L} = \omega \phi^{\eta} e^{\xi(\phi - 1.075)} (\frac{T}{T_{\rm ref}})^{\alpha} (\frac{P}{P_{\rm ref}})^{\beta}$$
(2.7)

In other terms, empirical methods are often used to characterize several parameters during thermal runaway and/or thermal abuse. This information is further analyzed to then proceed with the elaboration of models, which then are used to simulate by using CFD. Besides characterization purposes, CFD simulations are also useful to study other variables and processes of LIBs other than a thermal runaway. Jindal et al. (2022) Analyzed through simulations the cooling process in a multi-tier battery pack of NMC cells to explore the effect of additives such as graphene nanoplatelets (GNPs) during operation in electric vehicles. Two sets of different simulations were performed. On the first one, a common mixture of ethylene glycol (EG) and water was used acquiring readings of an approximate maximum temperature of 59.186 °C. A mixture of EG/water was used with 0.001 vol% of GNP on the second set of simulations, the lowest obtained temperature was 42.250 °C. By keeping the temperature between 35°C and 45°C the lifespan of a battery can be extended. Thus by research and development projects of this kind, thermal runaway and its propagation can be avoided in applications in which LIBs are used while optimizing the designs of battery coolant modules.

It is the purpose of this work to elaborate and obtain an equation for the laminar burning velocity based on the composition of the vented gases by LIBs, previous developed LBV equations have done so by using the composition of mixtures of methane or other hydrocarbons and an oxidant agent. After obtaining such correlation, CFD simulations will be executed to validate the obtained results with experimental data from the works of Henriksen et al. (2021)

# Chapter 3

# Numerical Modelling and Premixed Explosions

This section shows the underlying mathematical correlations that will be studied in this work, as well as the theoretical foundation of numerical modeling in premixed explosions. The study and application of governing equations such as mass, momentum, and energy conservation equations will be the first to be examined. Followed by a brief discussion of the Bray-Moss-lybby framework and the concept of laminar burning velocity and their relevance for this project. Finally, some closing remarks on turbulence will also be made. This section has the purpose of laying out the physical basis of this study.

### 3.1 Governing equations

The governing equations are considered to be the backbone of every CFD study. These equations are solved in every control volume of the computational domain by implementing discretization methods to obtain an approximate numerical solution. The discretization method in this study will be the finite volume method (FVM)(Versteeg and Malalasekera, 2007). Furthermore, in this section, the reader will find all the necessary information regarding the use and study of such elemental equations.

### 3.1.1 Mass Conservation

Also called continuity equation, considers that the variation of mass in a determined volume must be entirely due to an inlet and outlet flow through a differential volume(Versteeg and Malalasekera, 2007). The amount of mass in a control volume can be calculated by the following equation.

$$m = \rho V \tag{3.1}$$

where  $\rho$  is the specific mass or the fluid or gas mixture and V the is the volume of the cell. Then, the mass m of the defined grid can be determined by integrating equation 3.1.

$$\frac{d}{dt} \int_{cv} \rho dV = -\int_{cv} \rho \vec{v} \cdot \vec{n} dS \tag{3.2}$$

Then, by considering the flow in all areas of the control volume:

$$\frac{d}{dt}\int_{cv}\rho dV + \int_{cv}(\rho\vec{v})dA = 0$$
(3.3)

Applying Gauss theorem of Divergence;

$$\frac{d}{dt} \int_{cv} \rho dV + \int_{cv} \nabla \cdot (\rho \vec{v}) dA = 0$$
(3.4)

$$\int_{cv} \left(\frac{d\rho}{dt} + \nabla \cdot (\rho \vec{v})\right) dV = 0$$
(3.5)

The continuity equation has two terms: a transient term that defines the pace at which density changes over time, and a convective term that reflects the fluctuation of specific mass with spatial coordinates. Taking this into consideration, the following equation is given for X, Y, and Z

$$\frac{d\rho u}{dx} + \frac{d\rho u}{dy} + \frac{d\rho u}{dz} = 0$$
(3.6)

#### 3.1.2 Momentum Conservation Equation

The momentum equation can be explained as the representation of Newton's Second law. Total momentum in volume V is equal to the integral of the determined volume by the product  $\rho$ u. This equation primarily represents momentum variation to fluid-acting forces. The force exerted by the fluid out of the volume is given by the product between pressure P and the area S at any point of the volume.

$$\frac{d}{dt} \int_{cv} \rho \vec{u} dV + \int_{A} (\rho \phi) \cdot \vec{n} dA = \int_{A} (\rho \Gamma_{\phi} \phi) \cdot \vec{n} dA + \int_{cv} S_{\phi} dV$$
(3.7)

Again, using Gauss's theorem of Divergence Eq 3.7 yields;

$$\int_{cv} \frac{d(\rho \vec{u})}{dt} dV + \int_{cv} \nabla \cdot \rho \phi \vec{u} dV - \int_{cv} \Gamma_{\phi} \rho \phi dV - \int_{cv} S_{\phi} dV = 0$$
(3.8)

Equation 3.8 consists of four elemental terms. The transient term describes the change of  $\phi$  in the fluid element over time. The convective term expresses the total flow of  $\phi$  outside the fluid element. The diffusive term shows the increase rate of  $\phi$  due to viscous forces and the source term indicates the increase rate of  $\phi$ 

$$\frac{d(\rho\vec{u})}{dt} + \nabla \cdot \rho \phi \vec{u} = \Gamma_{\phi} \nabla^2 \rho \phi + S_{\phi}$$
(3.9)

#### 3.1.3 Energy Conservation Equation

The equation for conservation of energy can be used in many and different applications depending of the process upon study. For Newtonian fluids, a general form of this presentation can be presented as follows;

$$\rho C_p \frac{DT}{dt} = \nabla (k_t \cdot \nabla T) + \mu \phi_v + S_h \tag{3.10}$$

The differential form of this equation for a component i;

$$\frac{\partial}{\partial t}(\rho T) + \frac{\partial}{\partial t}(\rho u_i T) = \frac{\partial}{\partial x_i} \left(\frac{K}{C_p} \frac{\partial T}{\partial x_i}\right) + S^{\mathrm{T}}$$
(3.11)

### 3.2 Premixed Combustion

Before diving into the fundamental concepts of combustion, it is pertinent to define the concept of flame. A flame is the outcome of a combustion reaction and propagates at sub-sonic speeds in a self-sustaining way while consuming the flammable cloud (Turns, 2006). Premixed combustion is a process in which the fuel and oxidizer are mixed before ignition. The capacity to spread towards the premixed reactants mixture, burning them continually as it moves, is the most significant feature of premixed flames. It's worth noting that all of the explosion parameters investigated in this paper are for subsonic flames of gases expelled by failing LIBs, on a more technical language; deflagration. A premixed flame moves towards the flammable cloud in order to consume the remaining reactant mixture.

During combustion reactions, the number of involved chemical species is very high in occasions. For starters, hydrocarbon combustion reactions usually account more than 50 different species. Thus if a mixture is involved, the reaction kinetics become even more complex and the modelling of the reaction rate for each species will imply a higher computational cost. In order to make this task easier some assumptions and simplifications have to be made, starting with the reduction of the chemical species by considering a irreversible reaction, between fuel and the oxidiser agent reacting into products.

 $F + s O \longrightarrow (1 + s)P$ 

#### 3.2.1 BML Premixed Reaction Modelling

After assuming a one-step reaction, the flamelet approach proposed by Bray-Moss-Libby will be considered. One of the parameters studied by this approach is the reaction progress variable c. A value of 0 is assigned for the unburned reactant region and a value of 1 for the fully burned products during combustion (Bray et al., 1984)

$$c = \frac{Y_{\rm F} - Y_{\rm FR}}{Y_{\rm FP} - Y_{\rm FR}} \tag{3.12}$$

Where Y is the variable for the fuel mass fraction and the subscripts R and P, respectively represent the fuel mass fractions for reactants and products. Then, the Favre averaging

is introduced in the transport equation for the flammable mixture as;

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{c} + \nabla \cdot \left(\bar{\rho}\tilde{\mathbf{u}}\tilde{c}\right) = \nabla \cdot \left(\left(\frac{\mu + \mu_t}{\sigma_c}\right)\nabla\tilde{c}\right) + \bar{\omega}$$
(3.13)

In Eq 3.18 the term  $\mu + \mu_t$  expresses the effective viscosity, and  $\sigma$  is the turbulent Schmidt number for the reaction progress variable and finally,  $\overline{\omega}$  stands in for the mean reaction rate as a source term. Similarly, the transport equation for a flammable mixture (fuel and air) can be expressed as;

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{F} + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}\tilde{F}) = \nabla \cdot \left( \left( \frac{\mu + \mu_t}{\sigma_f} \right) \nabla \tilde{F} \right)$$
(3.14)

The turbulent Schmidt number for the fuel mixture is represented by  $\delta_{\rm f}$ . For both  $\sigma_{\rm f}$  and  $\sigma_{\rm c}$  a value of 0,7 is assumed.

#### 3.2.2 Equation of State and Thermodynamics

Considering the BML formulation, the main thermodynamic properties must be coupled to the reaction progress variable. It is also assumed. An additional transport equation must be introduced where it is considered the total energy E.

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{E} + \nabla \cdot \bar{\rho}u\left(\tilde{E} + \frac{\bar{P}}{\bar{\rho}}\right) = \nabla \cdot \left(\left(\frac{\mu + \mu_t}{\sigma_E}\right)\nabla\left(\tilde{E} + \frac{\bar{P}}{\bar{\rho}}\right)\right) + \nabla\mathbf{u}\bar{\tau}$$
(3.15)

Where  $\widetilde{E}$  is:

$$\widetilde{E} = \widetilde{e} + \frac{1}{2}\widetilde{u^2}u^2 + \widetilde{k}$$
(3.16)

In which e expresses internal energy, and it can be defined as:

$$\widetilde{e} = \int_{T_0}^T C_{\rm v} dT + H(Y_{\rm FR}(1-\widetilde{c}) + Y_{\rm FP}\widetilde{c})$$
(3.17)

Where H is enthalpy of combustion,  $C_v$  is the specific heat capacity at constant volume and T is temperature. P in Eq 3.30 can be determined from the equation for ideal gas.

$$\overline{P} = \frac{\widetilde{\rho}R\widetilde{T}}{\overline{W}_{\rm m}} \tag{3.18}$$

R is the universal constant of gases,  $\overline{W}_{m}$  is the mean molar mass and T represents the Favre mean temperature. These last two can be calculated by the use of the following equations:

$$T = \frac{\widetilde{e}}{C_{\rm VP}} + T_{\rm R}(1-\widetilde{c})\left(1 - \frac{C_{\rm VR}}{C_{\rm VP}} - \frac{H}{C_{\rm VP}}\left((1-\widetilde{c})Y_{\rm FR} + \widetilde{c}Y_{\rm FP}\right)\right)$$
(3.19)

$$W = \frac{W_{\rm R}(1-\tilde{c}) + W_{\rm p}\tilde{c}(1+\tilde{\tau})}{1+\tilde{\tau}\tilde{c}}$$
(3.20)

In both Eq. 3.24 and 3.25,  $\tau$  represents hear release rate and it can be expressed as:

$$\widetilde{\tau} = \left(\frac{\rho_{\rm R}}{\overline{\rho}_{\rm P}}\right) - 1 \tag{3.21}$$

#### 3.2.3 Reaction Rate Modelling

To conclude the set of equations shown in the previous section, it is necessary to further elaborate on the term  $\omega$ . The formulation considers that this parameter can be defined as follows:

$$\overline{\omega} = \rho_{\rm R} u_{\rm L} \Sigma \tag{3.22}$$

Where  $\rho_{\rm R}$  is the density of the reactants in the flammable mixture,  $u_{\rm L}$  represents the laminar burning velocity and  $\Sigma$  is the corresponding term for the surface of the flame per unit of volume. The latter can be represented as

$$\Sigma = \frac{gc(1-c)}{|\hat{\sigma}_{\mathbf{y}}|\hat{L}_{\mathbf{y}}} \tag{3.23}$$

In the previous equation the variable g and  $|\hat{\sigma}_y|$  is a constant and an orientation factor, respectively. These parameters have been studied extensively in the literature and empirical studies have established values for both of them. For g an approximate value of 1.5 and for  $|\sigma_y|$  a value of 0,5 is usually used.  $\hat{L}_y$  is the respective term for the integral length scale of wrinkling at it is also associated with the laminar length scale, as described in the following equation. The formulation of the BML framework has been revised very prominently in the literature, it has been found that the  $\hat{L}_y$  varies due to flame-to-wall interactions and local fluid motion. This has been reported in numerical and empirical tests (Ahmed et al.; s. Sattler et al., 2002).

$$\widehat{L}_{\rm y} = c_{\rm L} l_{\rm L} f \frac{u'}{u_{\rm L}} \tag{3.24}$$

The constant  $c_L$  is equal to 1 and  $l_L = (v/u_L)$ . The function f is based on experimental observations. The laminar length scale is directly proportional to  $(u'/u_L)$  until reaching a determined maximum value, later decreasing when the stretch of the flame causes the combustion reaction rate to decrease.

$$f\left(\frac{u'}{u_L}\right) = \left[\frac{1}{1 + \frac{c_{w1}}{(u'/u_L)}} \left(1 - \exp\left[\frac{-1}{1 + c_{w2}\left(u'/u_L\right)}\right]\right)\right]^{-1}$$
(3.25)

Usually, the function f is employed to determine the flame length scale by assumptions that this parameter is determined due to perturbations from the turbulent velocity field. Finally, the values of the constants  $C_{w1}$  and  $C_{w2}$  are 1.5 and 4.0, respectively.

#### 3.2.4 Laminar Burning Velocity

The propagation rate in laminar premixed flames is usually defined by the velocity of the advance of the flame relative to the reactants, in other words, laminar burning velocity. This parameter is highly dependent of the physical and chemical properties of the reactant mixture.

$$u_{\rm L} = u_{\rm L}(p, T_{\rm r}, Y_1, Y_2, ..., Y_{\rm n})$$
(3.26)

Cant and Mastorakos (2008) defined a laminar flame by considering the following characteristics traits as seen in Fig 3.1 the preheat region, the temperature is raised by the generated in the reaction and equilibrium zone. The reaction zone is where most of the combustion reactions take place, most of which have a fast reaction rate due to the high temperatures and volatility of the considered chemical species. Thus, this is the reason why this zone is very small. Finally, the equilibrium zone in which most of the generated heat is released and chemical equilibrium is reached. Variations in reactant and product temperatures can cause significant variations in laminar flame speed. The temperature of the reactants has a direct effect on the reaction rate since they are governed by the Arrhenius equation and changes in the temperature of the products may have repercus-



Figure 3.1: Variation of Temperature (T) and mass fraction (Y) Through a laminar premixed flame, Source: Adapted from Cant and Mastorakos (2008).

sions on the propagation of the flame, for example, lower temperature in products will cause a faster flame extinction whereas higher temperatures may increase flame propagation. Several empirical correlations have been presented and studied throughout the years. However, the scope of this paper will consider two equations on which this project is based. Henriksen et al. (2021) presented an expression for the laminar burning velocity of gases vented by failing LIBs by using the Gulder equation, as seen in Eq 2.7, and calculating the corresponding coefficients for their correlation. This study will introduce a new LBV equation for the mixture of gases expelled by failed LFP battery cells by using the expression presented by Abu-Orf and Cant (2000). This correlation for the laminar burning velocity of a gas is used in the framework of STOKES.

$$u_{\rm L} = a\phi^b e^{-c(\phi-d)^2} (\frac{T}{T_{\rm ref}})^{\alpha} (\frac{P}{P_{\rm ref}})^{\beta}$$
(3.27)

Where parameters a, b, c, d,  $\alpha$ ,  $\beta$ , are calculated by fitting them into Henriksen et al. (2021) experimental data for the mixture of LFP gases. By understanding the propagation of the flame in accidental explosions caused by lithium batteries.

### 3.3 Flammability Limits

Empirical studies have shown that there is a threshold of concentration of flammable compounds that will determine if the flame will eventually propagate. As mentioned in Chapter 2, these values are called lower explosive limit and upper explosive limit (UEL). Depending on the literature these parameters are also called lower and upper flammability limits (UFL). Said limits are determined by the physiochemical properties of the fuel-air mixture. Lean mixtures are characterized by having fuel to air ratio ( $\phi$ ) minor than 1 and on the other hand rich mixtures have a  $\phi$  higher than 1. The LEL for gas mixtures can be determined by using Le Chatelier's rule.

$$LEL_{\rm mix} = \frac{1}{\frac{X_1}{LEL_1} + \frac{X_2}{LEL_2} + \frac{X_3}{LEL_3} + \dots + \frac{X_n}{LEL_n}}$$
(3.28)

The same rule can be applied for the calculation of the UEL;

$$UEL_{\rm mix} = \frac{1}{\frac{X_1}{UEL_1} + \frac{X_2}{UEL_2} + \frac{X_3}{UEL_3} + \dots + \frac{X_n}{UEL_n}}$$
(3.29)

### 3.4 Remarks on the concept of turbulence

Turbulent flows are characterized by random and chaotic behaviors. Such flows are governed by high-momentum convection and low-momentum diffusion. in other terms, turbulence can be defined as the outcome of instabilities of laminar flows at high Reynolds numbers. Turbulent flows are always three-dimensional, the motion of the fluid particles is due to their many variations of position and time in a three-dimensional field (Versteeg and Malalasekera, 2007). Fig 3.2 is a representation of such fluctuations produced in turbulent regimes. The flows studied by computational scientists are turbulent by nature. The numerical modeling of these flows is one of the most important aspects of CFD studies, considering this selecting an appropriate turbulence model is the most important step towards obtaining solid and reliable results.


Figure 3.2: fluctuations of the turbulent velocity field, Source: Adapted from Versteeg and Malalasekera (2008).

#### 3.4.1 k- $\epsilon$ turbulence model

The k- $\epsilon$  model is considered to be a standard both in industry and academics since its stability and numerical accuracy. However, this method offers solutions that are not quite numerical accurate for unconfined flows. This model was elaborated by considering the variables and mechanisms that affect turbulent kinetic energy. Two variables are employed by this model to analyze the turbulent kinetic energy K and the turbulent dissipation rate  $\epsilon$ . The reader must consider that the previously defined variables will be used to define the velocity scale  $\vartheta$  and length scale l.

$$l = \frac{k^{3/2}}{\epsilon} \tag{3.30}$$

$$\vartheta = k^{1/2} \tag{3.31}$$

By considering the aforementioned variables, the turbulent eddy viscosity can be defined as:

$$\mu_{\rm t} = C_{\mu} \rho \frac{k^2}{\epsilon} \tag{3.32}$$

The parameter  $\mu_t$  is a constant of the employed model. Values for velocity and length scale can be obtained through the use of the following differential transport equations.

$$\frac{\partial}{\partial t}(\rho k) + \nabla(\rho \mathbf{u}k) = \nabla \cdot \left(\frac{u_{\rm r}}{\sigma_{\rm k}} \nabla k\right) + 2\mu_t E_{\rm i,j} E_{\rm i,j} - \rho \epsilon \tag{3.33}$$

$$\frac{\partial}{\partial t}(\rho\epsilon) + \nabla(\rho\mathbf{u}\epsilon) = \nabla \cdot \left(\frac{u_{\mathrm{r}}}{\sigma_{\epsilon}}\nabla\epsilon\right) + \frac{\epsilon}{k}(C_{1\epsilon}2\mu_{t}E_{\mathrm{i,j}}E_{\mathrm{i,j}} - C_{2\epsilon}\rho\epsilon)$$
(3.34)

The values of  $C_{1\epsilon}$ ,  $C_{1\epsilon}$ ,  $\sigma_k$  and  $C_{1\epsilon}$  can be observed in the works of Launder and Spalding (1974)

## Chapter 4

# Methodology

This Chapter will elaborate on the applied methodology for the execution of this study. Each of the stages that make up this study will be described in detail, starting from the construction of the implemented geometry and preprocessing to the calculations of the constants of the empirically based equation of Abu-Orf and Cant (2000) for the laminar burning velocity of the studied LFP battery cell gas mixture and its thermodynamic properties.



Figure 4.1: Flow diagram of the programs used in each of the stages of this study

Figure 4.1 illustrates the employed programs in this project and the output files generated with each software in every stage. The performed simulations were carried out by the software STOKES developed by Ferreira et al. (2016). This program will solve the main governing equations in each volume control for reacting flows.

## 4.1 Scenario of study

Following the guidelines of the experimental set-up from the literatureHenriksen et al. (2021), a 3-D model of a semi-confined explosion chamber was built using the open-source program Blender. It was elaborated With inner dimensions of 1m x 65mm x 11.65mm for length, width, and height, respectively. Several simulations were performed in order to analyze parameters such as pressure, flame velocity, and flame speed. Figure 4.2 displays the geometry used in this study.



Figure 4.2: Geometry and computational domain. (a) Front view; (b) Lateral view; (c) Upper view.

The simulations were executed with a mesh size of 5 mm in a computational domain of dimensions of 1.2m x 0.195m x 0.233m long, wide, and high, respectively. This mesh size led to 430 000 cells, as detailed in Figure 4.3. No subsequent sensitivity was carried out with smaller grids since the CFL and SF values have a strong correlation with the mesh size. Future works will investigate this issue.



Figure 4.3: Polygonal mesh superimposed over build geometry

As for the simulation set-up, the Courant-Friederich-Lewy number and smooth factor varied according to the type of employed flammable mixture. The LFP TR gas cases used 0.2 and 0.015 for CFL and SF, respectively for the first run of simulation cases. A subsequent set of simulations for the LFP flammable mixture in order to study the effects of different combustion rates in flame propagation, this is further explored in chapter five. Such cases used the same values for the aforementioned parameters. Finally, the cases with methane and propane used 0.5 and 0.04 for CFL and SF respectively.

Moreover, as part of the objectives of this research, cases with single hydrocarbon components such as methane and propane were carried out and later compared to the explosion cases executed with the mixture that constitutes the vented gases of a failed LFP battery cell. Table 4.1 displays the values for CFL and SF parameters in the proposed simulation cases

Simulation Cases	CFL	SF	$\Delta_{\mathbf{x}}(mm)$
LFP Flammable mixture	0.2	0.015	5
Methane	0.5	0.04	5
Propane	0.5	0.04	5

Table 4.1: Courant Friedrichs Lewy number, SF and mesh size for the considered simulations

The pressure history was probed using monitor points distributed along the geometry. In the results reported by Henriksen et al. (2021), four sensors were localised in different spots throughout the explosion chamber as depicted in table 4.2. However, only the data generated by the sensor close to the ignition source was considered. This approach is also adopted in the current investigation (monitor point 200mm from the ignition source). The ignition was placed in the back of the geometry's closed end as shown in Figure 4.4. Secondary parameters such as flame position and velocity were also part of this study.

Monitor Points	Х	Y	Ζ
1	-0,25	-0.0005075	0.1140
2	-0,05	-0.0005075	0.1140
3	0,15	-0.0005075	0.1140
4	0,35	-0.0005075	0.1140

Table 4.2: Localization of ignition source and monitor point in the simulation.



Figure 4.4: Localization of ignition source and monitor point in the simulation

Before starting the simulation process with the LFP mixture it was imperative to modify the source code of S.T.O.K.E. in order to simulate explosion cases with the studied mixture. The following section will elaborate in detail on the required modifications.

### 4.2 STOKES

The main objective of this research is to model the laminar burning velocity of the flammable mixture studied by Henriksen et al. (2021), Table 4.3 displays the volume composition of the mentioned mixture.

Type of Battery	$H_2(\%)$	$CH_4(\%)$	$\operatorname{CO}_2(\%)$	CO(%)	$C_2H_4(\%)$
LFP	34.9	15.0	20.1	25	5.0

Table 4.3: Studied flammable mixture in volume percentage.

S.T.O.K.E.S (Shock Towards Kinetic Explosion SIMULATION) is a premixed combustion CFD tool developed by the laboratory of industrial risk analysis (L4r1s4) of the University of Campinas. The code solves the full compressible Reynolds Averaged Navier-Stokes (RANS) using the finite volume method. The set of equations is integrated over time using fourth-order Runge-Kutta scheme. The turbulence problem is closed using the Boussinesq approach where two additional transport equations are solved for turbulent kinetic energy and its respective rate of dissipation. The combustion modeling is addressed by means of the Bray-Moss-Libby (BML)(Bray et al., 1984; Quaresma et al., 2021). The initial growth of the kernel at the early stages of the explosion is modeled based on a quasi-laminar approach as described by Vianna and Cant (Vianna and Cant, 2014).

A total of three pseudo-component were investigated, with the purpose of emulating the vented gases of a failed LFP battery cell. Implying the calculation of several thermodynamic and stoichiometric parameters such as combustion enthalpy, specific heat capacity as much for reactants and products, and upper and lower flammability limits, among others. A one-step mechanism was adopted where fuel (F) reacts with an oxidizer (Ox) and leads to products (P), as stated in equation 4.1. The following reaction mechanisms were considered in order to calculate the parameters displayed in Table 4.4.

$$F + Ox \rightarrow P$$

$$0,15 (CH_4 + 2 O_2 \longrightarrow CO_2 + 2 H_2O)$$

$$0,05 (C_2H_4 + 3 O_2 \longrightarrow 2 CO_2 + 2 H_2O)$$

$$0,25 (CO + O_2 \longrightarrow CO_2)$$

$$0,349 (H_2 + O_2 \longrightarrow H_2O)$$

$$(4.1)$$

Fuel/products	UEL	UEL	Cp (J/Kg*K)	MW (Kg/kmol)	$H_{comb}$ (KJ/Kg)
Fuel	4,52	0,34	1451,30	20,298	$41,4x10^{6}$
Products	-	-	1007,99	35,482	-

Table 4.4: Thermodynamic and combustion properties of the studied mixture

In order to execute simulation cases with a multiple-component flammable mixture, STOKES's source code must be modified by considering the elements of each component within the gaseous mixture. To do so, two of the subroutines of STOKE'S framework must be modified by adding a new stoichiometric relation to calculate the mass fraction of the burnt products in the following combustion reaction.

$$C_xH_yO_z + [x + y/_4 - z/_2]O_2 \longrightarrow xCO_2 + (y/_2)H_2O_2$$

Studying the explosion with only one pseudo-component would restrict the reach of this study. For this reason, three pseudo-components with very different atomic structures were proposed. The atomic structure of these components was based on the molecular weight of the studied mixture that was found based on the composition of the gases shown in Table 4.2. Table 4.5 depicts the three proposed simulation cases with their respective atomic structure.

CASE	С	Н	0
1	1.007	5.098	0.2
2	0.5	6.342	0.5
3	1.5	1.171	0.07

Table 4.5: Simulation cases according to the atomic structure of the pseudo-component

Besides the determination of thermodynamic and stoichiometric associated parameters, it is also imperative to calculate the coefficients for the expression for the laminar burning velocity of Abu-Orf and Cant (2000) used by STOKES. To do so, it was necessary to consider the provided experimental data for  $\alpha$  and  $\beta$  coefficients found by Henriksen et al. (2021, 2022). The value of these two coefficients is independent of the correlation that is used since they both are fuel dependent. Both equations were plotted by using different values for  $\phi$ , and the Abu-Orf equation was fitted to Gulder's to calculate the values for the a, b, c, and d constants. The values of these parameters are displayed in table 4.6.

Equation	$\alpha$	$\beta$	a	b	с	d
Abu-Orf	1.87347293753	-0,37383060658	0.49431	0.58447	4,10025	0,99129

Table 4.6: Values of LBV equation coefficients for the studied flammable mixture

Figure 4.5 displays the curve of the laminar burning velocity correlations implemented in Henriksen's Study and the correlation used by STOKES for different air-fuel ratios for the studied mixtures. Minor discrepancies can be observed at the beginning and the end of the plotted curves. Overall, the fitted values for the equation of Abu-Orf and Cant (2000) seem to adapt the data plotted with Gulder's.



Figure 4.5: Comparison of Laminar burning velocity using Gulder Equation and STOKES for composition 1

As a brief summary of this subsection, We investigated three pseudo-components with different atomic structures, but with the same thermodynamic and combustion parameters as the flammable mixture studied by Henriksen et al. (2021). Three different premixed simulation cases were carried out and numerical findings were compared with available experimental data. Table 4.5 displays the simulation cases with their respective atomic structures.

## Chapter 5

## Results

This chapter will present and formulate a discussion based on the results that were obtained throughout the duration of this research. Initially, flame propagation will be addressed, as well as key characteristics that will be compared to the flame analyzed in the experiments. Then, the numerical findings regarding pressure distribution, flame velocity, and position were also compared to the experimental data. Secondary comparisons with cases of single-component flammable clouds were also conducted. Moreover, a case study is presented where the studied flammable mixture is used in a premixed combustion case in a BESS. Then, a brief comparison between the simulation cases of LFP TR gas and single-component flammable clouds will be carried out. Parameters such as overpressure, flame velocity, and flame temperature will be considered. Finally, the results of a case study in a Baterry energy storage system will be compared by considering data from the available literature on this kind of facility.

### 5.1 Code Validation

### 5.1.1 Flame Propagation

After examining Figure 5.1, several early conclusions can be drawn. Subfigures (a), (b), and (c) demonstrate that the BML combustion framework can effectively convert reactants into products as the flame progresses through the geometry. Regarding the velocity field distribution, Subfigures 5.1 (d), (e), and (f) reveal that areas of lower pressure values generate drag, leading to an increase in the velocity field distribution in some

regions compared to others within the explosion chamber. By comparing these Subfigures with 5.1 (a), (b), and (c), it is evident that the highest velocities occur ahead of the flame front because the flame pushes the unburnt gases ahead of it, this is in line with the current understanding of premixed combustion. Additionally, Figure 5.1 (g), (h), and (i) show that the temperature of the premixed flame falls within an optimal range. This qualitative analysis provides a positive indication of the proposed model's ability to handle complex flammable mixtures.



Figure 5.1: (a) PV at 0.0107 s (b) PV at 0.0323 s (c) PV at 0.0647 (d) Velocity field at 0.0107 s (e) Velocity field at 0.0323 s (f) Velocity field at 0.0647 s (g) Temperature at 0.0107 s (h) Temperature at 0.0323 s(i) Temperature at 0.0647 s. The maximum temperature is above 2,000 K.

Figure 5.2 depicts the comparison of both flames, simulated and experimental at four different time instants. Following the analysis of the data, it was acknowledged that the propagation of the simulated flame is relativity faster than in the experiment. Besides, in the experimental snapshots, it is seen a tulip shape was not quite captured by the simulations that were carried out. The third and fourth-time instants display that the front of the flame collapses toward the products of the combustion reaction, this effect is most notorious in the last time-step. The shape of the flame in the previously mentioned snapshots is attributed to hydrodynamic effects that are originated by the acoustic waves superimposed on the backflow of burned gases (Ponizy et al., 2014). Although the differences between the numerical and experimental results can be considered insignificant, it is later seen that such differences may cause overestimations in pressure distribution calculations compared to experimental appreciations, as displayed in Figure 5.3.



Figure 5.2: 3-D representation of flame propagation and venting in different timesteps. Left: Simulation snapshots of STOKES. Right: High-speed pictures extracted from Henriksen's study - (a) Propagation at 0.0107 s (b) Propagation at 0.0323 s (c) Propagation at 0.0485 s (d) Propagation at 0.0647 s.

Moreover, turbulent flows are notoriously difficult to model accurately, since turbulence models can produce significantly different results for the same flow. Even though boundary conditions for the simulation cases perfectly emulate the conditions of the experiment the numerical schemes used in the simulations can also have an impact on flame propagation.

Finally, the chemical mechanism used to model the combustion chemistry can also impact flame propagation. Chemical mechanisms can vary in complexity, and a more detailed mechanism may better capture the behavior of the fuel and oxidizer mixture. However, a more complex mechanism may also require more computational resources and can lead to more numerical errors. The choice of mechanism should be carefully considered based on the specific problem being studied and the available computational resources. This is further elaborated in the following sections.

Despite the fact that this work is based on certain assumptions and simplified representations of the system, it can still produce results that closely match experimental observations. One possible explanation for the similarities in the flame front position and laminar burning velocity between the simulated and experimental data is that the model assumptions are reasonable approximations of the real-world conditions. Additionally, the pseudo-components used in the model may accurately capture the essential thermodynamic and kinetic properties of the fuel, leading to reasonable predictions of flame behavior. However, it is important to note that some differences in the data could be due to factors not accounted for in the model, such as turbulence or variations in the mixture composition. Overall, the similarities in the results suggest that the model is a useful tool for studying flame behavior and provides insight into the underlying physics of combustion.

#### 5.1.2 Pressure Distribution and Analysis

According to the provided experimental data, the highest overpressure was 2.194 (gauge). However, the calculated pressures using the pseudo-components depicted in ??, were 2.710 kPa (gauge), 3.020 kPa (gauge), and 14.570 kPa (gauge) for cases 1, 2, and 3, respectively. These pressure were higher than expected, also based on previous examinations of flame position and flame shape as displayed in Figure 5.2, it was noted that the reaction rate on the simulated explosions was faster compared to the experimental data, hence the model did not emulate the convex and concave sections of the flame front. It was suspected that the shape and orientation of the flame may have differed for this gas composition compared to hydrocarbons. These parameters are enclosed into a single constant within the S.T.O.K.E.S framework, as CC constant. To confirm this hypothesis, subsequent simulations were carried out in order to analyze the sensitivity of the variation of the CC constant.

The overpressure calculated by S.T.O.K.E.S. for case 1 is depicted in Figure 5.3 (a). The results indicate the best agreement when CC was set to 1.05 and 1.1. In case 2, Figure 5.3 (b) demonstrates that overpressure increases considerably when CC is set to 1.1. Figure 5.3 (c) illustrates the outcomes for case 3. The analysis of the graph indicates that the results were enhanced when CC was adjusted to 1.05 and 1.1. The examination implies that the propagation and heat release of the flame is significantly influenced by the gas composition, the shape and orientation of the flame, and the wrinkling of the flame front. Among all cases, it appears that case 1 with CC set to 1.05 was the most effective setup in reproducing the experimental data.



Figure 5.3: (a) recorded pressure in case 1 with different values for CC (b) recorded pressure in case 2 with different values for CC (c) recorded pressure in case 3 with different values for CC (d) Comparison between the three executed cases for different values for CC.

Table 5.1 exhibits a comparison between the highest calculated pressure and experimental data before the modification to the CC combustion parameter. Cases 1 and 2 were the closes to the experimental data, however, they were slightly overestimated. The pseudo composition used in case 1 yielded the most accurate results, with an absolute error of 23.54%.

Case	Pressure in experiments (Kpa-gauge)	Calculated pressure (Kpa-gauge)	%Diff	Absolute Error $\%$
1	2.194	2.710	-23%	23.54%
2	2.194	3.020	-37%	37.64%
3	2.194	14.720	-570%	570.09%

Table 5.1: Pressure data in experiments vs simulated for three study cases

Table 5.2 portrays the comparison of the calculated values after the modifications made to the CC parameters. Such changes included the shape and orientation factor and wrinkling of the flame. A substantial improvement is observed in all of the proposed cases, this being most noticeable, in case 1 with a CC value of 1.05, in which the absolute error was diminished to 7.56%.

Case	Pressure in experiments (Kpa-gauge)	Calculated pressure (Kpa-gauge)	%Diff	Absolute Error %
1	2.194	2.360	-7%	7.56%
2	2.194	3.020	-37%	37.64%
3	2.194	2.750	-25%	25.34%

Table 5.2: Pressure data in experiments vs simulated for three study cases

Figure 5.4 displays the variation of the time necessary to travel through the combustion chamber, according to the changes effectuated by the CC variable. Such findings were of good accordance with the hypothesis formulated in the flame propagation section, where it is shown that the numerical flame was propagating quite faster than the experimental flame. this may be due to changes and differences in reaction kinetics. Even though the proposed approach within the scope of this study has proven to be resourceful, reaction kinetics are far from similar to those of real explosions. The best result for the studied cases with CC set-ups of 1.05 is as much for pressure and global reaction time.



Figure 5.4: (a) Elapsed time in case 1 with different values for CC. (b) Elapsed time in case 2 with different values for CC (c) Elapsed time in case 3 with different values for CC (d) Comparison between the three executed cases for different values for CC. Elapsed time is the time required by the flame to travel the entire length of the combustion chamber.

Even though considering a pseudo-component for this study has proven to be quite interesting, it does not come without its downsides. An example of this, a lot of what would be ideal reaction kinetics are left out or simplified. The fact that the generation of pressure mitigating components like  $CO_2$  and CO during dissociation reactions could not be captured, can be an explanation of why the cases carried out with S.T.O.K.E.S. presented a slight overestimation of pressure distribution. It is worth mentioning that 20.1% of the mixture was  $CO_2$ . which may have had a mitigating effect on the experimental explosion.

Moreover, combustion kinetics play an important part in flame modeling. As stated in Section 4.2, a one-step reaction mechanism was adopted for all simulated cases. Although useful for this study, this assumption is a rather conservative approach to the kinetics of the combustion reaction of five different components.

Another important factor to consider is that the BML combustion model (see eq. 3.22) considers the density of the reactants. Given the differences in the atomic structure of each pseudo-component, it was expected that different combustion rates would be the cause of different overpressure values in each simulation case.

An example of this is the results for simulation cases 1, 2, and 3. Although they have the same thermodynamic and combustion properties, part of the differences in these results can be caused by their different atomic structures since each of the pseudocomponents represent a simplified version of a multi-component flammable mixture. However, other factors such as flame front propagation and the size of the combustion chamber could also play a role in the generated overpressure.

Although some disadvantages to the use of pseudo-components have been drawn, this approach remains a powerful tool for studying and modeling explosions of multi-component flammable mixtures since it can be difficult to model them directly due to the involved different chemical species and reactions. By using pseudo-components, flammable complex mixtures can be broken down into simpler components that can be easier to model, by doing so the computational costs to model the explosion is optimized, without sacrificing much fidelity of the results, as seen in Figure 5.3 and Figure 5.4. By carefully tailoring the pseudo-components presented in each of the cases to precisely emulate the LFP TR gas, the accuracy of the combustion framework can be improved. The use of pseudo-components in this research seeks to bring flexibility, as they can be designed for specific applications, to represent particular chemical species, or "emulate" reaction pathways that represent areas of interest. Furthermore, it must be clarified that the implementation of pseudo-components is consistent with the current modeling framework and software, grating a streamlined approach to modeling complex flammable mixtures, promoting synergy and the validation of results from this study. Additionally, pseudo-components represent a flexible approach for modeling and studying premixed combustion of flammable mixtures, enabling research to acknowledge complex chemical systems underlying mechanisms and behavior.

Similarities in pressure distribution values can also be explained by the employed correlation of the laminar burning velocity shown in the previous chapter since it displayed good agreement with the experimental results calculated by (Henriksen et al., 2021). If the laminar burning velocity of the pseudo-components is similar to the experimental data, then the combustion process is indeed comparable. This parameter is influenced by various factors such as temperature, pressure, and the composition of the reactants. The accuracy of the prediction of this variable is vital for the simulation process and therefore the calculation of pressure.



Figure 5.5: (a) Flame propagation and velocity field distribution at 0.03234 seconds (b) Flame propagation and velocity field distribution at 0.0539 second (c) Flame propagation and velocity field distribution at 0.072 seconds

Figure 5.5 displays the flame propagation of one of the subsequent simulations carried out with case 1 with a CC set-up of 1.1. Unlike Figure 5.1 the flame in these snap-shots is curved and the velocity field distribution is more symmetric around the front area. this is caused by lower velocity values caused by the decrease in combustion rate for this case. Contrary respect to Figure 5.1, the flame front is flattened due to higher velocity field distribution in the explosion chamber product of a higher combustion rate. Thus, it is assumed that lower combustion rates on these simulations tended to present pressure distribution values closer to the experimental data.

Accurately capturing the effects of turbulence also represents a major role in premixed combustion. It can be said that the implementation of the k- $\epsilon$  turbulence model could have led to very precise predictions of overpressure resulting from the combustion process when compared to the pressure distribution of experimental data. figure 5.6



Figure 5.6: Turbulent Reynolds number in simulation cases with CC 1.0 and CC 1.1 (a) Case 1 (C.C 1.0) at 0.0251 seconds (b) Case 1 (C.C 1.0) at 0.0531 seconds (c) Case 1 (C.C 1.0) at 0.0647 seconds (d) Case 1 (C.C 1.1) at 0.03234 (e) Case 1 (C.C 1.1) at 0.0539 (f) Case 1 (C.C 1.1) at 0.072

offers an insight into the turbulent Reynolds number in simulations carried out with a CC set-up of 1.0 and 1.1. The simulation with CC 1.0 showed a higher Reynolds, this is in good agreement with the observation made in Figure 5.5. In turbulent combustion, the interaction between the flame and turbulent eddies affect the combustion rate, flame position, and overpressure. When turbulent flow conditions are ideal, the flame front becomes convoluted and irregular as observed in the snapshots of Section 5.1.1. This lead to a higher surface area and increased flame transfer between the reactants and the flame, intensifying the combustion process and ultimately leading to higher overpressures.

Moreover, the fluctuations of eddies in turbulent flows can make way for localized areas of high pressures and temperature, thus causing pressure peaks during the combustion process. In other words, turbulent flows can enhance the transport of reactants, causing a faster combustion process and higher pressure distribution.

### 5.1.3 Flame Position

Regarding flame position, the numerical findings were really similar to those of the experimental data. Figure 5.7 displays the position of the flame in two different time instants, 0.033 and 0.063 seconds. It bears to be mentioned that the atomic structure of the proposed gases had little to no effect on the propagation of the simulated flame. The behavior of the simulated flame in the aforementioned time intervals had minor differences when compared to the experimental data.



Experiment vs STOKES

Figure 5.7: Flame position, S.T.O.K.E.S vs Experimental data for two instants of time.

Figure 5.7 displays a direct comparison of the obtained results by case 1 and the provided experimental data. Small discrepancies were observed at the verge of milliseconds in different time instants through the simulations. It can be said that the propagation of the simulated flame is alike to the experimental flame midway through the combustion chamber. this is also seen when the flame reaches the open end of the geometry. It can be assured that the flame position numerical findings are adequate enough to affirm that S.T.O.K.E.S. can predict flame propagation of flammable complex mixtures.

The results show that the laminar burning velocity  $(S_u)$  of the experimental and simulated data are in good agreement, indicating that the simulation model is capable of accurately capturing the fundamental characteristics of the flame. Additionally, the flame front positions of the experimental and simulated data are similar at the given time intervals, suggesting that the simulation model is able to predict the propagation of the flame front with reasonable accuracy. However, some differences can be observed outside of the given time intervals, which could be attributed to several factors such as variations in experimental conditions or model assumptions. Therefore, further analysis and evaluation are needed to better understand the sources of discrepancy between the experimental and simulated data.

Complementing the information regarding the last section, the flame front position can have an influence on overpressure because it affects the rate of heat release during combustion. As the flame front advances, the volume of the combustible mixture behind it decreases, which increases the pressure in that region. At the same time, the flame front releases energy through heat transfer and chemical reactions, which further contributes to the pressure increase. Therefore, the flame front position and its velocity can affect the pressure distribution during combustion.

In addition, the flame front position can also affect the shock wave generation during combustion. As the flame front advances, it can create a pressure wave that propagates ahead of it, which can interact with other pressure waves generated by the combustion process. These pressure waves can interfere with each other, leading to constructive or destructive interference patterns, which can affect the overall pressure distribution in the system. Therefore, the flame front position and its interaction with pressure waves can also affect the overpressure during combustion.

#### 5.1.4 Flame Velocity

The results presented in the table show the flame velocity of three pseudocomponents, as well as experimental data, at three different time intervals. The table reveals that the flame velocity of Case 2 is consistently higher than that of Case 1 and Case 3. At 0.018 seconds, Case 2 has a slightly higher flame velocity than Case 1, but lower than Case 3. However, at 0.038 seconds and 0.046 seconds, the flame velocity of Case 2 is considerably higher than the other two cases. On the other hand, at 0.038 seconds, Case 3 has the lowest flame velocity among all the cases, but it becomes the highest at 0.046 seconds. These differences suggest that there may be variations in the combustion parameters of the pseudo-components that are affecting the flame velocity. It must be mentioned that figure 4.1 used the data from the simulation cases with a CC value of 1.0



Figure 5.8: (a) Flame speed at 0.018 seconds (b) Flame speed at 0.038 seconds (c) Flame speed at 0.046 seconds (d) Global Comparison of flame speed in different time steps - STOKES vs Experimental data

Flame velocity discrepancies between the simulation cases were caused by the implementation of different combustion rates that are produced by the tuning done to the CC parameter. After comparing Figure 5.1 and Figure 5.5, the differences in velocity field distribution suggest that the changes done to the CC parameter affected flame velocity and ultimately flame propagation. This goes hand in hand with what is observed in 5.6 since the turbulent scale ( $Re_t$ ) decreases in the secondary simulation cases with different values of CC.

#### 5.1.5 Comparison with Single Component Flammable Cloud Cases

Preliminary simulation cases with single-component clouds were carried out at the beginning of this study with the purpose of findings values for CFL and SF parameters and avoiding numerical instabilities for the simulations in the explosion chamber. These values ended up being more or less approximate to the ones used in LFP flammable mixture.

Figure 5.9 depicts a direct comparison of overpressure between the experimental data, proposed pseudo-components, and single hydrocarbon flammable clouds of methane or propane. CH4-Air case reached a maximum value of 0.3 kPa(gauge) and the propane-Air mixture reacher a higher value of 1.74 kPa (gauge).

Direct analysis of the data of Subfigures 5.9 (a), (b), and (c) provides that the overpressure is higher in all of the cases that emulate the LFP TR gas than those of pure methane or propane. This is due to the fact that the pseudo-components used in the simulations ideally represent a more complex mixture of hydrocarbons and other compounds, consequently, the combustion in these cases is going to generate higher overpressure due to a large number of involved chemical species. The original mixture is composed of 34.9 % of hydrogen and smaller traces of other species of hydrocarbons, making this combination particularly reactive in combustion cases.

Subfigure 5.9 (d) displays pressure distributions through the entirety of the aforementioned cases. Upon reaching their greatest overpressure value major oscillations are observed in all of the pseudo-component cases when compared to methane and propane cases. This could be due to the combustion behavior of the pseudo-components being much more complex and the BML framework not being fully able to capture a streamlined behavior and which could have caused sensitivities to oscillations in pressure distribution.



Figure 5.9: Direct comparison of pressure distribution between the LFP pseudocomponent cases (a) Pressure distribution analysis between Case 1 with C.C 1.05, Methane case and propane case (b) Pressure distribution analysis between Case 2 with C.C 1.05, Methane case and propane case (c) Pressure distribution analysis between Case 3 with C.C 1.1, Methane case and propane case (d) Pressure distribution graph in all of the aforementioned cases

## 5.2 Case of Study - BESS Explosion

Recently, there has been a significant increase in the implementation of battery energy storage units. This is due to their capacity to integrate renewable energy sources such as lithium-ion batteries and the stability they can bring to electrical grids. However, the mass adoption of such systems has also led to an increase in the number of reported incidents in industrial scenarios(Zalosh et al., 2021). Thermal runaway is the first link of the chain of events that leads to explosions capable of turning the doors of these facilities into high-speed projectiles since the overpressure in some scenarios can reach up to 70 (Kpa-gauge). This section features a study of a particular case of an explosion in a BESS with the studied mixture within the scope of this research.

Experimental studies of explosions in energy storage systems are usually carried out in semi-confined enclosures similar to containers. The study presented by Jin et al. (2021) analyzed the hydrogen and carbon monoxide content of a failed LFP battery module at 100% SOC. Later, the authors proceeded to carry out controlled ignitions in an energy storage cabin of 12mx2,4mx3m for length, width, and height respectively. Although some flammable and toxic components were detected in the experiments, the composition of the gases expelled by the battery was not as detailed as other analyses of the literature(Golubkov et al., 2013, 2015).

However, it must be acknowledged that the flammable atmosphere in explosion incidents in battery energy storage units is not entirely composed of the gases studied in this research. Energy storage providers are aware of the challenges that the volatility of li-ion batteries can bring, for this reason, BESS facilities count on several safety measures to avoid or mitigate damages in case of fire or an explosion. Among them, is the fire suppression agent Novec 1230, This component is a fluoroketone that reduces the oxygen concentration of the surrounding area to suffocate the fire, it also evaporates fifty times faster than water. Moreover, when this component is deployed the heating, ventilation, and cooling systems are shut off to allow the emergent gases to concentrate. Consequently, the flammable cloud now is composed of a non-heterogeneous mixture that if it would come into contact with any remaining heat, could cause an explosion.



Figure 5.10: Illustration of mixture between ejected gases of a failed li-ion battery and anti-fire agent Novec 1230

This would end up in an even more complex mixture between the gases of the volatile electrolyte and Novec 12-30 as depicted in Figure 5.10. It is fair to mention, that the scope of this study only encompasses the mixture expelled by the battery during thermal runaway, however, it was sought to study the propagation of the flame in a facility that resembled a battery energy storage station. The pseudo-component presented in case 1 was used to carry out an explosion simulation. Additionally, the ratio between the shape and orientation factor (C.C) was adjusted to 1.5 for the simulation process. As for the geometry, a 3-D model of an energy storage system was elaborated, the design was based on the geometry presented by Jin et al. (2021).

Figure 5.11 depicts the elaborated geometry for this case, and it can be seen that the model consists of four main openings. The geometry consists of a corridor of 0.8 meters in width that extends to the open ends of the station as displayed in subfigure 5.11 (a). The two walls between the aforementioned corridor are designed to emulate the presence of battery racks on both lateral sides of the geometry as depicted in subfigure 5.11 (b). Moreover, Two smaller venting points were located at the side of the geometry at 2.4 meters of height and observed in subfigure 5.11 (c). The ignition (displayed as a red dot) was placed in the middle of the geometry and 1.70 meters above the ground as observed in subfigure 5.11 (c). The computational domain was designed to give the flame, space to propagate beyond the geometry with dimensions of 20mx11mx6m of length, width, and height respectively, as depicted in subfigure 5.12 (a). Finally, a uniform mesh of 5mm was applied in the entirety of the computational domain as displayed in subfigure 5.2 (b).



Figure 5.11: Geometry of ESC (a) front view (b) upper view (c) Lateral view



Figure 5.12: (a) Computational domain (b) Applied mesh

In a similar manner to the first part of this chapter; flame propagation, temperature, and pressure were studied and later compared to CFD simulations that have been carried out in the literature until now. Figure 5.13 displays the variable of progress and flame temperature respectively. Once again it was observed that the BML combustion framework successfully turned the reactants into combustion products while the flame advanced through the storage station, as depicted in subfigure 5.13 (a). Moreover, subfigure 5.13 (b) depicts flame temperature, the highest measured temperature was 3100 Kelvin, this parameter is entirely dependent on the thermochemical properties of the mixture, and further research is required to validate this finding. According to these images and judging by its shape, the flame that vented in the opening that is further south of the BESS displays a fairly turbulent behavior, so it was presumed that overpressure was higher at this point of the explosion.



Figure 5.13: Flame propagation and venting at 0,0863 seconds(a) Variable of progress (PV) (b) Flame temperature

Flame propagation can be observed in Figure 5.14. Subfigure 5.14 (a) depicts the ignition going off in the middle of the geometry at 1.70 meters of height. Naturally, the flame vented through the side openings of the model around 0.0575 seconds of the simulation. Finally, the flame reached and vented through both of the larger openings of the geometry at 0.0863 seconds as observed in sug-figure 5.14 (c). A particular trait about this last graph is that part of the flame front is pushed towards the flame that is going out of both openings. This is noticeable in both extremes of the geometry, however, it is more notable in the flame that is going out in the lower venting spot of subfigure 5.14 (c). This observation is in good agreement with the hypothesis presented in the analysis of Figure 5.13.



Figure 5.14: Flame propagation in different time steps (a) ignition at 0.0028 seconds (b) Flame venting through side openings at 0.0575 seconds (c) Flame going out of main corridor at 0.086 seconds



Figure 5.15: (a) flame propagation and pressure (b) 2-D slice of pressure field distribution

As expected the highest value for overpressure caused by the explosion was detected in one of the larger openings of the container, as displayed in 5.15 with 270 Kpa of inflicted pressure while the flame goes out of the geometry. So far the only. Although this value is exceedingly high for an explosion in such a scenario, it raised the question of the effect of the flammable mixture in battery energy storage units.

Explosion simulations in battery energy storage units can be quite challenging due to the complexity of flammable components in the gas mixture and the lack of experimental data. In this particular case, it considers that the use of a pseudo-component could simplify combustion kinetics and make the simulation more computationally feasible. This approach can often provide a reasonable approximation of the behavior of the actual mixture. Furthermore, the use of pseudo-components along with the calibration of the combustion framework of S.T.O.K.E.S, allowed for a better prediction of flame propagation and understanding of explosion hazards.

Furthermore, additional validation was required for overpressure in explosion cases in these facilities. The following sub-section will explore the explosion in BESS in the commercial software FLACS, the obtained information will be later compared to the numerical findings of S.T.O.K.E.S.

#### 5.2.0.1 Simulation cases - FLACS

As stated above, additional simulation runs were carried out using Gexcon FLACS, to validate and complement the results obtained by S.T.O.K.E.S. FLACS is widely considered a reliable tool for studying hazardous incidents. Besides studying overpressure in BESS explosions, it is also expected to compare flame propagation to validate the laminar burning velocity correlation explored within this research.

It is fair to mention that the same model of the energy storage station was used in these simulation trials. The simulations were carried out in a computational domain of 20mx11mx6m for length, width, and height respectively, the same as the domain of S.T.O.K.E.S to ease flame position analysis. Figure 5.16 displays the computational domain along the grid that was used. The sizes of the control volumes within the area of interest were 0.13, 0.03, and 0.08 meters for the X, Y, and Z directions. Moreover, The grid consisted of almost 400000 cells. The simulation setup followed the same instructions of S.T.O.K.E.S for cloud size and the location of the ignition.



Figure 5.16: Computational grid and domain

Post-processing of the simulation showed that the total elapsed time was 0.07 seconds, 18% less than the initial simulations on S.T.OK.E.S. Figure 5.17 depicts flame

propagation in different time steps. Early observations of this graph, show a good evolution of the flame kernel. It observed that the flame develops slower in the first instants of the explosion as displayed in subfigure 5.17 (a), after which displacement rate rises as observed in subfigures 5.17 (b) and (c). Thus, sudden changes in flame propagation would be the cause of pressure overprediction as previously mentioned. Moreover, An in-depth analysis shows the flame propagating almost in a similar way on the corridor, however, discrepancies in flame propagation are most prominent in the flame venting in the side openings of the geometry on the cases run by FLACS, as perceived in subfigures 5.17 (b), (d) and (f). It was perceived that the modeled flame with S.T.O.K.E.S did not manage to capture the effect of flame stretching observed in the aforementioned subfigures. This occurs when the local surface of the area of the flame is changed, either by hydrodynamic effects of curvature aided by propagation. Future works will explore the effects of straining and curvature in complex flammable mixtures.

Moreover, the differences in flame propagation are prominent in Figure 5.18.In order to evaluate flame position, it was necessary to analyse flame propagation in the X direction in the interval from 0 to 10 meters, in both FLACS and S.T.O.K.E.S. Three reference points were selected, namely, 2.05 meters, 4.65 meters, and 8.86 meters. From general observation, it is perceived that the discrepancies in flame position are more prominent as the simulation carries on. S.T.O.K.E.S propagated 13.23%, 17.49% slower than FLACS. Moreover, this is more noticeable around the 8.86 meters mark, the overall difference at this point was 18.63%. Table 5.3 may offer more insights into flame position.

Reference length	S.T.O.K.E.S - Time (s)	FLACS - time (s)	Absolute Error $\%$
2.05 meters	0.0415	0.036	13.23%
4.65 meters	0.0606	0.05	17.49%
8.86 meters	0.0806	0.07	18.63%

Table 5.5. Flame I ostion in various time steps, a comparison of 5.1.O.K.E.S and FLAC	Table 5.3:	Flame	Position	in v	various	time	steps,	a compar	rison (	of S.	T.O	.K.E.S	and	FLA	CS
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Figure 5.17: (a) Simulated flame with S.T.O.K.E.S at 0.0415 seconds (b) Simulated flame with FLACS at 0.036 seconds (c) Simulated flame with S.T.O.K.E.S at 0.0606 seconds (d) Simulated flame with FLACS at 0.05 seconds (e) Simulated flame with S.T.O.K.E.S at 0.086 seconds (f) Simulated flame with FLACS at 0.07 seconds



Figure 5.18: Comparison of flame position between S.T.O.K.E.S and FLACS

Finally, figure 5.19 provides a side-by-side view of flame venting in the last instants of the explosion. Overall, the results for flame propagation showed good agreement with the simulation in FLACS with minimal discrepancies in propagation considering the time scale of the explosion. As mentioned earlier, the simulation carried out in FLACS captured a flame that stretched out of the side opening of the geometry. Flame stretching is the result of both strain and curvature and the current iteration of the code does not capture the effects of flame stretch. This kind of flame increases its surface area by propagating. However, it is important to mention the curvature that is observed in the flame modeled with S.T.O.K.E.S in subfigure 5.19, was caused by the impulse pressure of the flame venting off the storage station.



Figure 5.19: 3-D representation of flame propagation (a) S.T.O.K.E.S at 0.086 seconds (b) FLACS at 0.07 seconds

Besides flame propagation, overpressure was also studied in FLACS simulation trials. The maximum overpressure probed was 2.741 bar, this is highly similar to the pressure calculated with S.T.O.K.E.S With 2.65 bar, less than 4% of the value calculated in FLACS simulations. This can be attributed to the differences in flame propagation between the two programs. However, in FLACS the highest pressure value was registered inside the storage station while the flame goes through the open end of the hallway as shown in Figure 5.20. whilst, in S.T.O.K.E.S the highest value was calculated in the flame front going out of the geometry.

It is important to clarify that the simulation set-up for this geometry considered that the whole section of the main corridor was filled with the gases of volatile electrolyte. Experiments of energy storage stations are partly filled with these gases. Also, in recent incidents, it was found that the flammable atmosphere in these facilities is usually a mixture of TR battery gas and fire extinguishing agents as observed in figure

### 5.10 DNV.GL (2020).



Figure 5.20: 3-D representation of flame propagation (a) S.T.O.K.E.S (b) FLACS
## Chapter 6

## Conclusions and future work

Various conclusions can be drawn from the simulations that were presented in this work. First, is that the BML combustion framework, can in fact predict and calculate flame propagation for a complex flammable mixture such as the gases expelled by a failed LFP battery cell. Though this mixture was emulated with pseudo-components several factors lead to differences from the experimental data extracted from the literature. The observed discrepancies could have been the product of the simplification of combustion kinetics. Although the one-step reaction mechanism adopted in this study proved to be useful, complex dissociation kinetics reactions are left out from the original mixture. This could be the cause of differences in flame propagation, flame velocity, and most importantly, pressure distribution.

Minor adjustments in the ratio between the shape and orientation factors led to numerical findings that were closer to the experimental data. However, case 1 with a CC set-up of 1.0 captured flame propagation better than the remaining simulation cases. The best numerical findings for pressure distribution were obtained with the pseudocomponent with a CC set-up of 1.1, with an absolute error of 7.56%. Thus, case 1 displayed the results that came closer to the experimental data in the three parameters studied during the validation stage. It was found that the chemical scale might play a role in the observed discrepancies. Since slower reaction rates are shown to favor kinetics rather than fluid mechanics.

Moreover, it must be mentioned that the new LBV correlation, adapted well for each of the simulation cases considering the differences in the atomic structure and density. Additional investigation is needed in order to analyze the propagation of such a complex mixture. Sadly, our approach failed to capture the effects of flame wrinkling in the flame front. Future studies will seek to analyze the effects of stretch and flame straining for single components and complex flammable mixtures.

The qualitative propagation test carried out in the geometry of the BESS showed good agreement with those executed in FLACS. Again, it must be mentioned that the intention of this case study is not a deterministic view of how explosions in energy storage systems must be studied using computational fluid dynamics. It was only expected to test the correlation used in this research to model the flames of flammable mixtures produced during thermal runaways. The general consensus after analyzing the results was, that the numerical flame simulated with S.T.O.K.E.S was highly similar to the one simulated in FLACS. Minor differences were spotted, such as the flame stretch in the side openings of the geometry, this detail was not captured by S.T.O.K.E.S.

In general, empirical BESS explosion studies must consider the changes that are done to the flammable atmosphere inside the station in TR incidents. Since the mixture, in this case, is not fully "pure" volatile electrolyte gas as seen in 5.10. future experimental studies must study the laminar burning velocity of the mixture between the gases of evaporated electrolyte and fire extinguishing agents. Finally, future works regarding the study of this composition through CFD will seek to implement kinetics that can represent the behavior of the mixture after the combustion reaction.

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