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EFFERVESCENT BREAKUP AND COMBUSTION OF LIQUID FUELS: EXPERIMENT AND MODELLING

EFFERVESCENTNÍ ROZPRAŠOVÁNÍ A SPALOVÁNÍ KAPALNÝCH PALIV: EXPERIMENT A MODELOVÁNÍ

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1 INTRODUCTION

Liquid breakup, or atomization, is a complex process that transforms bulk liquid into a spray and thus increases its surface area. It is a key ingredient in many industrial applications ranging from pharmaceutics, fire suppression, spray coating and spray cooling to diesel engines and – significantly for the present thesis – liquid (spray) combustion. Liquid fuels have been, and still are, one of the main resources in the process and power industries. Spray combustion is therefore a crucial and essential process in achieving the final product - heat. A great deal of effort is constantly being put into understanding the fundamental phenomena and processes governing spray formation. In many industrial burners, spray combustion is accompanied by another complex phenomenon: swirling flow. The swirling aspect of combustion is essential as it enhances the mixing of reactants and stabilizes the flame. These efforts are motivated by the need to achieve better performance, lower emissions and longer lifetime of furnaces and combustors in various industrial applications.

In the last few decades Computational Fluid Dynamics (CFD) tools have been employed to facilitate the designs of combustors and furnaces. However, the modelling of an atomization process presents a formidable challenge. Since for the majority of industrial applications it is prohibitively expensive to model these problems using state-of-art approaches, careful compromises must be made and appropriate models need to be applied for various stages of the atomization process as well as turbulence, chemistry, or radiative heat transfer.

Despite the importance of liquid breakup (or atomization), its principles are not yet fully understood. Moreover, the behaviour and local properties of sprays are not always fully known, specifically in the case of effervescent atomization. The deficiencies of published experimental spray characteristics are aggravated in CFD spray combustion simulations by additional assumptions and simplifications. In order to enhance our ability to model swirling spray combustion it is therefore necessary to address an array of problems. And the purpose of this work is to help in this effort.

1.1 OBJECTIVES AND THESIS OVERVIEW

This dissertation thesis aims to investigate a novel spray forming approach - effervescent atomization, with emphasis on atmospheric spray combustion. The long term goal toward which this research is aimed is to improve the predictability of swirling spray combustion, with focus on the distribution of heat loading (wall heat fluxes) in the combustion chamber of a fired heater. In order to contribute to the accomplishment of this goal many partial tasks were carried out.

- Literature review of the current state of the art in the area of effervescent sprays
- Experimental investigation of effervescent spray combustion

- Validation of current spray models against available drop size data
- Evaluation of effervescent spray combustion simulation and comparison to experimental data
- Detailed experimental investigation of multiple effervescent sprays

The subject of the research is very broad and the research was occasionally strayed into unexpected directions. Firstly, current spray models were tested and compared to available experimental data of effervescent sprays (5.1). At this point the first shortcomings of current spray models have been discovered, but their effect was underestimated. It was only after the model's application to the large-scale combustion simulation and comparison with experimental data (5.2) that these shortcomings were fully recognized. In order to make sure the cause of the discrepancies lied in the spray model as opposed to other aspects of the simulation (mainly turbulence, chemistry and radiation) a comparative study on gas combustion has been performed (5.3). Moreover a review on swirling flow modelling and its validation has been performed (5.4). The focus of the research has therefore been shifted into better understanding the effervescent spray formation, which of course necessitates experimental data. According to the methodology presented in chapter 5.5 extensive experimental measurements of effervescent sprays have been performed. Analysis of the results presented in chapters 5.6 and 5.7 shows dependencies that, to the author's knowledge, have not yet been published.

1.2 THESIS STRUCTURE

The presented thesis is written in a form of an annotated collection of research articles. The text is composed of 6 chapters. Chapters 1-4 form an introductory and unifying part which aims to provide a description of the phenomena involved in spray combustion, as well as methods and tools that were used in the course of this work. Chapter 5 contains the collection of published articles and represents a mapping of the author's research findings. Finally, summary and conclusions are provided in chapter 6.

Chapter 2 first covers the underlying phenomena taking place during spray combustion, namely primary and secondary atomization principles, basic ideas behind turbulence and combustion. In the following section the reader can familiarize himself with the notion of effervescent atomization. Experimental methods both for spray and combustion measurement are described in chapter 3 and the numerical approaches to the problem are explained in chapter 4. The results in the form of research articles are presented in chapter 5 and an overview and synthesis of all results is presented in chapter 6 along with a discussion and future work proposals. The experimental data obtained during the research of effervescent atomization are disclosed in the thesis' appendixes in full detail in order to facilitate future research and provide validation data for spray models.

2 UNDERLYING PHENOMENA

Spray combustion is a very complex process where several physical and chemical phenomena occur simultaneously. Moreover it is quite sensitive to physical properties of the fluids involved. The scope of the following sections is to describe and explain the phenomena involved and to clarify the impact of physical properties.

2.1 PRIMARY ATOMIZATION

The primary atomization is a process in which the bulk liquid disintegrates into drops (ligaments, filament usually appear as intermediate products of the disintegration process). This process can be understood as a disruption of the consolidating influence of the surface tension by the action of internal and external forces. In the absence of such disruptive forces the surface tension tends to pull the liquid into the form of a sphere, since it has minimal surface energy. The liquid viscosity acts as a damping force trying to prevent deformations of the system geometry, while the aerodynamic forces promote the disruptive process by distorting the bulk liquid. Breakup occurs when the disruptive forces exceed the consolidating surface tension forces (Lefebvre, 1989).

Different mechanisms are responsible for the disintegration depending on the nature and also shape of the flow of the bulk liquid.

2.2 SECONDARY ATOMIZATION

When primary atomization occurs, a great variety of drops is produced. Some of them are still susceptible to further breakup depending on their size and the nature of the surrounding flow. The process during which these drops break up or disintegrate into smaller drops is called secondary atomization.

2.3 TURBULENCE

Turbulence is a physical phenomenon the fundamentals of which are not yet fully understood. It is a quasi-chaotic time dependent behaviour seen in many fluids that causes the formation of swirling eddies of different length scales. We can mathematically describe turbulence only in a phenomenological sense – we are not talking about causes but about consequences. Turbulent flow arises in all kinds of problems when the Reynolds number surpasses a certain critical value. Turbulent flows are characterized by fluctuating velocity fields. These fluctuations mix transported quantities such as momentum, energy, and species concentration, and cause the transported quantities to fluctuate as well. Since these fluctuations can be of small scale and high frequency, they are too computationally expensive to be simulated directly, at least in all practical engineering applications. Instead, the instantaneous (exact) governing equations are averaged, in order to remove the small scales, resulting in a modified set of equations that are computationally less expensive to solve. However, the modified equations contain additional unknown

variables, and turbulence models are needed to determine these variables in terms of known quantities (Warnatz et al., 2001).

2.4 COMBUSTION

Combustion is a chemical process, where a sequence of exothermal chemical reactions occurs between a fuel and an oxidant. The reactants (fuel and oxidizer) are conversed into products (flue gasses) and due to the exothermal nature of the process heat is released. The production of heat can result in a visible flame. The key process in combustion is mixing of the reactants and oxidizer. If the fuel and oxidizer are in a turbulent region of the flow, the mixing process is enormously enhanced. This in turn leads to quicker combustion, shorter and more controllable flames, minimization of pollutants that arise as a result of imperfect combustion. It is therefore evident that the vast majority of industrial combustion applications heavily rely on turbulent flow fields.

2.5 EFFERVESCENT ATOMIZATION

Sprays are produced in a variety of ways. There are a number of nozzles, in this context referred to as atomizers, which facilitate the atomization process using different mechanisms. Conventional atomizers disintegrate the liquid by creating high relative velocity between the liquid and gaseous phase. This can be achieved either by ejecting the liquid at high velocity into quiescent air (pneumatic or pressure atomizers, pressure-swirl atomizers) or by exposing the liquid to a high-velocity gas stream (airblast atomizers). Due to the need to fulfil specific industry requirements other atomizers using different mechanisms have been devised, such as electrostatic, ultrasonic or vibrating atomizers. One of the most recent spray formation mechanisms is effervescent atomization, which was pioneered by Lefebvre and his colleagues (Lefebvre et al., 1988) and is gaining popularity especially for combustion purposes ever since.

Effervescent atomization is often confused with flash atomization. Unlike flash atomization, where an atomizing gas is dissolved in the liquid inside the nozzle, effervescent atomization does not require solubility of the atomizing gas. Instead, the principle of effervescent atomization is based on the formation of a two-phase flow inside the nozzle. A small amount of gas (usually air) is introduced in the liquid before it exits the atomizer and a two phase flow is formed (Figure 1). When the mixture exits through the nozzle, pressure suddenly drops. The pressure drop causes fast expansion of gas bubbles, which in turn leads to the disintegration of the atomized liquid into drops. The spray formation process in effervescent atomizers therefore does not rely solely on high liquid pressure and aerodynamic forces. This breakup mechanism allows the use of lower injection pressures and larger nozzle diameters without compromising the drop-size distribution and preventing clogging and fouling. In contrast to airblast atomizers the amount of atomizing air is minimal (Babinsky and Sojka, 2002). On the other hand the atomizer body is quite

complicated and usually consists of multiple parts, whose structure, size and dimensions have an effect on the resulting spray (Jedelský et al., 2009a).

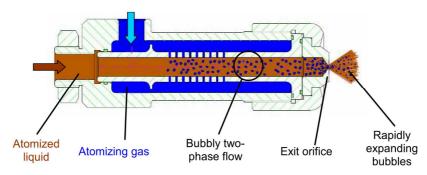


Figure 1 Schematics of effervescent atomization, courtesy of (Jedelský et al, 2007)

Effervescent sprays often suffer from unsteadiness; the involved spray forming process is after all inherently unsteady (Luong and Sojka, 1999). This phenomena has been thoroughly investigated in many research papers, such as (Jedelský et al., 2009b; Luong and Sojka, 1999; Gadgil et al., 2011; Liu et al., 2011). The most important conclusion in terms of industrial applications is that the unsteadiness can be minimized by carefully choosing the operating conditions.

3 EXPERIMENTAL METHODS

Experimental measurements are arguably the most important part in the process of model development. Regardless of how carefully the model is developed, without proper validation it cannot be employed in industrial applications. Clearly the scope of measurement is to obtain as much relevant data as possible without compromising measurement accuracy and while minimizing measurement errors. Two types of experimental measurement are essential in case of spray combustion: measurement of the spray characteristics and measurement of the combustion characteristics. The present chapter provides an overview of experimental approaches employed within the dissertation.

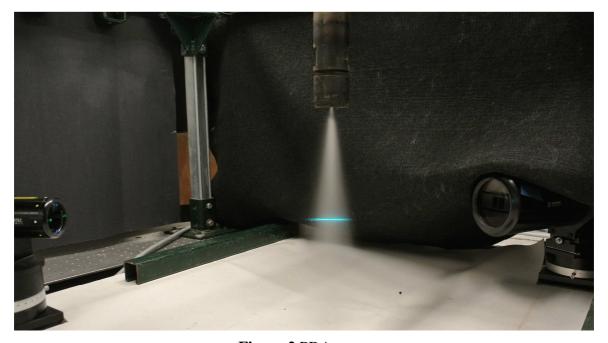


Figure 2 PDA setup

3.1 SPRAY MEASUREMENTS

When setting up a spray measurement, the sought variables are usually drop size (drop diameter) and drop velocity. The following paragraphs provide the reader with an overview of the most used measurement with emphasis on the Phase/Doppler Particle Analyser (P/DPA) or sometimes also called Phase Doppler Anemometry (PDA).

For the current research, experimental measurements were performed at three axial locations – 5, 10 and 15 cm. Measurements performed at closer distances yielded no results (probably due to high spray density). At each axial distance, several radial measurements points were established. First, equidistant radial measurement points 1 cm apart were chosen – a total of 3, 5 and 6 radial measurement points for distances 5, 10 and 15 cm respectively. In order to increase the measurement resolution, at axial distance 5 cm the respective distance of radial

points was lowered to 0.5 cm, which finally yielded 6 radial measurement points. This division proved to be adequate as it captured well the drop size variations and no major fluctuation between adjacent radial points was observed.

One of the parameters influencing the quality of measured data is the number of sampled droplets. It is reasonable to expect, that the actual drop size distributions are smooth, including the peripheries or so called tails, where the droplet fraction is small. To obtain such distribution it is important to sample a sufficient number of droplets. Various sampling numbers are adopted, form 2,000 (Li et al., 2012), 10,000 (Panchagnula and Sojka, 1999), 20,000 (Jedelský et al., 2009a) up to 50,000 and 100,000 (Liu et al., 2010). There is no universal rule to determine this number, but it can be derived during the measurement itself by judging on the convergence of the drop size distribution. In some cases the smoothness of the drop size distribution might be also compromised by a wrong choice of mask, or by high noise. The latter case can be remedied by shielding the measurement area from any other light sources and/or by increasing the PDA lasers power.

During experimental drop size measurements performed in the current research (5.5, 5.6 and 5.7) the goal was to collect ideally 20,000 samples at each location. At certain operating conditions and spray locations it was not possible to reach this number due to local spray properties (spray density) and therefore less samples were collected. The average number of samples collected was 10,000. Seven measurements (out of 136) yielded less than 1,000 samples.



Figure 3 Combustion test facility

3.2 COMBUSTION EXPERIMENTS

Wall heat fluxes in combustion chambers, furnaces and boilers are one of the most important parameters in process and power applications. It is therefore very important to be able to predict them and to have experimental data for model validation. The distribution of local heat flux across heat exchanging areas is of special interest due to material strength and durability implications. In the last two decades, a number of research papers can be found where wall heat fluxes are investigated either experimentally (Hayes et al., 2001) or numerically using CFD tools (Vondál and Hájek, 2009).

The combustion experiments presented in this work relied on a water-cooled horizontal combustion chamber (1 m internal diameter and 4 m length) which is located in the Institute of Process and Environmental Engineering of Brno University of Technology (Figure 3). The shell of the chamber is divided into seven sections; each of which has a separate water inlet and outlet and is equipped with a water flow meter and temperature sensors, allowing for accurate local heat transfer rate measurement along the flame. The experimental facility is described in detail in (Kermes et al., 2007) and (Kermes and Bělohradský, 2008).

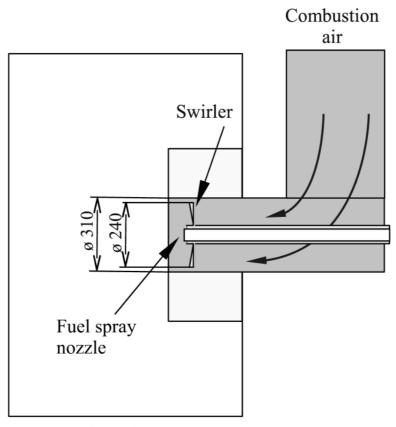


Figure 4 Cross-section of the burner

4 NUMERICAL METHODS

The problem of spray combustion is a highly complex one. Different phenomena (turbulent flow, atomization, evaporation and combustion) interact with each other causing the solution to be very sensitive. Swirling combustion alone (gaseous) still represents an uneasy problem (Vondál and Hájek, 2009; Vondál et al., 2010) and the presence of spray drops further increases the complexity of predicting such flames. Clearly, to minimize the uncertainties and errors that are caused by numerical representation of sprays, appropriate atomization models need to be found and validated. The following sections discuss numerical approaches adopted in the current work.

4.1 GOVERNING EQUATIONS OF THE FLUID FLOW

Before focusing on more detailed aspects of the two phase flow problems in question, it is helpful to review the governing equations of fluid flow, the so called Navier-Stokes equations. These equations are fundamental to almost any flow problem imaginable and the engineering world relies heavily on them when looking for a solution. A peculiar thing about the Navier-Stokes equations is that we expect them to give us a solution that is unique. However, this has only been proven for two-dimensional flows, not yet for three-dimensional flows. According to the Clay Mathematics Institute this is one of the Millennium Prize Problems.

4.2 TURBULENCE

As mentioned in paragraph 2.4, turbulence is a very complex phenomenon which causes the flow properties fluctuate. However, when dealing with industrial turbulent flow problems the main interest is usually not in the instantaneous properties, but in the mean values. We can therefore use certain averaging techniques which eliminate the fluctuating components from the governing Navier-Stokes equations, thus getting the so called RANS equations. Nevertheless, this approach introduces new variables called Reynolds stresses which need to be modelled in addition the filtered governing equations.

Turbulence models generally differ in the way they model the Reynolds stresses. A variety of models has been developed ranging from the simplest algebraic models, through one and two equation models to more complex Reynolds stress models. The most common models used in industrial applications are the two equation models, mainly k- ε and k- ω and their variations. A detailed comparison of two equation turbulence models for gas combustion can be found in (Broukal et al., 2012). Over the past few years a great deal of research is being performed around the LES models. These models represent an interesting hybrid combining DNS, where all the fluctuations are resolved, with the RANS models. However promising LES surely is, at the present time it is still not ready to be widely employed in real-life applications.

4.3 SPRAY REPRESENTATION

At the present time, two predominant methods for numerical spray representation are used: the Euler–Euler and Euler–Lagrange approach. The first approach is handles both the liquid and gaseous phase as impenetrable continua and tracks their interfaces. Therefore two sets of Navier-Stokes equations (one for each phase) need to be solved along with the coupling interface equations. However, this approach is computationally demanding and so far is used almost exclusively for spray formation investigations without combustion as for example in (Riber et al., 2009; Shinjo and Umemura, 2011). The latter approach is on the other hand less demanding since only the gaseous phase is treated as a continuum while the liquid (or dispersed) phase is handled in a discrete fashion. Only one set of Navier-Stokes equations needs to be solved and the discrete particles (drops) are tracked in a Lagrangian frame of reference using a set of relatively simple ordinary differential equations. The coupling between phases is represented by source terms in the Navier-Stokes equations.

Due to its simplicity the Euler-Lagrange approach allows employment in combustion applications as for example (Yan et al., 2008; Nieckele e al., 2010). However, the simplicity and low computational costs of the Euler-Lagrange approach are compensated by the need to find or develop appropriate sub-models for primary breakup (to determine initial drop parameters like diameter and velocity and their angular variations) and secondary breakup (breakup of drops that occurs further downstream from the nozzle) as well as for all other processes concerning the drops, like momentum, heat and mass transfer in the evaporating spray. Even when taking into account the aforementioned simplification, the problem would still be complex due to the enormous number of particles to track. Another simplification is therefore made which consists in introducing parcels. Parcels are objects that associate particles with similar location, diameter, velocity and other variables of interest. In the tracking algorithm parcels are being tracked instead of individual particles, which greatly reduce the computational time. The concept of parcels also applies to other submodels (secondary breakup, collisions). In the following paragraphs the Euler-Lagrange approach will be discussed in more detail. This approach is adopted in the numerical analyses performed in this work. A comprehensive overview and review of the spray modelling area can be found in (Jiang et al., 2010).

4.3.1 Particle Tracking

Ansys Fluent predicts the trajectory of a discrete phase particle/parcel (in this case a drop) by integrating the force balance on the particle, which lives in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle.

In order to take into account the turbulent flow effects on particle motion, the Discrete Random Walk (DRW) can be applied. The DRW model simulates

interactions of a particle with a succession of discrete stylized fluid phase turbulent eddies (Gosman and Ioannides, 1983).

4.3.2 Primary Breakup Models

The most crucial step when modelling a spray in the Euler-Lagrangian framework is the primary breakup. The model responsible for this process should ideally provide us with an initial drop size distribution, velocity distribution and mass flow rates, all dependent on spray angle. Available advanced methods that try to approach this idealized model include for example the Maximum Entropy Formalism (MEF) or Discrete Probability Function (DPF) method. These two methods are able to provide us with drop size and velocity distributions (in the case of DPF only with drop size distribution) and can also, to some extent, predict multimodal distributions, as demonstrated for example by Chin et al. (1995). Unfortunately both have also significant drawbacks. MEF requires two representative drop diameters and good predictions are achieved only after adjustments of the model parameters in order to fit experimental data. In the case of DPF, probability density functions of the fluctuating initial conditions are needed. Such fluctuations can be caused by a number of factors, some of which are vibrations of the atomizer, fluctuations in liquid delivery rate, fluctuations in liquid properties (in the case of non-homogenous liquids), fluctuations in exit velocity, etc. However, at the present time we are not able to measure these functions (Babinsky and Sojka, 2002). So far these drawbacks disqualify such methods from being widely used in industrial applications, although they represent a promising research direction.

Since advanced models able to predict the whole range of diameters are not applicable at the moment, simpler primary breakup models are being used. These models usually focus on predictions of a single representative diameter. Papers can be found, e.g. (Qian et al., 2010; Wu et al., 1992), where authors propose empirical correlations between the representative diameter and various physical conditions based on measured data. Such correlations are unfortunately valid only for a small range of atomizers or even for a small range of operating conditions. In industrial combustion applications, operating conditions are not constant, therefore more flexible models need to be employed. To overcome this obstacle, analytical formulas derived from first principles are needed.

Jet breakup in simple plain orifice atomizers is often modelled by introducing large droplets of the size of the nozzle orifice (Ashgriz, 2011). One of the analytical approaches to describe primary atomization was performed by Senecal et al. (1999). He relates to the pioneering work on jet disintegration by Weber (1931). In his work he investigates liquid sheet atomization and develops the so called LISA (Linearized Instability Sheet Atomization) model. This model predicts the maximum unstable growth rate and wave length, the sheet breakup length and the resulting drop size for pressure-swirl atomizers. The approach of Lund (et al., 1993) is, similarly to the previous case, based on Weber's work (Weber, 1931), but when formulating the

model a simpler instability analysis is used to predict a mean drop size of effervescent atomizers. An improvement of Lund's model is proposed by Xiong (et al., 2009), by applying the more rigorous Senecal's instability analysis. As Xiong pointed out, in numerous experimental observations of effervescent atomizers it was concluded that the primary atomization of the liquid undergoes three stages. First, assuming that the two phase flow in the nozzle is annular, an annular sheet forms and breaks up into cylindrical filaments. Second, the filaments break into ligament fragments. Finally, the ligament fragments stabilize to form individual drops. The model assumes that the annular liquid sheet breaks into several cylindrical filaments with almost the same diameter as the thickness of the annular sheet (Figure 5). The filaments then break into ligament fragments at the wavelength of the most rapidly growing wave and each fragment only forms one drop. The predicted SMD is later used as the initial diameter of injected drops during the numerical simulation.

The initial particle velocity is yet another unknown, which has to be approximated. One of the possible approximating formulas was derived in Appendix 2 of (Jedelský et al., 2009a). However, such formulas only give us a single velocity value and for the sake of precision angular dependency might be necessary.

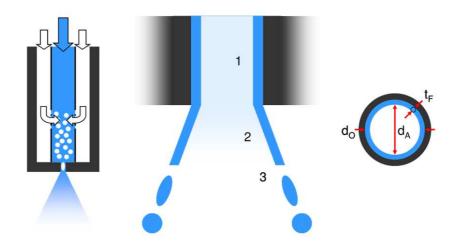


Figure 5 Simplified model of effervescent atomization, courtesy of (Schröder et al., 2010)

4.3.3 Secondary Breakup Models

Once the initial drop diameter (or diameter distribution) is obtained, we are interested in how will the drop size change in space and time. When primary breakup model provides a single diameter, the expectation from the secondary breakup model is to create an approximation of the actual drop size distribution. There are two main branches of secondary breakup models. The first branch is based upon Taylor's analogy between an oscillating and distorting drop and a spring mass system (Taylor, 1963) and it is called Taylor Analogy Breakup (TAB) model, used for example in (Senecal et al., 1999). The second model branch is based on the wave breakup model of Reitz (1987). Here the drop breakup is considered to be induced by the relative velocity between the liquid and gas phase. The relative velocity

causes the growth of Kevin-Helmholtz instabilities which are responsible for the final breakup. By using this model it is assumed, that atomization occurs only in the region close to the spray nozzle, since further downstream the relative velocity decreases due to drag and the model no longer predicts any breakup. The model was used for example in (Park et al., 2009) in a study of biodiesel fuel injector.

There are also other approaches to secondary breakup modelling. Xiong (et al., 2009) employs Cascade Analogy Breakup model proposed by Tanner (2004) to simulate an effervescent atomizer. The secondary breakup model based on Fokker – Planck equation proposed Apte (et al., 2003) is adopted by Vuorinen (et al., 2010). These recent models however have yet to be extensively validated and thus have not reached wide acceptance.

4.3.4 Drop Collision Models

There are different models that handle drop collisions. One of the most employed is the algorithm of O'Rourke (1981). Rather than using geometry to see if parcel paths intersect, O'Rourke's method is a stochastic estimate of collisions. Two particles can collide only if they are in the same computational cell. Once it is decided that two parcels of drops collide, the algorithm further determines the type of collision. Only coalescence and bouncing outcomes are considered.

New models are being proposed to address the drawbacks of O'Rourke's algorithm. Most recently, Taskiran and Ergeneman (2014) proposed a new collision model taking into account parcel location and velocity data to derive the impact parameter. Their model is therefore no longer mesh dependent but suffers from dependency on parcel number used in the calculations. The authors argue that this drawback could easily be solved in the near future as advances in computer technology will enable us to abandon the parcel approach and track individual droplets.

4.3.5 Drop Drag Models

Accurate determination of drop drag coefficients is crucial for accurate spray modelling and therefore every computational software has a wide array of models to choose from. Ansys Fluent, for example, provides a variety of methods that determine the drop drag coefficient ranging from simple models (Spherical drag law) to dynamic models (Dynamic drag model), where variations in the dropt shape are taken into account. The shape of drops is often assumed to be spherical, but in the case of high Weber numbers, this assumption can distort the final results. The dynamic drag model accounts for the effects of drop distortion, linearly varying the drag between that of a sphere and a value of 1.54 corresponding to a disk.

4.4 COMBUSTION

The challenge of modelling turbulent reacting flows consists of two interrelated parts, namely the representation of chemical reaction mechanism and its coupling with turbulence. The basic and simple model is Eddy-Dissipation pioneered by

Magnussen and Hjertager (1977). This model assumes that combustion is "mixing limited". This means that turbulence slowly mixes fuel and oxidizer into reaction zones where they burn quickly. Due to the Eddy-Dissipation assumption, the model cannot predict intermediate products (e.g. radicals) and can therefore be used only with one-step or two-step global reaction mechanisms. An ignition source is not required, since combustion occurs wherever turbulence is present (Broukal, 2009).

Eddy-Dissipation Concept can be viewed as an extension to the Eddy-Dissipation Model that allows the use of detailed chemical mechanisms and is therefore able to model phenomena such as local extinction and flame lift-off. This advantage comes however with a great computational price.

A compromise between detailed chemistry and computational time may be found in the use of models based on the mixture fraction concept. The power of the mixture fraction modelling approach is that the chemistry description is reduced to two transport equations. Under the assumption of chemical equilibrium, all thermochemical scalars (species fractions, density, and temperature) are uniquely related to the mixture fraction. When taking into account adiabatic systems, the instantaneous values of mass fractions, density and temperature depend only on the instantaneous mixture fraction. The turbulent nonpremixed flame problem is now reduced to tracking the turbulent mixing of the mixture fraction. This tracking can be done from wide variety of levels including DNS, LES and RANS.

4.4.1 Drop Evaporation

As the droplets are heated up by the reaction heat, mass transfer occurs between the discrete Lagrangian entities (fuel droplets) and the continuous gas phase. To take into account such interaction between phases, mass source terms are introduced to the gas phase in appropriate cells, whereas the mass and temperature of droplets are adjusted simultaneously. The evaporative mass fluxes are governed by gradient diffusion, with the flux of droplet vapour into the gas phase related to the difference in vapour concentration at the droplet surface and the bulk gas. No flow inside the droplet is considered and droplet properties such as temperature and density are considered to be uniform over the droplet volume.

5 RESULTS

This chapter contains an overview of relevant results in a form of excerpts of published papers. Since some results have been restated in subsequent publications to lay the groundwork for a new contribution, several articles have been omitted from this overview. The paper excerpts collected in this chapter are as follows:

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The last section (5.8) contains additional results that have not yet been published. These results are not in a form of a scientific article, since their meaning is to complement the published results and provide additional information to the reader.

5.1 EFFERVESCENT ATOMIZATION OF EXTRA-LIGHT FUEL-OIL: EXPERIMENT AND STATISTICAL EVALUATION OF SPRAY CHARACTERISTICS

This paper presents an experimental and statistical analysis of an effervescent atomizer. The spray data were obtained from experimental measurements by means of a Dantec phase/Doppler particle analyser (P/DPA) and analytical and statistical analysis was performed using MATLAB software. The main goal of this work was to analyse the spray characteristics and to find analytical functions that would fit the experimentally obtained drop size distributions. The fitted distributions were then discretized for modelling purposes and the modelled spray was verified against the experimental data. The discrete spray characteristics will be later used for combustion modelling.

Raw data from experimental spray measurement were analysed and fitted using a software tool developed in the MATLAB programming environment. The obtained distribution characteristics were used as input in Ansys Fluent to set up appropriate injections. The spray was properly discretized and represented by a sufficiently large number of computational droplets. The spray simulation was finally validated by comparing the computed data with the experimental data.

It has been shown that Ansys Fluent is able to represent reasonably well sprays in terms of overall drop size distribution. However, in case one is interested in a more detailed spray description then more sophisticated atomizer models or complex injections may be necessary.

5.2 VALIDATION OF AN EFFERVESCENT SPRAY MODEL WITH SECONDARY ATOMIZATION AND ITS APPLICATION TO MODELING OF A LARGE-SCALE FURNACE

The present work consists of a validation attempt of an effervescent spray model with secondary atomization. The objective is the simulation of a 1 MW industrial-type liquid fuel burner equipped with effervescent spray nozzle. The adopted approach is based on a double experimental validation. Firstly, the evolution of radial drop size distributions of an isothermal spray is investigated. Secondly, the spray model is tested in a swirling combustion simulation by means of measured wall heat flux profile along the flame.

In the first part of the paper, both experiments are described along with the measuring techniques. Drop sizes and velocities measured using a Dantec phase/Doppler particle analyser are analysed in detail for six radial positions. Local heat fluxes are measured by a reliable technique along the furnace walls in a large-scale water-cooled laboratory furnace.

In the second part Euler – Lagrange approach is applied for two-phase flow spray simulations. The adopted spray model is based on the latest industrially relevant (i.e. computationally manageable) primary and secondary breakup sub-models

complemented with droplet collision model and a dynamic droplet drag model. Results show discrepancies in the prediction of radial evolution of Sauter mean diameter and exaggerated bimodality in drop size distributions. A partial qualitative agreement is found in radial evolution of drop size distributions. Difficulties in predicting the formation of small drops are highlighted. Comparison of the predicted wall heat fluxes and measured heat loads in swirling flame combustion simulation shows that the absence of the smallest droplets causes a significant elongation of the flame.

The present work provides a detailed analysis and an unsuccessful validation attempt of a modern industrially relevant (i.e. computationally manageable) effervescent spray modelling approach. The investigated application is a 1 MW swirling flame of light fuel oil in a large-scale water-cooled laboratory furnace. Data for validation include spray characteristics in six locations along the spray radius at 150 mm axial distance from the nozzle and distribution of local heat flux along furnace walls. The following conclusions were drawn:

- The measured number-based drop size distribution of effervescent spray is unimodal around the axis and bimodal in the external part of the spray. Volume-based distributions are much less smooth and rather than bimodality they display irregularities among the larger drops. The volume-based distributions are clearly much more sensitive to the number of measured drops.
- The measurements prove that in effervescent sprays it is insufficient to measure a single total drop size distribution for a given axial position, as the distributions change very significantly in the radial direction. Single SMD value that is often provided in the literature is even less representative.
- Comparisons between predicted and experimentally measured radial drop size distributions show that the spray model implemented in this work based on Lund's primary breakup model (Lund et al., 1993) and secondary breakup model by Reitz (1987) is insufficient to describe the formation of effervescent spray.
- The computational model does not predict the formation of small drops below 30 μ m, which is in contrast with drops down to 3 μ m observed in the measurements.
- Comparison of the predicted and measured heat loads on furnace walls shows that the real flame is significantly shorter. As predictions for natural gas combustion in the same furnace with a similar gas burner do not display this discrepancy (Vondál and Hájek, 2009), it may be attributed to the deficiencies of the spray model, mainly to the missing small drops below 30 µm.

- Drop dynamics at the atomizer exit seems to be an important factor that should be reflected by the primary breakup model. Drop size, velocity, and mass flow rate should be functions of the spray angle.
- The C_2 parameter value in the secondary breakup sub-model (Reitz, 1987) is shown to have only little effect on the drop size distributions studied in this case.
- The proposed method of spray model validation by analysing radial (i.e. depending on spray angle) drop size distributions provides valuable insights and indeed seems to be necessary for effervescent sprays.

5.3 EXPERIMENTAL AND NUMERICAL INVESTIGATION OF WALL HEAT FLUXES IN A GAS FIRED FURNACE: PRACTICABLE MODELS FOR SWIRLING NON-PREMIXED COMBUSTION

Natural gas combustion and combustion of other light hydrocarbon gases is still one of the primary means of gaining heat. This applies especially for process and energy industries, where gas combustion is used as heat source for various processes. It is therefore of crucial importance, that the combustion chamber is designed properly in order to optimize the heat transfer process. Recently, CFD (Computational Fluid Dynamics) tools have proved themselves as a great potential aid for designers and engineers. These tools allow predicting of various phenomena of practical interest.

The main focus of this study is to validate a numerical model for swirling combustion in terms of wall heat fluxes using reliable measured data. The first part of this study deals with the experimental measurement of wall heat fluxes. Two burner duties are taken into account: 745 kW and 1120 kW. The second part consists in a numerical analysis of the problem. The simulations are performed using unsteady RANS with four different turbulence models coupled with chemistry and radiation models. Boundary conditions are set identically to the experiment.

Two simulations are performed (one for each burner duty) and fine-tuned. The measured and simulated wall heat flux profiles are finally compared and shortcomings if the numerical model are reported and discussed.

This study addresses the issue of turbulent swirling gas combustion. Two cases with different burner duties (745 kW and 1120 kW) were addressed both experimentally and numerically. Four commonly used turbulence models were compared in terms of local wall heat fluxes predictions and confronted with experimental measurements. The results indicate that in the case of higher duties (case 2) the used models struggle to capture the swirling effect, which results in slower mixing of fuel and oxidizer leading to longer flames and mismatch between predicted and measured wall heat fluxes. It can be argued, that there are turbulence models able to overcome these shortcomings, but unfortunately they are still too

computationally expensive to be employed across the board. Furthermore it is shown that the advanced RSM model has difficulties predicting total wall heat fluxes as accurately as simpler two-equation models. More research is therefore needed to better understand the swirling process and to find efficient ways to improve current models or to develop new ones.

5.4 REVIEW ON VALIDATION OF CFD MODELS OF SWIRLING FLOWS BY EXPERIMENTAL DATA

Efficient research and development of combustion applications is not possible without an experimental facility. Recently, development has also been supported by Computational Fluid Dynamics (CFD). CFD models, however, have to be validated against experimental data to become reliable tools for predictions. This article reviews available experimental data that are necessary for validation of CFD models of swirling turbulent reacting or nonreacting flows. The review is primarily concerned with measurements and CFD model validations of swirling turbulent combustion. However, swirling turbulent isothermal flows are included as well for sake of completeness. Experiments under well-defined conditions are stressed. These experiments are identified as popular with CFD modelers as they provide for complete experimental data that are appropriate for validation.

The review has revealed, that quality experimental data for validation of numerical models of swirling turbulent reactive flows are available mainly for gas swirl burner with tangential inlet swirl generators such as Sydney burner. This is supported by a large number of validation reports, in which LES and DES are the most often used methods for predictions. However, other turbulence models are also tested as they still dominate in practical industrial applications due to lower computational requirements. Other types of configuration (e.g. burners with guide vanes swirl generators) seem to be less frequently studied, which is given probably by the fact that the experimental database is not so extensive with respect to the number of different case studies. Available documentation of such experimental setups for tests under well-defined conditions includes description of TECFLAM burners (with movable blocks) and several gas combustion turbine configurations (e.g. based on Turbomeca design). A set of measurements on burners with axial guide vanes is very limited. To the best author's knowledge, no experimental measurement for validation of CFD turbulent combustion models is available for natural-draft burners, which are typical in process engineering applications.

5.5 DROP SIZE DISTRIBUTIONS IN EFFERVESCENT SPRAYS: AN EXPERIMENTAL STUDY USING PDA TECHNIQUE

Although effervescent atomizers (twin fluid atomizers with internal mixing) represent one of the most recent atomization techniques, they have already shown great usability especially in combustion applications. Due to their different drop formation mechanism they are able to produce smaller droplets than many other

conventional atomizers at similar operating conditions, thus making the combustion process more efficient. However, one of the shortcomings of effervescent atomization is the complexity of the atomization mechanism, which involves a twophase flow. This complexity presents a challenging obstacle when trying to devise computational models describing effervescent sprays. In the past few years many various models have been proposed, but their verification and validation often relies only on very limited data, such as only few representative diameters or global drop size distribution. The purpose of this paper is to review the previous experimental studies on effervescent atomization in order to identify areas that need to be more deeply investigated. The parameters that need more detailed analysis include especially radially (or angularly) and axially dependent representative drop diameters or drop distributions and mass fluxes. It is shown that previous measurements did not collect sufficient amount of data across the whole spectrum of drop sizes and thus parts of the previously measured spectra might be unreliable. A methodology for effervescent spray measurement for verification and validation of numerical models for combustion applications is suggested. Preliminary results are shown indicating the importance of appropriate mask choice.

The present work provides an overview of spray measurements with emphasis on effervescent spray formation and stresses the need of experimental data for verification and validation of numerical spray models for combustion purposes. It is shown that a great deal of available experimental results are insufficient for validation of numerical models, since only a coarse and global representation of the spray is given. Furthermore it is highlighted, that higher spatial resolution of measurements is needed, although recently detailed studies started to appear (Li et al., 2012).

Furthermore, a methodology for effervescent spray measurement using PDA technique is suggested that produces experimental results suitable for numerical model validations. Ideally, at least two sets of radial measurements points at various axial locations should be performed focusing on drop size and velocity distributions and also on mass flux distribution. Attention must be paid to the mask choice in order to prevent trimming of the drop distributions. The issue of unreliable mass flux measurements using PDA is addressed, but it is shown, that the Dual PDA extension of the original technique is able to at least partially overcome this problem. However, a similar study to that of (Dullenkopf et al., 1998) needs to be performed for the case of effervescent atomization.

In the last section experimental data are shown that demonstrate how a wrong mask choice can greatly skew obtained drop size distributions. Moreover, such mistake might be hard to notice, therefore a great caution should be addressed to this issue.

5.6 EXPERIMENTAL ANALYSIS OF SPATIAL EVOLUTION OF MEAN DROPLET DIAMETERS IN EFFERVESCENT SPRAYS

Effervescent atomization has established itself in the past decade as a promising alternative to conventional spray formation mechanisms. A great effort is currently being put into understanding the involved phenomena and developing numerical models to predict outcomes of processes relying on effervescent atomizers (i.e. spray combustion, coating, drying). This still proves to be a formidable challenge as effervescent atomization is a complex process involving two phase flow.

The presented paper focuses on mean droplet sizes and how they vary throughout effervescent sprays at different operating conditions. The experiment was performed using Phase Doppler Anemometry (PDA) and the droplet data were collected in multiple locations varying both axially and radially. At each measurement location the Sauter Mean Diameter (SMD) was computed. The preliminary results show that closer to the spray nozzle the bigger droplets are concentrated in the spray core, while the small droplets are in the peripheral regions. However, this trend is slowly reversing with increasing distance from the spray nozzle. Finally, from a certain distance the initial trend is completely reversed with the small droplets being in the spray core, while larger droplets are found closer to the edge of the spray. Moreover, this phenomenon seems to be independent of operating conditions. Reasons for such behaviour are suggested and discussed. Furthermore, SMD sensitivity to operating conditions is analysed.

The present work discloses results of an experimental study focused on local SMD values in industry-scale effervescent sprays. The effect of mass flow rate and GLR on local SMD has been investigated based on numerous experimental data. Examining SMD values varying both axially and radially has shown that while in the regions closer to the spray nozzle SMD decreases toward the spray edge, in the regions further downstream this trend is completely opposite. This finding holds true regardless of the operating conditions. An explanation is proposed to explain this behaviour. The presented results furthermore accentuate the effervescent spray complexity and can be used as a solid foundation ground on which future numerical models for effervescent sprays can be validated.

5.7 AN EXPERIMENTAL STUDY OF EFFERVESCENT SPRAYS: AXIAL EVOLUTION OF MEAN DROP DIAMETER

Effervescent atomization is a spray formation technique pioneered by Lefebvre and his colleagues in the late 1980s. It is becoming more and more frequently used in many industrial applications, ranging from pharmaceuticals, spray drying and coating to both internal and atmospheric combustion. Such interest obviously necessitates development of predictive models that would help us gain insight into the complexities of effervescent atomization and also help industry-based engineers

and designers with their decision-making. As shown in previous author's work, spatial drop size data is needed in order to validate numerical effervescent spray models. The purpose of this paper is to perform a deep investigation of the axial evolution of SMD in effervescent sprays. The influence of liquid mass flow rate and gas-liquid ratio will be taken into account both on cross-sectional SMDs and local SMDs.

The present work investigates SMD evolution along the spray axis. Three different SMDs are investigated - ID₃₂ (or cross-sectional SMD), axial SMD (local SMD values along the spray axis) and boundary SMD (local SMD values along the spray edge). It has been shown, that each of these evolutions behave quite differently and also have different dependencies on liquid mass flow rate and GLR. In general it can be said that the ID₃₂ seems to be rather constant at any given operating conditions. On the spray axis the SMD generally decreases, while on the edge of the spray SMD increases. The effects of liquid mass flow rate and GLR seem to be dominated by the transition in the two-phase flow regime inside the atomizer body, although further experiments would be needed to fully investigate this proposition. However, in the majority of cases increase of GLR leads to smaller SMD which is in agreement with previous studies (Ghaffar et al., 2012; Ochowiak, 2013). A similar, although less strong, dependency has been found also for the liquid mass flow rate.

6 SUMMARY AND CONCLUSIONS

As stated in the first chapter, the long term goal to which this work tried to contribute, is the predictability of swirling spray combustion, with focus on the distribution of heat loading (wall heat fluxes) in the combustion chamber of a fired heater. In order to achieve this goal much ground needs to be covered and this work represents an effort in this direction. The thesis consists of a general theoretic introduction into the area of effervescent spray combustion and a collection of published articles disclosing the author's findings.

6.1 RESULTS SUMMARY

This section tries to summarize and mutually relate the results contained in individual papers from chapter 5.

The article in chapter 5.1 acts as a more rigorous introduction in the discussed area for the reader. As a matter of fact, at the time of its writing it was also an introduction to the doctoral research for the author. The main aim was to assess the suitability of simple (readily available) numerical spray models to represent effervescent atomization. Experimental data was used to set up the primary atomization model in terms of a Rosin-Rammler distribution of drop sizes. The question was whether the radial change in the drop size distribution found in the experimental data will emerge in the relatively simple numeric simulation. Only partial agreement was achieved. It was concluded, that more sophisticated models need to be used in order to represent adequately effervescent sprays.

A second attempt to model effervescent atomization is described in chapter 5.2. A spray model comprising a primary atomization model derived from first principles along with a secondary atomization model was applied to a large-scale swirling combustion simulation. First, the spray itself was analysed and compared to experimental data. Although the predicted mean drop sizes were in qualitative agreement, the spray model was not able to predict droplets smaller than 30 µm as well as the radial evolution of SMD observed in the experimental data. It was concluded, that these two deficiencies are responsible for the poor predictions of the wall heat fluxes. This further strengthened the opinion, that a single SMD is not a sufficient representation of an effervescent spray and spatial evolutions need to be accurately predicted in order to get acceptable wall heat fluxes predictions.

A small detour from effervescent atomization has been taken in chapter 5.3 where the goal was to try and confirm the conclusions from chapter 5.2, that the failure to predict the wall heat fluxes was indeed caused by the spray model. An analogous gas combustion simulation was performed with identical turbulence, chemistry and radiation models and good agreement with experimental measurements was found. The previous conclusion was therefore confirmed as well as the need of more complex effervescent spray models. Moreover, an extensive literature review on numerical approaches in swirling flow was performed (5.4).

In order to develop a new effervescent spray model validation data are needed. During an extensive literature review it was found that well documented experimental data are rarely available, especially in the case of drop size data of effervescent sprays. It was therefore essential to perform experimental measurements. Due to a fortunate turn of events a possibility arose to experiments and it was fully utilized. Chapter 5.5 presents an overview of experimental approaches and puts forward a measurement methodology that is believed to be appropriate for the present case, i.e. acquiring data suitable for validation of effervescent sprays.

The work presented in chapter 5.6 aims to investigate radial variations of experimental SMD at various axial distances and sensitivity to operating conditions. It was observed that closer to the spray nozzle the SMD decreases with radial distance, while further downstream the relationship is completely reversed. This phenomenon was preserved regardless of operating conditions. The effect of GLR and liquid mass flow rate is more unclear. In the spray core the relationship was difficult to determine, while in the outside spray region their increase led to smaller SMD. This investigation revealed complexities in the effervescent spray formation that have, to the author's knowledge, not yet been published.

The investigation of the experimental data continued in a follow up study (5.7) where both global and local axial evolutions of SMD were investigated. A technique for calculation of cross-sectional SMD was adopted (ID₃₂) and its axial evolution was compared to two axial evolutions of local SMDs – one consisting of local SMD computed on the spray axis and the other of local SMD computed on the spray edge. It has been shown that each of these three evolutions behave quite differently. Irregularities in the effect of GLR on individual SMD evolutions has been attributed to change in the two-phase flow regime inside the atomizer body. In general however, increase of GLR leads to smaller SMD and a similar, although less strong, dependency has been found also for the liquid mass flow rate.

6.2 CONCLUSIONS AND FUTURE WORK

The main conclusions of this thesis can be summarized as follows:

- Simple spray models contained in today's commercial computational software products are not able to represent effervescent sprays in a sufficient manner.
- In order to predict wall heat fluxes in effervescent spray combustion simulations, the spray model needs to be able to predict radial drop size variations.
- Experimental validation data for new spray models must reflect the model's purpose. Moreover, multiple radial and axial measurements provide valuable insight into the spray formation phenomena.

- A new phenomena was observed, where in the area close to the effervescent spray nozzle drop sizes decrease with radial distance, while further downstream the trend is completely opposite.
- The effect of GLR on drop sizes reported in numerous articles was confirmed.
- A new method in the investigation of axial drop size evolution was proposed based on a comparison of cross-sectional, axial and boundary SMDs evolutions.

During this research it has been recognized that a significantly more detailed effervescent spray model is needed instead of the commonly used ones. The results put forward in this thesis represent a solid foundation for development and validation of such models with emphasis on spray combustion applications. Implementation of the given guidelines and ideas into a numerical model is however a very challenging task that deserves a separate research of its own.

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ABSTRACT

This thesis presents an investigation of effervescent sprays and their application to spray combustion with emphasis on large-scale combustors. Both aspects – modelling and experiment – are addressed.

The thesis contains a general introductory part, where underlying phenomena of spray forming and turbulent combustion are explained and effervescent atomization is presented. Then, adopted experimental approaches are described both for the spray measurement and for the measurement of wall heat fluxes during combustion experiments. In the following chapter numerical models and their philosophy is discussed. Models for spray formation, turbulence and combustion adopted during the research are introduced and explained.

The actual results of the thesis are presented in form of separate papers (published or accepted for publication) with an additional section devoted to unpublished relevant results. It is found that standard spray models can to some extent represent effervescent sprays. However, in order to predict a spray flame more detailed spray models are needed in order to describe accurately radial and axial variations of drop sizes. Numerous experimental measurements of effervescent sprays are performed using a proposed methodology. Drop size data are analysed with emphasis on radial and axial drop size evolutions and some new phenomena are described. The inverse relationship between gas-liquid-ratio and mean diameter has been confirmed. Moreover a complete reversal in radial mean diameter trends for various axial locations has been described. Finally, a result summary is put forward that recapitulates the main accomplishments and conclusions. In the closing remarks possible future research is outlined. Experimental data for future effervescent model validations are disclosed.

ABSTRAKT

Tato práce se zaměřuje na oblast effervescentních sprejů a jejich aplikace na kapalné spalování s důrazem na průmyslové spalovací komory. Oba aspekty – modelování a experiment – jsou řešeny.

Práce obsahuje obecný úvod, ve kterém jsou vysvětleny základní jevy rozpadu kapaliny a vířivého spalování a dále je představena effervescentní atomizace. Poté jsou popsány použité experimentální postupy jak pro měření spreje, tak pro měření tepelných toků do stěn při spalování. V následující kapitole jsou popsány numerické modely a jejich podstata je vysvětlena. Jsou zde uvedeny modely pro rozpad spreje, turbulenci a spalování použité během výzkumu.

Vlastní výsledky práce jsou uvedeny formou samostatných článků (vydaných nebo přijatých) s dodatečnou částí věnovanou nepublikovaným relevantním výsledkům. Bylo zjištěno, že standardní modely sprejů jsou do jisté míry schopny popsat effervescentní spreje. Nicméně aby bylo možné predikovat plamen kapalného spreje, jsou zapotřebí detailnější modely sprejů, které dokáží přesně zachytit změnu průměrů kapek v radiálním a axiálním směru. Experimentální effervescentních sprejů bylo provedeno pomocí navrhnuté metodiky. Výsledky měření byly analyzovány s důrazem na radiální a axiální vývoj průměrů kapek a některé nové jevy byly popsány. Nepřímá úměrnost mezi gas-liquid-ratio a středním průměrem kapek byla potvrzena. Dále by popsán jev, kdy pro různé axiální vzdálenosti které dojde k úplnému převrácení závislosti středního průměru na axiální vzdálenosti. V závěru je uvedeno shrnutí, které rekapituluje hlavní výsledků a závěry. V závěrečných poznámkách je nastíněn možný budoucí postup. Experimentální data pro ověřování budoucích effervescentních modelů jsou poskytnuta.