

Computational Fluid Dynamics Simulation and Validation of Wall Wetting for Methanol Port Fuel Injection

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Ghent, June 2026
Spruytte Lien

Preface and Acknowledgments

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The global maritime industry faces pressure to reduce greenhouse gas emissions from frameworks such as the EU's fit for 55 package. Methanol has emerged as a promising alternative fuel for retrofitted dual fuel engine operation. However, methanol's high latent heat of vaporization and low volatility makes it prone to wall wetting. This can cause problems for the mixture homogeneity and engine stability.

As a first step, this study presents a comprehensive literature review. The background of methanol as an alternative fuel is discussed, along with its key implications for engine operation. This is followed by a critical assessment of the current state of knowledge on wall wetting phenomena in port fuel injection (PFI) systems. From this review, a clear research gap is identified and the research questions are defined.

This thesis develops and validates a Computational Fluid Dynamics (CFD) based framework in CONVERGE to model wall wetting behavior in methanol port fuel injection systems. The framework employs a Lagrangian-Eulerian approach combined with the Bai-Gosman spray-wall interaction model and conjugate heat transfer. The numerical model is validated against experimental data and limitations of the model are discussed. Subsequently, a systematic Latin Heuristic Sampling study investigates the influence of the injection pressure, fuel temperature, and ambient temperature on film thickness, film area, and film mass.

Keywords: Methanol, Port fuel injection, Wall wetting, Computational fluid dynamics, CONVERGE

COMPUTATIONAL FLUID DYNAMICS SIMULATION AND VALIDATION OF WALL WETTING IN METHANOL PORT FUEL INJECTION

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ABSTRACT

Methanol is a promising alternative fuel for the maritime sector, but its high latent heat of vaporization and low volatility lead to significant wall wetting in port fuel injection systems. This study implements and validates a Lagrangian-Eulerian CFD model of a methanol spray on a quartz glass wall. After a systematic parameter simulation campaign, a Spearman correlation reveals that the fuel temperature and injection pressure are dominant input parameters, while the ambient temperature has negligible influence. An iso-contour analysis further shows that fuel temperature and injection pressure can partially compensate for one another in controlling film thickness.

INTRODUCTION & MOTIVATION

The maritime sector accounts for roughly 2.9% of the global greenhouse gas emissions. International institutions have started to introduce legislation targeting the emissions from the shipping sector, such as the EU's Fit for 55 package. These regulations have motivated the exploration of alternative fuels, where methanol stands out. This is due to its high octane number, possibility for liquid storage, and potential for renewable production [1]. Methanol's high octane number and high latent heat of vaporization make it well-suited for spark ignition (SI) engines. Existing compression-ignition marine engines are being retrofitted with methanol port fuel injection (PFI) to work in dual fuel operation. However, methanol's high latent heat of vaporization and low volatility also introduce challenges during mixture formation when applied in low pressure PFI systems. One of the most critical issues is the wall wetting that occurs. The liquid film strongly influences evaporation, mixture homogeneity, combustion stability, and emissions, especially under cold-start conditions [2].

NOMENCLATURE

P	[bar]	Pressure
T	[K]	Temperature

Subscripts		
amb		ambient
inj		injection

Wall wetting phenomena have been studied extensively for gasoline and diesel applications, using both numerical and experimental approaches. In contrast, methanol wall wetting behavior remains far less studied and understood. Existing numerical research for PFI conditions often focuses on the spray atomization, penetration, and droplet size. Methanol wall wetting is mostly examined at high pressure direct injection in both numerical and experimental research [3]. Furthermore, existing methanol wall wetting studies often rely on single-parameter analysis, but not on the interaction effect. As a result, there is a clear research gap in the availability of validated, methanol-specific CFD frameworks that can systematically investigate wall wetting under PFI conditions.

METHODOLOGY

In this study, simulations are performed in CONVERGE using a Lagrangian-Eulerian (L-E) framework in which the gas phase is solved using the Reynolds-averaged Navier-Stokes (RANS) equations with the Re-Normalization Group (RNG) $k-\epsilon$ turbulence model. The liquid fuel is represented by Lagrangian parcels. The spray breakup is modeled using the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) framework. The droplet evaporation is described using the Frössling correlation while taking the convection effects and Stefan flow into account. To model the Spray-Wall interaction, the Bai-Gosman model is used to categorize the outcome of the impinging droplets into sticking, rebound, spreading,

and splashing regimes. To solve the dynamic heat conduction in the wall, conjugate heat transfer (CHT) is implemented to allow for a prediction of the thermal interaction of the fuel film and the wall.

The parametric study uses a discrete Latin Hypercube Sampling (dLHS) design covering three input variables: ambient temperature T_{amb} (5–45°C), fuel temperature T_{fuel} (20–60°C), and injection pressure p_{inj} (5–20 bar). Twenty simulation runs systematically cover this parameter space to capture both main effects and interactions

VALIDATION

Before conducting the parameter investigation, the numerical model is validated against experimental data from an optical spray-impingement study by Zhang et al.[4]. Their experiments investigate methanol spray impingement and wall wetting under PFI conditions using the refractive index matching (RIM) technique to measure liquid film thickness on a quartz glass surface. The RIM method is particularly interesting because it provides a simpler and more cost-effective alternative compared to more commonly used laser-based film thickness measurement techniques. As such, it could potentially be an accessible experimental approach for future validation studies if its limitations are well understood.

The numerical model successfully captures the observed trends with respect to the injection pressure. Both the experiments and simulations show an initial increase in wall film thickness with increasing injection pressure. For even higher pressures, the thickness reduces due to enhanced atomization and splashing. In the wall temperature validation case, the trend of decreasing film thickness is followed when the wall temperature is increased from 293 K to 373 K. However, at high temperatures, the model predicts stronger evaporation than observed in the experiment. Possible model limitations are the following:

1. The Bai–Gosman spray–wall interaction model may not be fully calibrated for methanol-specific splashing behavior, and wall roughness effects are not fully resolved.
2. Simplified thermal coupling with the quartz glass wall may overestimate the heat flux and cause excessive evaporation.
3. The Lagrangian wall film representation limits the resolution of film spreading and evaporation near the contact line.

PARAMETER STUDY & KEY FINDINGS

The parameter study revealed that the fuel temperature is the dominant factor for the film thickness. Increasing the fuel temperature from 20°C to 60°C reduces the average film thickness by approximately 3–4 μm , while the film area slightly increases due to the lower surface tension and viscosity. It is the absolute fuel temperature that drives the outcome. In contrast, the ambient temperature was noted to have very little effect on the wall wetting behavior. It is however the main driver in evaporation of the suspended droplets. Furthermore, the study also revealed that the injection pressure strongly controls the wetted area and the film mass. Higher pressure reduces the film thickness, however this is not a linear correlation. Beyond 10 bar, the reduction diminishes. Another notable threshold is observed between 5 and 10 bar, where the fraction of injected mass adhering to the wall increases before declining at higher pressures.

Interestingly, an iso-contour mapping of the pressure–temperature space shows that a reduction in fuel temperature can be partially offset by an increase in injection pressure to maintain the same film thickness. Vice versa, a lower injection pressure can be fully compensated by raising fuel temperature within the studied range.

CONCLUSION & FUTURE OUTLOOK

This study implemented and validated a CFD model for methanol wall wetting under PFI conditions and used it to assess the effects of fuel temperature, ambient temperature and injection pressure. The ambient temperature had little impact on film formation due to methanol’s high latent heat of vaporization. On the other hand, the fuel temperature was a dominant factor. Higher fuel temperatures reduce the film thickness while increasing the area. The same trend, but more nuanced, was visible upon increasing the injection pressure. The iso-contour shows that these two parameters can partially compensate each other.

In future work, the limitations of the model should be addressed by incorporating more realistic engine port geometry, an improved CHT model with stainless steel walls, and additional parameters such as the injection angle. Including the intake airflow in the parameter study would make the results more realistic for PFI conditions. After that, full engine simulations should be used to study how the input parameters affect the wall wetting over multiple injections and how this affects mixture formation, combustion efficiency, and cold-start emissions in methanol PFI engines.

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Nomenclature

Abbreviations

AMR	Adaptive Mesh Refinement
ASOI	After Start Of Injection
CFD	Computational Fluid Dynamics
CHT	Conjugate Heat Transfer
CI	Compression Ignition
DBI	Diffuse Back Illumination
DF	Dual Fuel
DI	Direct Injection
dLHS	Discrete Latin Hypercube Sampling
DNS	Direct Numerical Simulation
DoE	Design of Experiments
ETS	Emission Trading System
GHG	Greenhouse Gas
HFO	Heavy Fuel Oil
ICE	Internal Combustion Engine
IMO	International Maritime Organization
KH	Kelvin–Helmholtz
L-E	Lagrangian–Eulerian
LES	Large Eddy Simulation
LIF	Laser-Induced Fluorescence
MGO	Marine Gas Oil
MON	Motor Octane Number
NTC	No Time Collision
OA	O’Rourke–Amsden Model

PFI	Port Fuel Injection
PISO	Pressure Implicit with Splitting of Operators
RANS	Reynolds Averaged Navier–Stokes
RIM	Refractive Index Matching
RNG	Renormalization Group
RON	Research Octane Number
RT	Rayleigh–Taylor
SGS	Sub-Grid Scale
SI	Spark Ignition

Greek Symbols

α_{spray}	Spray evaporation model constant
β_{spray}	Heat transfer correction factor
δ_{ij}	Kronecker delta
η	Non-dimensional strain rate parameter
κ	Thermal conductivity
λ	Air–fuel equivalence ratio
Λ_{KH}	Wavelength of fastest-growing KH instability
Λ_{RT}	Wavelength of fastest-growing RT instability
μ	Dynamic viscosity
μ_g	Dynamic viscosity of gas
μ_l	Dynamic viscosity of liquid
μ_t	Turbulent dynamic viscosity
ν	Kinematic viscosity
ω	Growth rate of instability
Ω_{KH}	KH instability growth rate
ω_{RT}	RT instability growth rate
ϕ	Fuel–air equivalence ratio
ϕ'	Sub-grid scale unresolved variable
ρ	Density
σ	Surface tension
σ_{ij}	Viscous stress tensor

τ_{ij}	Reynolds stress tensor
τ_{KH}	KH breakup time
τ_{RT}	RT breakup time
ε	Turbulent dissipation rate

Letters

$\dot{m}$	Mass flow rate
$\tilde{S}_{ij}$	Mean rate-of-strain tensor
A	Area
A_d	Droplet surface area
A_f	Fuel film area
A_n	Nozzle cross-sectional area
b	Impact parameter
B_0	KH size constant
B_1	KH breakup time constant
B_M	Spalding mass transfer number
b_{crit}	Critical impact parameter
Bi	Biot number
C_D	Drag coefficient
C_d	Discharge coefficient
c_l	Specific heat capacity of liquid
C_{bl}	Breakup length constant
C_{RT}	RT size and time constant
D	Mass diffusivity
d	Droplet diameter
d_0	Initial droplet diameter
D_{imp}	Impingement distance
d_{nozzle}	Nozzle diameter
e	Specific internal energy
E_2	Droplet impact energy parameter
$E_{2,\text{crit}}$	Critical droplet impact energy parameter
$F_{p,i}$	Force acting on parcel in direction i

g	Gravitational acceleration
h	Convective heat transfer coefficient
H_{vap}	Latent heat of vaporization
k	Turbulent kinetic energy
K_s	Equivalent roughness height
k_s	Thermal conductivity of solid
k_{air}	Thermal conductivity of surrounding air
L_b	Breakup length
L_c	Characteristic wall length
La	Laplace number
m_d	Droplet mass
Nu	Nusselt number
P	Pressure
P_k	Production of turbulent kinetic energy
Pr	Prandtl number
Q_d	Heat flux to droplet
r	Radius
r_p	Parent droplet radius
r_s	Spearman rank correlation coefficient
Re	Reynolds number
S	Volumetric source term
S_{mom}	Momentum source term
Sc	Schmidt number
Sh	Sherwood number
T	Temperature
T_d	Droplet temperature
T_f	Average film thickness
T_{amb}	Ambient temperature
T_{fuel}	Fuel temperature
T_{wall}	Wall temperature
u_i	Velocity component in direction i
V_p	Parcel volume
V_{cell}	Eulerian cell volume
We	Weber number

Chapter 1

Literature Review

1.1 Introduction

The global shipping industry is responsible for approximately 2.9% of the annual global greenhouse gas (GHG) emissions [1]. This share continues to grow as the global trade market and the importance of maritime transport also increase. To address climate change, the Paris Agreement aims to limit global warming below an increase of 2°C. In response, both the European Union and other international institutions have introduced legislation targeting emissions from the shipping sector. The EU's Fit for 55 package is set to cut greenhouse gas emissions with 55% by 2030, compared to 1990 levels. As part of this package, the shipping industry has been included in the EU Emission Trading System (ETS), which requires shipowners to pay for their CO₂ emissions when operating in EU territory [2].

Globally, the International Maritime Organization (IMO) proposed a net-zero framework that aims to reach net-zero emissions around 2050. It also sets intermediate checkpoints for a reduction of at least 20% by 2030 and 70% by 2040. This framework includes measures such as the setting of efficiency standards for new and existing vessels, the development of low- and zero-carbon fuels, and a carbon pricing system [3]. However, the formal implementation of the framework is currently on hold due to further negotiations among member states. These legal measures are expected to push shipping companies towards greater efficiency and making investments in green technologies.

Most ships today run on heavy fuel oil (HFO) or marine gas oil (MGO), which is burned in large two-stroke or four-stroke diesel engines. While these engines are powerful and reliable, they emit high levels of CO₂ and other emissions such as NO_x and unburned HC molecules [4].

To comply with new regulations, several alternative fuels have been considered for maritime transportation such as hydrogen, ammonia, methane, methanol, and ethanol [5]. Each of these offer advantages and challenges in terms of production, storage, and combustion characteristics. In this study, the utilization of methanol as a fuel is chosen because of its promising properties.

1.2 Methanol as a Fuel

This part of the literature study focuses on the chemical and physical properties of methanol, its production pathways, environmental and safety aspects, and the technical feasibility of using methanol as a fuel in internal combustion engines.

Table 1 shows the key properties of methanol compared to typical fossil fuels such as gasoline, diesel, and hydrogen.

Property	Unit	Methanol [6]	Gasoline[7]	Diesel[7]	Hydrogen[8]
Chemical formula	–	CH ₃ OH	various	various	H ₂
Molecular weight	kg/mol	32.0	95–120	150–250	2.02
Density (vap., 20°C, 100 kPa)	kg/m ³	1.42	3.88	n/a	0.08
Density (liquid)	kg/m ³	790	730–780	820–845	0.08
Dynamic viscosity (20°C)	mPa·s	0.57	0.60	3.0	0.009
Boiling point (100 kPa)	°C	65	25–215	150–380	–253
Reid vapour pressure (37.8°C)	kPa	31.7	50–90	n/a	n/a
Lower heating value	MJ/kg	20.09	42.9	43.2	120
Autoignition temperature	°C	465	192–470	230	585
Heat of vaporisation	kJ/kg	1100	180–350	225–280	461
Flash point	°C	11	–45	55	n/a
Stoichiometric air–fuel ratio	kg air/kg fuel	6.5	14.7	14.7	34.2
Upper flammability limit (λ)		0.23	0.26	0.32	0.15
Lower flammability limit (λ)		1.81	1.60	3.5	10.57
Research octane number (RON)	–	109	95	n/a	130
Motor octane number (MON)	–	92	85	n/a	n/a
Cetane number	–	3	8–14	53	n/a

Table 1.1: Comparison of fuel properties for methanol, gasoline, diesel, and hydrogen [6][7] [8] .

Methanol has a higher octane number than gasoline, which means that it is less likely to auto-ignite. This allows for higher compression ratios, improving thermal efficiency. Additionally, methanol also has a higher latent heat of vaporization, which can cool the air-fuel mixture. This combination of properties increases the volumetric efficiency and creates a higher power output. However, methanol’s lower volumetric energy density means that more fuel is required to achieve the same energy output compared to gasoline. Methanol has twice the volumetric energy density of hydrogen and it is significantly easier to store and handle. These properties make it a more practical alternative for marine applications.

Currently, methanol is primarily produced from natural gas or coal. The process involves three main steps: syngas production, conversion to crude methanol, and purification [9]. Syngas is a mixture of hydrogen (H₂), carbon monoxide (CO), and carbon dioxide (CO₂). It can be generated via steam reforming, auto-thermal reforming or partial oxidation of methane. The conversion of syngas to methanol occurs under low pressure and moderate temperatures while using a copper-based catalyst. This process is efficient and has been economically viable for decades, but faces sustainability challenges due to its reliance on fossil feedstock [9].

Methanol has the potential to be produced from renewable sources such as biomass and renewable hydrogen. Biomass, including agricultural waste and solid waste, is gasified to produce syngas. This is a thermochemical process that uses high temperatures and gasifying agents like steam or oxygen. It is a technically complex process with additional challenges such as the production of tar and a low hydrogen output [9]. The process also relies on the availability of biomass, which is a limit to the scalability of this method. In 2022, an estimate of 0.38% of the global methanol production came from biomass [10].

Another sustainable way to produce methanol is through catalytic hydrogenation of CO₂, also known as e-methanol [11]. In this process, CO₂ captured from industrial flue gases, reacts with hydrogen over a catalyst to form methanol and water. The reaction:



This reaction requires a significant amount of energy to break the strong carbon-oxygen bonds in CO₂. However, when both the hydrogen and energy input are derived from renewable sources, like solar or wind, this method offers a carbon neutral route to methanol production [9].

Due to methanol's high octane number and low tendency for knock, it is an ideal fuel for spark-ignition (SI) engines. On the other hand, its low cetane number makes it unsuitable for compression-ignition (CI) engines, which require fuels with a much higher cetane rating (e.g. diesel has a cetane rating that ranges from 40 to 55) [12]. Since most internal combustion engines in maritime vessels are CI-based, using methanol in these engines requires either modifying the fuel or adapting the engine design.

A possible approach is to add additives to the methanol, as a result of which the cetane number increases. However, many of these additives contain nitrogen compounds that are toxic [13]. Therefore, it is better to look at technologies to retrofit the existing CI engines so that they can operate on methanol using SI-based strategies.

1.3 Port Fuel Injections

Two main types of fuel injection methods are used to convert heavy-duty maritime engines into dual-fuel (DF) engines. The first and oldest method is port fuel injection (PFI). In this system, the fuel is injected into the intake port, which is located upstream of the intake valve. The air and fuel mix before entering the combustion chamber. This method gives time to form a relatively homogeneous air-fuel mixture.

The second method is direct fuel injection (DI). In this system, the fuel is injected directly into the combustion chamber during the compression stroke. This method gives more control over the injection timing and mixture formation.

When considering methanol as a fuel, both strategies have been analyzed in experimental studies. According to experiments by Yin et al.[14], the methanol DI strategy shows more advantages regarding the combustion characteristics, combustion rate, and CO₂ emissions. Although this paper focuses on the benefits of DI systems, it also states that PFI remains the more practical choice. This is because a PFI system involves less complex hardware and thus is easier for retrofits. PFI uses lower pressure injectors and intake manifolds compared to DI [15]. As a result, converting existing engines to methanol PFI is more cost-effective and simpler than adding high-pressure DI systems. Both researchers and industry experts agree that PFI is the most practical and cost-effective solution for converting marine and heavy-duty engines to run on methanol [16] [17].

However, retrofitting existing marine internal combustion engines (ICEs) also comes with challenges [16] [17]. Methanol has a lower heating value, which is about half that of diesel or gasoline. This means that a higher flow rate and larger injector capacity are required to maintain the equivalent power output [4]. Methanol's high latent heat of vaporization introduces strong cooling. This increases volumetric efficiency but often leads to cold-start difficulties and incomplete evaporation [18]. Furthermore, existing compression ratios, combustion chamber geometries, and ignition systems are typically optimized for fossil fuels. Thus, conversion of these engines can result in increased ignition delay and sub-optimal combustion [16] [19].

Methanol combustion has low soot and NO_x emissions due to its oxygenated nature and high heat of vaporization, but it still has several challenges regarding emissions. Cold-start and low load conditions can lead to incomplete combustion. This can increase the CO, HC, and unburned methanol emissions [6]. Recent research shows that using advanced combustion strategies can improve this, but there will be trade-off between reducing the emissions of HC, CO₂ and No_x [20].

Overall, converting existing engines to fit methanol PFI systems comes with a lot of challenges and requires a lot of new research. One of the most critical issues in methanol PFI is cold-starting. Methanol's high latent heat of vaporization makes it difficult for the fuel to evaporate under certain ambient conditions. According to Li et al.[21], cold-start becomes an issue for ambient temperatures below 289 K. The engine can no longer start reliably without an auxiliary heating system. Methanol droplets can no longer completely evaporate below a temperature of 263 K. In a single-droplet analysis, increasing the ambient temperature from 263 K to 293 K as well as reducing the droplet diameter was shown to be optimal for promoting methanol evaporation. Increasing the fuel temperature did not promote better evaporation [22].

These findings highlight the importance of understanding how methanol behaves and evaporates during the mixture formation. One key phenomenon that influences evaporation, mixture homogeneity, and combustion stability is wall wetting [17]. Research into wall film formation and its dynamics is thus essential to optimize methanol use in retrofitted engines.

1.4 Wall Films

When fuel is injected into the intake port, not all of the fuel immediately mixes with the incoming air flow. Some of the fuel droplets impinge on the walls or valve surfaces and form a liquid film. This film gradually evaporates and the fuel eventually enters the combustion chamber. Due to methanol's high latent heat of vaporization, low volatility, and increased injected fuel amount, this wall wetting phenomenon becomes increasingly important.

Understanding and predicting wall film behavior has therefore become a key focus in both numerical modeling and experimental research. Over the past decades, researchers have developed models to simulate spray-wall interactions and film dynamics. These models are the foundation for useful Computational Fluid Dynamics (CFD) simulations.

1.4.1 Numerical Research

Numerical research on PFI wall wetting started in the early 1980s when a groundwork was put in place using basic fluid mechanics and heat transfer principles. P.G. De Gennes laid the theoretical groundwork for understanding how different liquids interact with solid surfaces [23]. De Gennes described the physics of contact angles, surface tension, and wall wetting transitions. These elements are crucial for modeling fuel behavior in engine intake systems and film formation.

In the 1990s, researchers began developing simplified models to simulate droplet behavior and film formation. For example, a 1D airflow model, combined with a 2D droplet flow model and film models, was used to predict mixture behavior in SI engines [24]. These models showed phenomenologically correct results but also highlighted the need for experimental validation and model improvements.

The transition to CFD-based modeling began in the mid-1990s. Two influential wall film models were introduced in 1996. The O'Rourke-Amsden (OA) model and the Bai-Gosman model.

- **O'Rourke-Amsden:** The O'Rourke-Amsden model introduced the first Lagrangian droplet-wall interaction and wall-film model [25]. Their particle-based approach simulated wall film dynamics and evaporation in gasoline in PFI SI engines. The model assumes a thin film, laminar flow, and negligible inertia. With those assumptions the governing equations could be simplified.
- **Bai-Gosman:** The Bai-Gosman model uses a semi-empirical regime-based approach with transition criteria for stick, rebound, and splash [26]. It accounts for droplet impact pressure, tangential momentum transfer, and gas shear forces acting on the film while solving the mass, momentum, and energy equations within a boundary layer framework.

Further progress came from Curtis et al. [27], who developed a quasi-dimensional wall wetting model to predict transient air-fuel ratio excursions. Their model incorporates multi-component fuel behavior, backflow-induced film redistribution, and laminar boundary-layer film flow. This model made accurate simulation of evaporation and liquid fuel transport possible. With this model the influence of intake valve deposits and operating temperature on fuel film behavior was highlighted.

Between 1997 and 1999, researchers significantly improved wall film modeling by adding the effects of shear and evaporation. Han and Reitz' model is built on the O'Rourke-Amsden model by introducing non-isothermal evaporation and film spreading driven by shear stresses [28]. This made the model more realistic for both diesel and gasoline PFI sprays. A year later, Stanton and Ruland extended previous models by coupling the wall film's momentum with the in-cylinder gas flow [29]. The model solves the continuity, momentum, and energy equations for a thin liquid film over complex 3D surfaces. The model accounts for shear forces, dynamic pressure, and evaporation effects and includes impingement regimes such as stick, rebound, spread, and splash. This allowed the film to respond dynamically to the engine airflow and improves the accuracy of the model.

In the beginning of the 21st century, commercial CFD codes such as KIVA-3V and VECTIS began integrating the improved wall film models. The models included film evaporation, wall heat transfer, and energy balance equations, which linked wall wetting phenomena to hydrocarbon emissions and engine performance [30]. In particular, the O'Rourke-Amsden model was significantly improved in 2000 to include splash modeling, film inertia, and a pressure gradient [31]. Improved numerical methods made it more accurate for cold-start and transient conditions in PFI engines.

In recent years, more research has been done on various wall wetting phenomena using the three-dimensional CFD software.

A notable example is the study of Liu et al. [32] in 2016. They performed a detailed numerical study on wall film formation during cold-start and evaporation in PFI engines using an iso-octane fuel mixed with 5% 3-pentanone. Under low injection pressures (0.25-0.3 MPa), poor atomization led to large droplets impinging on the intake surfaces and formation of a liquid film. It was previously noted that these films, especially at low wall temperatures, do not fully evaporate. This can lead to an increase in unburned hydrocarbon emissions and poor mixture preparation [33]. To numerically investigate these phenomena, the authors developed a three-dimensional simulation framework using the commercial CFD software Ansys Fluent. They combined an Eulerian-Lagrangian Discrete Phase Model with a refined spray-wall interaction and wall film evaporation sub-models. Their results showed that higher injection pressures, longer impingement distances, and more oblique angles improved atomization and reduced film thickness. Higher wall temperatures significantly accelerated the evaporation process, especially at the film edges where the thickness was lower. On the other hand increasing the injection duration led to more fuel mass and thicker fuel films. This also increased the thermal resistance within the film, which limited the evaporation efficiency.

Like the study by Liu et al., most of the previous research on wall wetting has focused on gasoline-like fuels. This means that there is a gap in understanding the methanol-specific wall wetting behavior. Methanol's high latent heat of vaporization, low volatility, and low heating value cause challenges for mixture formation and combustion stability in retrofitted heavy-duty engines.

To address this, Singh et al. [34] present a recent study that investigates the retrofitting of heavy-duty engines to operate on 100% methanol using PFI. The authors report that the work combines experimental testing and CFD modeling to assess the combustion characteristics, emissions, and wall wetting behavior. While the detailed methodology and the results are

not accessible, the authors highlight methanol’s potential for clean combustion and improved thermal efficiency, but also emphasize the need for a deeper understanding of mixture formation and wall film dynamics.

A more detailed study was done by Zoumpourlos et al. in 2025 [17]. They present a CFD-based investigation using CONVERGE v3.0 to examine methanol spray behavior under PFI conditions in marine ICEs. Their CFD framework incorporates Lagrangian-Eulerian coupling and Reynolds-averaged Navier-Stokes (RANS) turbulence models. The study focuses primarily on spray modeling. In the study, the authors vary the injection pressure from 6 to 200 bar. The results show that higher injection pressures improve atomization, reduce droplet size, and enhance evaporation rates. The authors confirmed that poor atomization and low intake temperatures can lead to wall film formation, which disrupts the mixture homogeneity and engine stability. However, this research does not simulate the wall wetting phenomena. The authors identify it as a key issue and suggest that future work should couple the spray modeling to wall wetting models to better understand these methanol-specific wall wetting effects.

Lastly, a very targeted investigation was done by Kontkanen O. [35], who modeled methanol wall film formation and evaporation using OpenFOAM. The study simulated a simplified intake stroke with static valves and non-deforming surfaces. The results showed that over 90% of the injected methanol formed wall films. Evaporation is dominated by boiling on the hot valve surface, while evaporation from the runner is slow. At the end of the stroke 20-25% of the fuel remains as a liquid film. However, the author mentions that this study has several limitations. Wall films are only modeled on static surfaces and thus do not take the dynamic valve motion into account. Secondly, fixed wall temperatures prevent realistic heat transfer and cooling effects.

The reviewed literature shows that wall wetting in PFI engines is a complex phenomenon that is influenced by intake conditions, fuel properties, and the implementation of the spray. Early models have provided a good foundation for modern CFD simulations. Over time these CFD models have improved in their accuracy when more physical elements were taken into account in the sub-models. For methanol, the problem of wall wetting is even more prominent. Its high latent heat of vaporization and low volatility promotes wall films and hinder the homogeneity of the mixture. Despite progress, the amount of research and modeling on this problem is still limited.

1.4.2 Experimental Research

Experimental studies on wall films in PFI systems are also scarce. This is mostly due to the limited in-engine visibility. To analyze the liquid film inside the intake runner and on the valve, an optical intake runner and engine are needed. To avoid this, most studies on wall wetting adopt a simplified approach where an injection spray is directed at a flat surface, either at an angle or perpendicular to the spray axis. Although this setup does not fully replicate real engine conditions, it is widely accepted as a standard method [36][37].

From experimental research on fossil fuels, several factors are widely recognized to increase wall wetting in fossil fuel engines.

Firstly, the injection pressure plays a critical role. High pressures increase the velocity of the droplets. This causes droplets to splash off the surface rather than stick to it to form a film. Additionally, higher injection pressures produce finer droplets, which stick less easily to the walls. For moderate pressures, the film thickness is increased [38][39].

Secondly, the wall temperature strongly influences the fuel-film formation after impingement. With increasing wall temperature, the film mass decreases and evaporates more rapidly due to the increased heat transfer. Several studies on gasoline wall wetting report a reduction in maximum film height or faster film evaporation at higher wall temperatures. However, near and above the Leidenfrost regime (for gasoline around 420 K) a vapor layer forms between the liquid film and the wall. This layer reduces the direct wall-liquid heat transfer and changes the impingement regimes of the droplets [40]. Depending on the fuel type, pressure, and surface material, this either further reduces the film or, in some cases, suppresses evaporation and enlarges the film area [41][42][40].

Thirdly, the impingement distance and angle also influence the wall film formation. Short distances and steeper angles decreased the fuel mass of the film because of the high kinetic energy and splashing. With larger distances, the kinetic energy is reduced and more fuel sticks to the wall [38][43].

Lastly, ambient conditions also influence wall film formation during fossil fuel injection. A higher ambient pressure tends to reduce film formation [38] [43] [44]. Similarly, increasing the ambient temperature decreases the film thickness in diesel sprays, as reported by [45].

A concrete example of experimental research is the work of Dhanji et al.[37], who investigated the behavior of gasoline direct injection sprays impinging on cold and heated surfaces. Their study focuses on fuel film formation, evaporative cooling, and surface temperature, using the Engine Combustion Network (ECN) Spray G injector. Experiments were done in a constant-volume chamber where the film thickness was measured using low-coherence interferometry. After the start of injection (SOI) the film thickness first increases slightly and then reduces until 40 ms after SOI, where it stabilizes. The film thickness remains constant. The authors suggest that the heavier components stay on the wall for a prolonged time. To complete these measurements, the authors performed CFD simulations using a Lagrangian-Eulerian framework with the modified O'Rourke-Amsden wall film model and a 1D Conjugate Heat Transfer approach. While the simulations showed the general trends such as initial cooling and film distribution, they underpredicted the magnitude of cooling and film distribution. The authors investigated that this happens because the system does not anticipate how much the fuel droplets will cool as they evaporate. Another reason is that the free spray heats up to a temperature higher than the fuel's initial injection temperature.

The above findings are all based on fossil fuels such as gasoline and diesel. While they can provide valuable insights, it is important to note that methanol has different chemical and physical properties that makes it even more prone to wall wetting. Therefore, it is essential to have dedicated research on methanol's wall wetting behavior. Only a small number of studies have examined methanol wall film formation and their results are not always consistent.

An important study performed in 2022 by Zhang et al. [36], who used an innovative optical platform to study methanol spray impingement and wall wetting. They used the diffuse back-illumination (DBI) and the refractive index matching (RIM) method. Their setup included a 14-hole low-pressure methanol injector, a temperature controlled quartz glass wall, and a high speed camera. With this setup they were able to capture the spray and film formation. Experiments were conducted under varying boundary conditions: impingement distances (62, 91, 120 mm), wall temperatures (293–423 K), and injection pressures (300–500 kPa). Methanol properties and ambient conditions were carefully controlled, and each test was repeated five times for statistical accuracy. From the results, the authors conclude that increasing the spray distance also increases the wall wetting due to the kinetic energy decrease of the droplets. Secondly, when the injection pressure is initially increased, wall wetting also increases. However, beyond an injection pressure of 400 kPa, splashing also increased and less fuel stuck to the wall. Finally, the effect of wall temperature was analyzed. An increase in wall temperature from

293 K to 373 K, reduced the amount of fuel sticking to the wall due to faster evaporation. However, when the wall temperature reached 423 K, the wall wetting increased again due to the Leidenfrost effect.

In contrast, Yuan et al. [46] studied methanol spray impingement on a curved intake valve while using a transparent intake port. This setup matches more closely the real PFI conditions. The study shows that increasing the fuel injection pressure improves spray breakup and penetration, but also leads to a larger fuel film on the intake port wall. This observation is the opposite of earlier mentioned findings. Another point this paper examined was the effect of the wall temperature of the valve. They state that raising the valve temperature above the Leidenfrost point prevents fuel droplets from sticking to the surface and losing momentum. Instead, the droplets slide off. According to these authors, this greatly reduces wall wetting.

Overall, it is clear that wall wetting from methanol shows unique and sometimes contradictory behaviors. While certain trends are in line with the trends from fossil fuel studies, others are not. Furthermore, there is no full consensus on the influence of several key factors. This highlights the importance of continuing experimental and numerical investigation into methanol wall wetting phenomena in PFI.

1.5 Research Gap

1.5.1 Define Gap

Wall wetting in PFI systems is a critical phenomenon because it affects mixture formation, combustion stability, and emissions. Although wall wetting has been widely studied in gasoline and diesel engines, little attention has been given to methanol film formation. This is an important gap, since methanol's high latent heat of vaporization, low volatility, and lower heating value can intensify wall wetting effects and make mixture preparation more challenging. This is especially the case during cold-start operation.

Previous experimental and numerical research has focused mostly on fossil fuel engines. While recent work has begun to investigate methanol spray behavior and wall wetting, several limitations remain.

Firstly, existing studies often concentrate on spray atomization and penetration without fully taking the wall wetting dynamics into account. Such models are often simplified by assuming static surfaces and neglecting heat transfer effects. As a result, the coupling between spray dynamics, wall temperature, and film evaporation is not yet sufficiently understood.

Secondly, experimental evidence on methanol wall wetting remains limited and sometimes inconsistent. This shows the need for systematic investigations under controlled conditions.

Thirdly, only a small number of studies have examined the combined influence of operating parameters such as intake conditions, injection settings, and wall temperature. In most cases, these variables have been analyzed individually rather than in a systematic matrix. A study with a systematic matrix could capture the interactions and relative importance of the examined parameters.

1.5.2 Research Questions

To address these gaps, this thesis develops and validates a CFD-based framework in CONVERGE v5.0 for simulating wall wetting phenomena in methanol PFI systems. Methanol-specific properties, wall film sub-models, and heat transfer models will be implemented and validated against experimental data from the study by Zhang et al. [36]. The model will also be critically assessed to identify its limitations and to discuss possible improvements.

After validation, a systematic simulation campaign will be conducted to investigate wall wetting behavior of a methanol spray on quartz glass. The study will examine the influence of the following key operating parameters: injection pressure, wall temperature, and ambient intake conditions. Their impact on fuel film thickness, film area, and evaporated mass will be analyzed. The results are intended to improve the understanding of methanol wall wetting and to support the development of more effective modeling.

This thesis is guided by the following main research question:

Which operating parameters most strongly influence wall wetting behavior in methanol-fueled PFI systems?

This question is addressed through the following sub-questions:

1. How does the temperature difference between the injected methanol and the intake air affect wall wetting formation and film evolution?
2. How do injection pressure and fuel temperature interact to influence wall wetting behavior, and are there critical threshold regions within the investigated parameter ranges?
3. Which parameters and parameter interactions most strongly influence wall wetting behavior across the investigated operating space, and what correlation trends can be identified?

1.6 Outline of the Thesis

With the formulation of the research questions for this thesis, the literature review of this chapter can be concluded. The following chapters will build upon this foundation. First, chapter 2 provides an extensive overview of the numerical framework implemented in CONVERGE CFD. The chapter opens with an introduction into the physical phenomena that occur, followed by a detailed explanation of the implemented sub-models. The chapter concludes with a description of the computational mesh, the numerical solvers, and the data extraction procedure.

Second, Chapter 3 addresses the validation of the implemented model against the experimental data from Zhang et al. [36]. The chapter critically assesses the capabilities of the numerical model, as well as the reliability of the experimental measurement technique used by Zhang et al.

After the validation study, Chapter 4 contains the simulation study and discussion to answer the research question of this thesis. The influence of the three key operating parameters is analyzed individually, as well as in terms of their interaction and relative importance. Finally, the Chapter 5 summarizes the key findings of this thesis and directions for future work.

1.7 Responsible Use of Artificial Intelligence

During the course of this thesis, Artificial Intelligence (AI) tools were used for various purposes. During the implementation of the models in CONVERGE, AI tools were used as an aid to navigate the software in combination with the manual. Secondly, AI tools were used to support writing post-processing codes such as plotting scripts and latex formatting. Lastly, AI tools were used to rephrase sentences to improve the readability.

It is important to note that all conceptual decisions, hypotheses, data interpretation, and scientific arguments were made by the author. All AI output was reviewed, and where necessary adapted, by the author. All final decisions regarding wording, structure, and written content are the responsibility of the author.

Chapter 2

Methodology

2.1 Introduction to the Numerical Framework

Simulating methanol wall wetting under PFI conditions requires a numerical framework that captures several physical phenomena. Figure 2.1 provides an overview of the key processes that occur during an injection. Starting from the injector, liquid methanol is introduced into the domain as discrete parcels. As these parcels travel through the ambient gas, they undergo different phenomena. The aerodynamic forces cause the droplets to break up and the droplets also collide with each other. Simultaneously, droplets evaporate into the surrounding gas. The injection causes turbulent flow in the domain that influences the droplet trajectories and mixing of the fuel vapor. Finally, droplets that reach the wall interact with the surface.

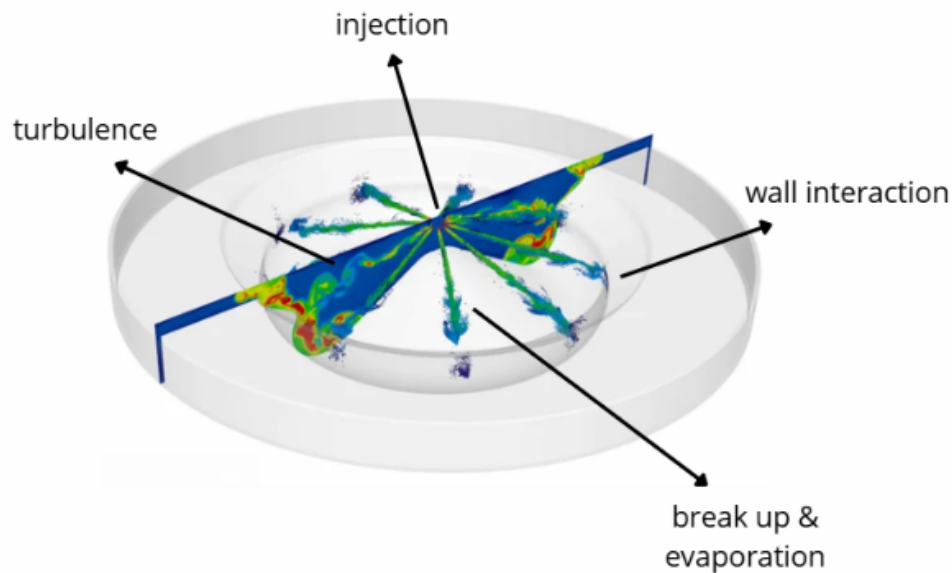


Figure 2.1: Lagrangian spray with physical phenomena adapted from [47].

Each of these phenomena is represented by a sub-model within the Lagrangian-Eulerian (L-E) framework implemented in CONVERGE CFD. The following sections describe each sub-model in detail based on the information in the CONVERGE 5 Manual [48].

2.2 Lagrangian-Eulerian Framework

The fuel spray injection is modeled using the Lagrangian-Eulerian (L-E) framework. The gas phase is treated as a continuum and resolved using the Eulerian conservation equations. On the other hand, the liquid phase is treated as discretized Lagrangian parcels [49].

2.2.1 Lagrangian Parcel Modeling

Directly tracking and calculating every individual droplet is impossible. Instead, the liquid phase is represented by parcels. Each parcel represents a group of identical droplets with the same diameter, velocity, and temperature. The parcel velocity is obtained from Newton's second law:

$$\rho_p V_p \frac{dv_i}{dt} = F_{p,i} \quad (2.1)$$

where ρ_p is the density of the parcel, V_p is the parcel volume, and $F_{p,i}$ is the total force acting on the parcel. For liquid methanol parcels, $F_{p,i}$ is defined as the sum of the aerodynamic drag force and the gravitational force:

$$F_{p,i} = \frac{1}{2} C_D \pi r_p^2 \rho |U_j| U_i + \rho_p V_p g_i \quad (2.2)$$

$$U_i = u_i + u'_i - v_i \quad (2.3)$$

In Equation 2.2, C_D is the drag coefficient, r_p is the parcel radius and U_i represents the relative velocity between the parcel and the gas phase. This relative velocity accounts for both the mean fluid velocity u_i and the turbulent fluctuating velocity u'_i . This allows the model to capture turbulent dispersion.

2.2.2 Eulerian Gas-Phase Conservation

The gas-phase is solved as a continuum by the Navier-Stokes equations. To account for the spray, the equations are adapted to include source terms. The source term represents the exchange of momentum, mass, and energy between the gas and the liquid spray.

The momentum equation for the gas becomes:

$$\frac{\partial(\rho u)_g}{\partial t} + \nabla \cdot (\rho u u)_g = -\nabla p + \nabla \cdot \tau + S_{mom} \quad (2.4)$$

where τ is the viscous stress tensor, ρ is the gas density, and u the gas-phase velocity. The momentum source term S_{mom} is calculated by a summation of the momentum change of all the parcels passing through a specific Eulerian grid cell:

$$S_{mom} = -\frac{1}{V_{cell}} \sum_{parcels} \dot{m}_p \left(\frac{du_p}{dt} - \mathbf{g} \right) \quad (2.5)$$

where V_{cell} is the volume of the Eulerian control volume, $\dot{m}_p$ is the mass flow rate from parcel p , $\mathbf{u}_p$ is the parcel (droplet) velocity, $\frac{du_p}{dt}$ is the parcel acceleration obtained from its Lagrangian equation of motion, and $\mathbf{g}$ is the gravitational acceleration.

2.2.3 Numerical Coupling

The coupling between Eulerian fluid cells and Lagrangian parcels is calculated iteratively at each time step. Parcels transfer mass, momentum, and energy to the gas phase through the source terms. The parcels also receive updates on the velocity, temperature, and turbulence in the gas-phase. This two-way coupling approach is essential for accurately representing the interaction between the phases.

2.3 Reynolds-Averaged Turbulence Modeling

The governing Navier-Stokes equations for turbulent flows cannot be solved analytically for most practical engineering problems. Numerical simulations with simplified models are necessary to limit the computational cost. Different methods exist on how to deal with turbulence. Direct Numerical Simulations (DNS) resolve all turbulent scales down to the smallest Kolmogorov scale, and thus these simulations are very computationally expensive. Large Eddy Simulations (LES) capture only the largest turbulence scales. However, these are still expensive calculations and LES is very sensitive to the initial turbulence conditions. Instead of capturing these eddies explicitly, models are often used that represent the effects of turbulence. One such approach is Reynolds-averaged Navier-Stokes (RANS), in which flow variables are decomposed into a time-averaged component and a fluctuating component.

2.3.1 Reynolds Averaging

The Reynolds-averaged Navier-Stokes (RANS) method uses time-averaged equations that describe the flow [50]. The instantaneous compressible Navier-Stokes equations are given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (2.6)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} \quad (2.7)$$

where u_i is the instantaneous velocity component in the i -direction, x_i the spatial coordinate, p the instantaneous pressure, ρ the fluid density, and σ_{ij} is the viscous stress tensor defined as

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (2.8)$$

In the RANS approach, each instantaneous variable is decomposed into a mean value, $\tilde{u}_i$, and a fluctuating component, u_i'' . For compressible flows, velocity is decomposed using Favre averaging:

$$u_i = \tilde{u}_i + u_i'' \quad (2.9)$$

$$\tilde{u}_i = \frac{\overline{\rho u_i}}{\bar{\rho}} \quad (2.10)$$

Pressure and density are decomposed as

$$p = \bar{p} + p', \quad \rho = \bar{\rho} + \rho' \quad (2.11)$$

Substituting these decompositions into Equations 2.7 and 2.6 gives the Reynolds-averaged Navier-Stokes equations:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho} \tilde{u}_i)}{\partial x_i} = 0 \quad (2.12)$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\bar{\sigma}_{ij} - \bar{\rho}\widetilde{u_i''u_j''} \right) \quad (2.13)$$

This substitution results in an additional term, the Reynolds stress tensor:

$$\tau_{ij} = -\bar{\rho}\widetilde{u_i''u_j''} \quad (2.14)$$

It represents the additional momentum transport caused by turbulent velocity fluctuations.

The introduction of τ_{ij} results in more unknowns than available equations. To close the system, turbulence models are required. The most common closure approach is the Boussinesq eddy viscosity hypothesis. It assumes that the Reynolds stress tensor behaves similarly to the molecular viscous stress tensor. More specifically, the Reynolds stress tensor is related to the mean rate-of-strain tensor by

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i} \right) \quad (2.15)$$

Therefore, the Boussinesq hypothesis is represented by

$$\tau_{ij} = 2\mu_t\tilde{S}_{ij} - \frac{2}{3}\bar{\rho}k\delta_{ij} \quad (2.16)$$

where $k = \frac{1}{2}\widetilde{u_i''u_i''}$ is the turbulent kinetic energy and δ_{ij} is the Kronecker delta.

The eddy viscosity μ_t can be determined by solving transport equations for the turbulence together with the continuity and momentum equations. For closing these equations several different transport models exist.

2.3.2 k - ε Turbulence Model

In the standard k - ε model, the turbulent viscosity is defined as

$$\mu_t = \bar{\rho}C_\mu \frac{k^2}{\varepsilon} \quad (2.17)$$

where ε represents the rate at which turbulent kinetic energy is converted into thermal energy by viscous effects.

The transport equation for ε is:

$$\frac{\partial(\bar{\rho}\varepsilon)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\text{Pr}_\varepsilon} \right) \frac{\partial\varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^2}{k} + C_{\varepsilon 3} \bar{\rho} \varepsilon \frac{\partial\tilde{u}_i}{\partial x_i} + S_\varepsilon \quad (2.18)$$

where:

- $\mu_t = \bar{\rho}C_\mu \frac{k^2}{\varepsilon}$: turbulent dynamic viscosity
- Pr_ε : turbulent Prandtl number for ε
- $P_k = \tau_{ij} \frac{\partial\tilde{u}_i}{\partial x_j}$: production of turbulent kinetic energy

- $C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\varepsilon 3}$: empirical constants
- S_{ε} : source term

The transport equation for k is:

$$\frac{\partial(\bar{\rho}k)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\text{Pr}_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \bar{\rho}\varepsilon + S_k \quad (2.19)$$

where:

- $\bar{\rho}$: mean fluid density
- $k = \frac{1}{2} \widetilde{u'_i u'_i}$: turbulent kinetic energy
- $\tilde{u}_j$: Favre-averaged velocity component
- x_j : spatial coordinate
- μ : dynamic (molecular) viscosity
- μ_t : turbulent dynamic viscosity
- Pr_k : turbulent Prandtl number for k
- $P_k = \tau_{ij} \frac{\partial \tilde{u}_i}{\partial x_j}$: production term
- ε : turbulent dissipation rate
- S_k : additional source term

RNG k - ε Model

The Renormalization Group (RNG) k - ε model introduces an additional term R_{ε} in the right hand side of the dissipation equation to improve the prediction of turbulence in flows with strong recirculation. This makes it more suitable for injection spray simulations, where intense mixing, jet spreading, and rapidly changing turbulent structures can occur [51]:

$$R_{\varepsilon} = C_{\mu} \bar{\rho} \frac{\eta^3 \left(1 - \frac{\eta}{\eta_0} \right)}{1 + \beta \eta^3} \frac{\varepsilon^2}{k} \quad (2.20)$$

with

$$\eta = \frac{k}{\varepsilon} \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}} \quad (2.21)$$

where:

- η : non-dimensional strain rate parameter
- η_0 : model constant (typically 4.38)
- β : model constant (typically 0.012)

2.4 Injection Model

To introduce the methanol into the computational domain, a Blob injection model is implemented. The Blob model assumes that the liquid is injected as discrete parcels with an initial diameter equal to the nozzle diameter d_{nozzle} . These "blobs" interact with the ambient gas and breakup according to the selected breakup model.

The mass flow rate of these parcels is defined by the implemented rate shape. In this study, a constant rate shape is used rather than a transient injection profile. This simplification avoids introducing the complex needle-lift dynamics and isolates the examined parameters in this study.

The spray injector introduces fuel into the domain through nozzles with a certain diameter d_{nozzle} . For liquid parcels, the injection pressure is not set directly as a value, but is computed from the set injection timing, the total injected mass, the nozzle geometry and the discharge coefficient. The discharge coefficient, C_d takes the nozzle contraction and flow losses into account, causing the effective flow area to be reduced. Equation 2.22 shows the mass flow rate for incompressible flow through a nozzle. From this equation, the corresponding pressure drop can be calculated.

$$\dot{m} = C_d A_n \sqrt{2\rho_l \Delta p} \quad (2.22)$$

In this study, the methanol injector is modeled with a fixed spray cone angle set at 20° for every nozzle defined in Figure 2.2. The model uses a solid spray cone with the parcels evenly distributed throughout the cone. The effect of this parameter and its chosen value is discussed in Section 3.4.1.

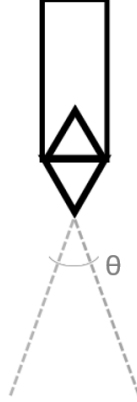


Figure 2.2: Schematic of an injector nozzle.

2.5 Droplet Breakup

The breakup model controls the droplet atomization of the injected fuel. This plays a crucial role in the accuracy of the simulation. The Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) framework is a widely used approach. It is a hybrid model that takes two distinct instabilities into account, the Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instabilities.

2.5.1 KH Instability

The KH instability predicts the primary breakup of the droplets in the liquid core due to shear forces generated by the velocity difference between the liquid jet surface and the ambient atmosphere. The high relative velocity between the liquid and gas creates waves on the droplet surface. When these waves reach a critical frequency, the droplet breaks.

In this model, the initial parcel diameters are set equal to the nozzle hole diameter d_0 . The radius of the breakup droplets r_{KH} is proportional to the wavelength of the fastest-growing unstable surface wave, Λ_{KH} . This relationship is given in Equation 2.23, where B_0 is a model constant.

$$r_{KH} = B_0 \Lambda_{KH} \quad (2.23)$$

The rate of change of the parent droplet radius (r_p) is given by Equation 2.24, where τ_{KH} represents the KH breakup time.

$$\frac{dr_p}{dt} = \frac{r_p - r_{KH}}{\tau_{KH}} \quad (2.24)$$

$$\tau_{KH} = \frac{3.788 B_1 r_p}{\Omega_{KH} \Lambda_{KH}} \quad (2.25)$$

The breakup time constant B_1 is related to the initial disturbance level of the liquid jet. The value of this factor varies from one injector to another [52].

2.5.2 RT Instability

The RT instability causes the secondary breakup further downstream. Unstable RT waves are triggered by the rapid deceleration of droplets due to the drag force and density difference between the fuel droplets and gas. The resulting droplet radius (r_{RT}) is calculated from Equation 2.26

$$r_{RT} = \frac{1}{2} C_{RT} \Lambda_{RT} \quad (2.26)$$

Λ_{RT} is the wavelength corresponding to the RT wave with the maximum growth rate ω_{RT} and C_{RT} is a model constant. When the viscosity of the liquid (μ_l) and the gas (μ_g) are included, it can be shown that the maximum growth rate can be written by Equation 2.27, with k_{RT} the wavenumber [53].

$$\omega_{RT} = -k_{RT}^2 \left(\frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right) + \sqrt{k_{RT} \left(\frac{\rho_l - \rho_g}{\rho_l + \rho_g} \right) a - \frac{k_{RT}^3 \sigma}{\rho_l + \rho_g} + k_{RT}^4 \left(\frac{\mu_l + \mu_g}{\rho_l + \rho_g} \right)^2} \quad (2.27)$$

The variation rate of the parent droplet over time in the RT breakup is expressed as:

$$\frac{dr_p}{dt} = \frac{r_p - r_{RT}}{\tau_{RT}} \quad (2.28)$$

where τ_{RT} , the RT breakup time, is calculated in Equation 2.29 with C_τ the model time constant:

$$\tau_{RT} = \frac{C_\tau}{\omega_{RT}} \quad (2.29)$$

2.5.3 Breakup Length

The above described models are dominant in different stages of the injection spray. Initially, only the KH instability is active. At a certain length the influence of the RT instability becomes significant. This length is defined as the primary breakup length L_b . Beyond this point both KH and RT models are activated. The liquid core is further atomized and the detached droplets are broken into smaller droplets, as visualized in Figure 2.3.

The breakup length L_b is defined in Equation 2.30 [54].

$$L_b = C_{bl} \sqrt{\frac{\rho_l}{\rho_g}} d_0 \quad (2.30)$$

$$C_{bl} = A \times \ln(\rho_{amb}) + 4.74 \quad (2.31)$$

In this equation, C_{bl} is a fuel depended characteristic constant that can be determined from Equation 2.31. According to a study by Zhang et al., the characteristic A for methanol is approximately 4.9 [55].

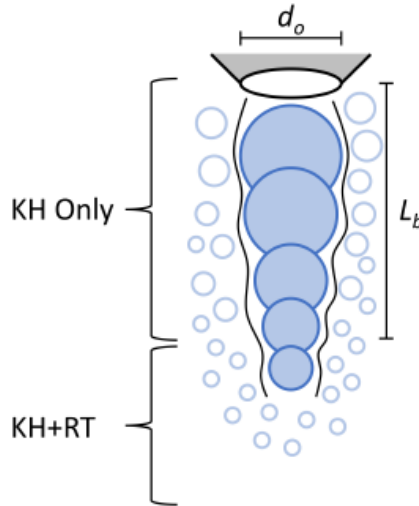


Figure 2.3: Schematic of the KH-RT spray breakup model extracted from the CONVERGE manual [48].

2.5.4 Implemented Parameters

In this section an overview of the implemented parameters of the KH-RT model is given for the methanol spray. An overview is given in Table 2.1 for ambient temperature equal to 293 K .

Table 2.1: KH-RT model constants

Parameter	Symbol	Value
KH size constant	B_0	0.61
KH velocity constant	C_{KH}	0.188
KH breakup time constant	B_1	10
Shed mass constant	C_s	0.25
Fraction of injected mass	f	0.03
RT size constant	C_3	0.8
RT breakup length constant	C_{bl}	5.6
RT breakup time constant	C_{RT}	1.0

2.6 Collision Model

The parcel-parcel interactions are computed with two complementary submodels. Firstly, The No Time Collision (NTC) model determines when collisions occur. Secondly, The post-collision outcome model of Post and Abraham (2022) describes the physical result of a collision between liquid parcels. Together, they describe the spray interaction inside each cell.

2.6.1 NTC Collision Model

Checking every possible parcel collision in a cell with N_p parcels would require N_p^2 collision checks. This can become very computationally expensive. Instead the NTC method uses a stochastic sampling technique. The algorithm identifies candidates based on a statistically representative sample. For two particles i and j , the chance that they collide depends on how big they are [56].

2.6.2 Post-Collision Outcome Model

Once a candidate collision has been selected, the post-collision outcome model of Post and Abraham determines its outcome [57]. For liquid parcels, there are 4 possible outcomes: bounce, permanent coalescence, stretching separation, and reflexive separation. The first criterion is the bouncing threshold, given in Equation 2.32. If the Weber number in the collision is smaller than We_{bounce} , the parcels bounce of each other and the new velocities are updated.

$$2We_{coll} < We_{bounce} \quad (2.32)$$

If the collision has more energy and the threshold is reached, the model checks further for stretching separation, reflexive separation, and coalescence. The stretching outcome depends on the impact parameter b and a critical value b_{crit} . The parameter b measures how off-center the collision is. If b equals 0, then the collision happens head on. For values bigger than 0, the droplets graze past each other. If $b > b_{crit}$, the collision is sufficiently off-center and stretching separation can occur. Secondly, if the criterion of Ashgriz and Poo in Equation 2.33 is satisfied, reflexive separation is possible [58].

$$2We_{coll} > 3 \left[7(1 + \Delta_p^3)^{2/3} - 4(1 + \Delta_p^2) \right] \frac{\Delta_p(1 + \Delta_p^3)^2}{\Delta_p^6\eta_1 + \eta_2} \quad (2.33)$$

This equation couples the collision Weber number, the dimensionless size ratio parameter Δ_p , and the deformation-related parameters η_1 and η_2 . When neither separation criterion is activated, the model assumes coalescence.

2.7 Evaporation Model

In the Lagrangian parcel approach, droplet evaporation depends on two processes that happen at the same time: heat transfers from the surrounding gas to the droplet, and mass transfer of fuel vapor from the droplet surface [59].

2.7.1 Mass Transfer

The rate of evaporation depends on the temperature of the droplet, the local gas-phase conditions, and the relative velocity between the droplet and the surrounding gas region. The d^2 law for modeling droplet evaporation states that the square of the droplet diameter decreases linearly with time under quasi-steady conditions. This captures the physics of diffusion-controlled evaporation for a stationary droplet. However, when there is a relative velocity difference between the droplet and the gas region, a correction is needed for the convection phenomena. This correction is taken into account in the Frössling correlation, given in Equation 2.34. The Sherwood number represents the ratio of the convective to diffusive mass transfer.

$$Sh = (2.0 + 0.6 Re_d^{1/2} Sc^{1/3}) \frac{\ln(1 + B_M)}{B_M} \quad (2.34)$$

Re_d is the droplet Reynolds number, Sc is the Schmidt number of the gas mixture, and B_M is the Spalding mass transfer number. The Spalding number represents the thermodynamic driving force for evaporation and is defined as the ratio of the vapor mass fraction difference between the droplet surface and the far field. The correction factor $\ln(1 + B_M)/B_M$ accounts for the blowing effect of the outward Stefan flow on the boundary layer surrounding the droplet [60].

The rate of change of the droplet radius is then given by

$$\frac{dr_0}{dt} = -\frac{\alpha_{\text{spray}} \rho_g D}{2\rho_l r_0} B_M Sh \quad (2.35)$$

where ρ_g and ρ_l are the gas and liquid densities, D is the mass diffusivity of the fuel vapor in the gas, r_0 is the instantaneous droplet radius, and α_{spray} is a model constant.

2.7.2 Energy Transfer

The uniform temperature model is used to determine the droplet temperature T_d . This model assumes that the internal thermal conductivity of the liquid is infinite, and thus that the droplet temperature is uniform. The energy balance is defined in Equation 2.36.

$$A_d Q_d = c_l m_d \frac{dT_d}{dt} - \frac{dm_d}{dt} H_{\text{vap}} \quad (2.36)$$

A_d is the surface area of the droplet, Q_d is the heat flux to the droplet, c_l is the specific heat capacity of the liquid, and H_{vap} is the latent heat of vaporization. The energy transferred to the droplet will either cause the droplet to heat up or supply heat for vaporization. The rate of the heat conduction to the surface of the droplet is given by Equation 2.37

$$Q_d = \frac{\beta_{\text{spray}} \text{Nu}_d k_{\text{air}}}{d_0} (T_{\text{gas}} - T_d) \quad (2.37)$$

where β_{spray} is a scaling factor and k_{air} is the thermal conductivity of the surrounding atmosphere. Similar to the mass transfer model, the Nusselt number includes a correction for the blowing effect:

$$Nu = \left(2.0 + 0.6Re_d^{1/2}Pr^{1/3}\right) \frac{\ln(1 + B_M)}{B_M} \quad (2.38)$$

where Pr is the Prandtl number of the gas.

In the simulation, these equations are solved iteratively. First, an intermediate droplet radius r_0^* is calculated using the Frössling correlation in 2.35. This intermediate value is used to determine the updated droplet temperature T_d using the energy balance, using (Eq. 2.36). Finally, the updated temperature is fed back into the mass transfer equations to finalize the droplet radius for the current time step.

2.8 Spray-Wall Interaction

The way these droplets react upon impingement has direct consequences for film formation.

2.8.1 Bai-Gosman Model

The Bai-Gosman model is a regime-based model to predict the behavior of a droplet impinging on a wall. Two key dimensionless groups that determine the regime transitions are the Weber number and the Laplace number, that can be calculated from Equations 2.39 and 2.40.

$$We = \frac{\rho v^2 d}{\sigma} \quad (2.39)$$

$$La = \frac{\rho \sigma d}{\mu^2} \quad (2.40)$$

Where ρ is the liquid density, v the droplet impact velocity, d the droplet diameter, σ the surface tension, and μ the dynamic viscosity.

The Weber number represents the ratio of inertial forces to the surface tension forces. It characterizes how strongly the droplet deforms when it impinges against the wall. The Laplace number represents a ratio of the surface tension and viscous forces. It determines how the droplet dissipates energy during spreading.

Additionally, the droplet-wall interaction also depends on the temperature difference between the wall temperature and the fuel's boiling point, the impact angle of the droplet, the surface roughness, and the pre-existing thickness of the film.

The regimes of the Bai-Gosman model are based on experimental observations. Figure 2.4 shows a schematic overview of the different regimes.

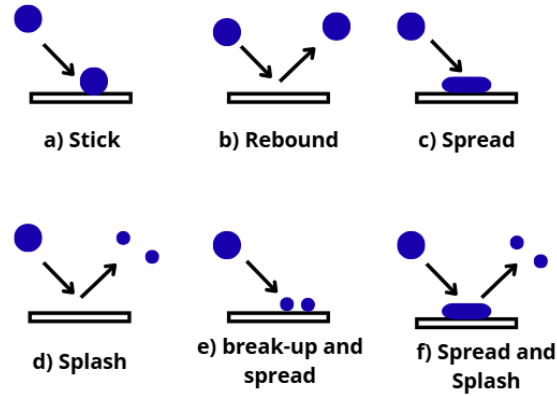


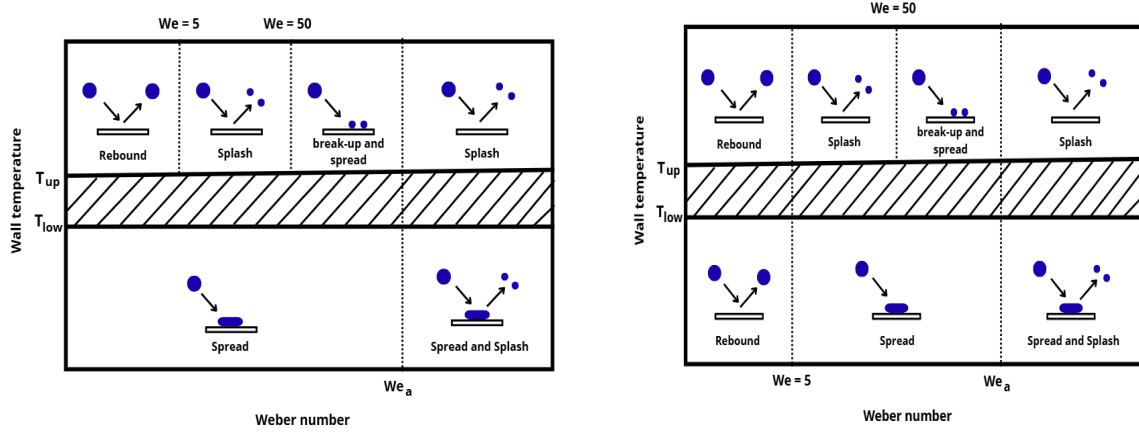
Figure 2.4: Schematic overview of impact regimes adapted from Smith et al. [61].

The regimes can be described as the following [26].

- a) **Stick:** The spherical droplet adheres to the wall.
- b) **Rebound:** The droplet deforms when hitting the wall but keeps enough surface energy to bounce completely off the wall.

- c) **Spread:** The impinging droplet spreads out and forms a film, or merges with a pre-existing liquid film.
- d) **Splash:** The droplet rebounds from the wall while simultaneously breaking into smaller droplets.
- e) **Break-up and spread:** The droplet breaks up upon impact and spreads along the surface.
- f) **Spread and splash:** Upon impact the droplet breaks up. A part of the droplets attaches to the wall while other parts rebound off the surface

The boundaries between these regimes are illustrated in Figure 2.5. However, it is important to note that in reality these transitions happen more gradually. The critical Weber number that separates the spread and splashing regimes is a function of the Laplace number and the presence of a pre-existing wall film. A wet wall lowers the splash threshold compared to a dry wall. On a wet wall the kinetic energy of the impinging droplet is transferred to the film, where it causes the formation of secondary droplets that splash up.



(a) Regime diagram for dry wall conditions

(b) Regime diagram for wet wall conditions

Figure 2.5: Bai-Gosman regimes adapted from Smith et al. and the CONVERGE manual [61][48].

In this study, $We = 5$ is used as a threshold for the rebound Weber number. Droplets with $We < 5$ are associated with sticking or rebound behavior, due to the fact that surface tension is dominant. $We > 5$ represents the minimum condition for a droplet to deform and spread on the wall. The traditional Bai-Gosman Weber splashing threshold is given by Equation 2.41. O'Rourke and Amsden proposed a framework to use the dimensionless parameter E^2 to improve the reaction behavior with the wall. The transition to the splashing regime is therefore determined by the critical energy parameter $E_{crit}^2 = 3300$ as set in the framework. A droplet is said to be in the splashing region when the E^2 of the impinging drop is greater than the critical value E_{crit}^2 [31][62].

$$We_{crit} = A \cdot La^{-0.18} \quad (2.41)$$

$$E^2 = \frac{\rho v^2 D}{\sigma} \cdot \frac{1}{\min(h/D, 1) \cdot \frac{\delta_{bl}}{D}} \quad (2.42)$$

2.9 Conjugate Heat Transfer

In this study, the thermal interaction between the gas-phase, methanol spray, and solid wall is modeled using the Conjugate Heat Transfer (CHT) approach. This allows for a more dynamic calculation of heat transfer compared to the assumption that the wall temperature is fixed.

2.9.1 Biot number

It is important to determine whether the temperature gradients within the solid wall are significant, as this influences how the heat is distributed from the methanol spray into the engine components or how the wall influences the wall film. The way the wall heat transfer is modeled directly impacts the accuracy of the resulting wall wetting and evaporation. The Biot number (Bi) gives the ratio of the heat transfer resistance inside the wall to the the heat resistance at the surface [63].

$$Bi = \frac{hL_c}{k_s} \quad (2.43)$$

In Equation 2.43, h is the convective heat transfer coefficient, L_c is the characteristic length of the solid wall, and k_s is the thermal conductivity of the solid wall.

If the Biot number is less than 0.1, the temperature gradients within the solid region are minimal and a lumped capacitance model can be used. However, when the Biot number exceeds 0.1, significant temperature gradients develop within the solid. It is then required to use the transient heat conduction equations to accurately take the internal thermal resistance and temperature distribution into account.

In this study, the solid wall is modeled to be a quartz glass wall with thickness 1 *cm* and assumed to have a constant k_s equal to 1.38 [64]. The calculated convective heat transfer coefficients lie in a range between 105 - 320 W/m^2K . With these values the Biot number is always bigger than 0.1, which indicates that the internal temperature gradients are not negligible. In this simulation, the lumped wall model would be inaccurate. The quartz glass density, specific heat, and electrical conductivity are assumed constant at 2.2 g/cm^3 , 739 $J/(kgK)$, and 1.0×10^{-15} S/m , respectively [65].

2.9.2 Energy Transport Equations

Within the solid region, the energy transport is dictated by conduction and described by Equation 2.44.

$$\frac{\partial \rho e}{\partial t} = \frac{\partial}{\partial x_j} \left(k_s \frac{\partial T}{\partial x_j} \right) + S \quad (2.44)$$

With e the internal energy, k_s the thermal conductivity, and S represents the volumetric heat sources.

This solid-phase equation can be coupled with the fluid phase energy equation through boundary conditions at the wall.

The transport equation for the specific internal energy (e) in the fluid domain is given by

$$\frac{\partial \rho e}{\partial t} + \frac{\partial (u_j \rho e)}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S - \frac{\partial q_{R,j}}{\partial x_j} \quad (2.45)$$

From left to right, the terms in Equation 2.45 represent: the internal energy change over time and convective transport on the left-hand side. On the right-hand side, pressure work, viscous dissipation, heat conduction, species diffusion, volumetric source term, and radiative heat source in the medium.

The coupling of Equation 2.44 and Equation 2.45 ensures that the wall temperature responds realistically to the cooling from the fuel impingement.

2.9.3 The INTERFACE Boundary

The coupling between the fluid and the solid region is modeled by an INTERFACE boundary in CONVERGE. It consists of a single geometrical boundary layer but it maintains two sets of boundary conditions to represent both the fluid side and the solid side. At every point on the boundary the temperature and the heat flux are matched. With these conditions, the simulated heat transfer behaves as it would physically.

$$T_{\text{fluid}} = T_{\text{solid}} \quad (2.46)$$

$$-k_f \left(\frac{\partial T}{\partial n} \right)_{\text{fluid}} = -k_s \left(\frac{\partial T}{\partial n} \right)_{\text{solid}} \quad (2.47)$$

2.10 Computational Mesh and Grid Control

Two regions are defined in the geometry for this study: one for the liquid spray injection and one for the solid wall.

2.10.1 Liquid Domain

A cylindrical geometry, with a height of 62 mm and a radius of 150 mm, was used as the control volume. The simulation uses a Cartesian base mesh with a cell size of 4.0 mm across the x , y , and z dimensions in accordance with previous spray modeling studies [17]. However, to refine the direct spray area, a fixed embedding and adaptive mesh refinement (AMR) were used.

Firstly, a conical refinement zone was defined from the injector nozzles reaching all the way to the end wall. This takes the increasing spray width into account. The cone is defined with an initial radius of 2 mm and expands to 20 mm. The mesh density within this region is controlled by a scaling parameter n , which reduces the cell size according to the relationship given in Equation 2.48.

$$EmbeddedCellSize = \frac{BaseGrid}{2^n} \quad (2.48)$$

Based on the grid independence study, described in Section 2.10.3 a scale of 3 was selected. This results in a local cell size of 0.5 mm.

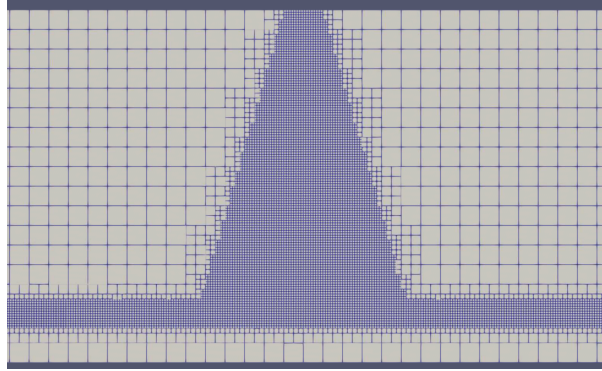


Figure 2.6: Close up of the mesh.

Secondly, AMR is added with the Sub-Grid-Scale (SGS) theory. A numerical grid can never perfectly resolve a continuous field. The SGS term ϕ' represents the unresolved portion of a variable ϕ .

$$\phi' = \phi - \bar{\phi} \quad (2.49)$$

with $\bar{\phi}$ the resolved (cell averaged) value. The unresolved component can be written as an infinite series of higher-order spatial derivatives. In practice it is approximated using the second order term.

$$\phi' \simeq -\alpha_{[k]} \frac{\partial^2 \bar{\phi}}{\partial x_k \partial x_k} \quad (2.50)$$

This approximation gives a measurement of how poorly the variable is resolved in a cell. During the simulation, if the calculated value ϕ' exceeds a specific SGS criterion, the cell is refined according to the maximum embedding level. And the other way, if the SGS value drops below the critical value, the cell can be coarsened.

In this study, AMR is applied to both velocity and temperature fields in the liquid domain. A sub-grid scale of 2.5 is used as critical value and a maximum embedding level of 3.

2.10.2 Solid Domain

A cylindrical disk with a thickness of 1 cm is added at the base of the fluid control volume. Capturing the temperature gradients at this interface requires a fine resolution. To achieve this, a fixed embedding is applied to the boundary of the solid cylinder and the liquid domain. The base grid of 4 mm is refined with a parameter $n = 3$. This reduces the local cell size to 0.5 mm. To ensure a smooth transition and avoid abrupt cell size changes, the refinement transitions gradually into the base grid size over 5 embedded layers. These layers act as intermediate refinement zones which improves the solution and ensures that the thermal gradients are resolved accurately.

2.10.3 Grid Independence Study

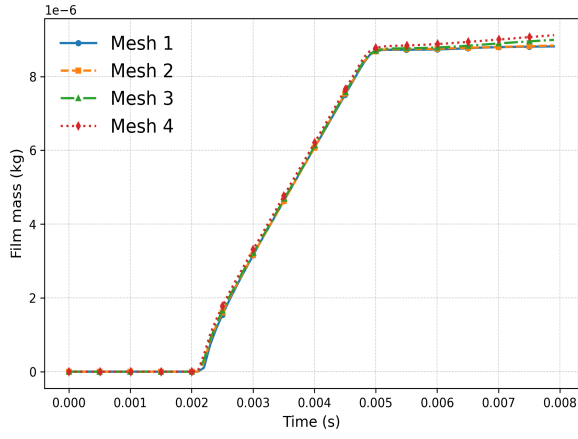
To ensure that the numerical results are independent of the cell sizes, a grid independence study was conducted. The base mesh was set to 4.0 mm in line with common spray modeling studies. Four levels of refinement were checked by varying the mesh scaling parameter (n) from 1 to 4 for the AMR and embedded mesh. An overview of the corresponding grid sizes is given in Table 2.2 at a timestamp of 8 ms ASOI. The benchmark for grid convergence is given by the total film mass.

Table 2.2: Overview of the grid refinement levels and corresponding cell sizes.

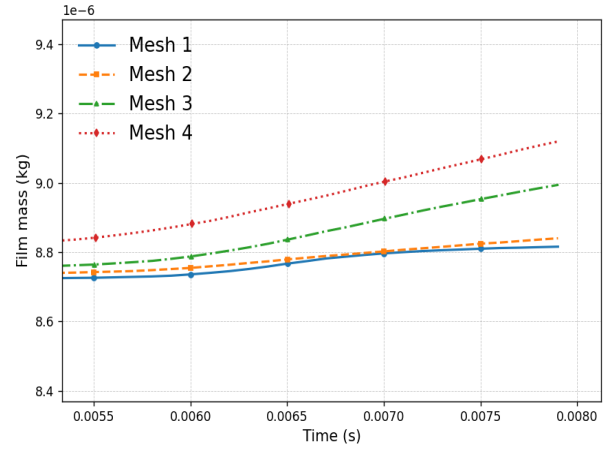
Case	Scale (n)	Local Cell Size [mm]	Number of Cells	Computational Time (s)
Mesh 1	1	2.0	235 302	385
Mesh 2	2	1.0	982 215	850
Mesh 3	3	0.5	3 727 267	2836
Mesh 4	4	0.25	15 926 699	21753

Figure 2.7 shows the total film mass evolution for different mesh sizes. From Figure 2.7a it is clear that all four meshes show nearly identical trends in film mass evolution. However, the close up from 5.5 ms to 8 ms reveals a divergence. Mesh 1 and mesh 2 compute the lowest film mass values and remain close in value. In contrast, Mesh 4 shows a divergence from the other cases. However, considering that the solver issued warnings that the maximum number of iterations was exceeded, this deviation may be due to numerical artifacts. This suggests that the simulation did not fully converge. Additionally, the computational cost of Mesh 4 is approximately ten times higher than that of Mesh 3.

From this independence study, mesh 3 is selected as the optimal compromise. It showed sufficient convergence, follows the overall trend of mesh 4 but maintains a much higher computational efficiency. Mesh 3 gives a balanced trade-off between acceptable numerical accuracy and the computational cost of running the simulation.



(a) film mass evolution



(b) close up of film mass evolution

Figure 2.7: Grid independence study: film mass evolution for different refinement levels over 8 ms.

2.11 Numerical Solvers

2.11.1 PISO

The simulation uses a Pressure Implicit with Splitting of Operator (PISO) algorithm, with a density-based convergence criterion to solve the transport equations. PISO is designed for transient pressure-velocity coupling and can handle rapidly changing fields better than a steady solver. The algorithm starts with a predictor step to solve the momentum equation. From this the velocity field is estimated. Next, a pressure equation is derived and solved to ensure conservation of mass. This produces a correction that is applied to the momentum equation. This correction process is applied multiple times until the following convergence criterion is met:

$$error_{PISO} < p_{iso_{tol}} \quad (2.51)$$

The PISO tolerance is set at 0.001, with at least two and at most nine iterations per time step. A full description of the algorithm is given in [66].

2.11.2 Rhie Chow

All variables are stored in cell centers. This could lead to oscillations in pressure and velocity fields due to weak coupling. The Rhie-Chow method resolves this problem by modifying the face velocities. Specifically, a pressure correction term, derived from the momentum equation, is added to the interpolated face velocities. This method strengthens the pressure-velocity coupling and reduces oscillations which means that the solution is more stable. However, it is important to note that this method can introduce a small amount of numerical dissipation [67].

The legacy Rhie-Chow method is used in this study due to its robustness and proven effectiveness in preventing checkerboarding. This is important because the pressure gradients and near wall-velocities can be steep in a spray-wall interaction. Using the Rhie-Chow method ensures numerical stability and prevents non-physical oscillations.

2.12 Data Processing and Film Metrics

Once the simulation is complete, the wall film characteristics are extracted using a post-processing routine that distinguishes between the bulk liquid film and secondary droplets on the wall in Tecplot for CONVERGE. An important aspect of this methodology is the implementation of a thickness threshold for geometric measurements. To ensure a meaningful parameter analysis, the film area and average film thickness are calculated exclusively for regions where the liquid film thickness is equal to or larger than 1 μm . This lower limit was selected to isolate the 'main' film from the microscopic secondary droplets. Including these regions below 1 μm would artificially lower the calculated average thickness and preventing a meaningful analysis of how operating parameters influence the bulk film structure.

In contrast, the accumulated film mass takes into account all liquid present on the surface, regardless of local thickness. The post-processing workflow in CONVERGE Studio's Line Plotting tool only provided this method for extracting film mass. Within the Tecplot environment, it was not possible to compute the cumulative liquid mass of the film (only an averaged value could be obtained). This inclusive approach ensures that the total mass balance remains accurate and that evaporation rates can be more accurately calculated.

However, this dual measurement approach requires a more nuanced interpretation of the wall-wetting phenomena. While the film mass provides a complete picture of the total liquid to wall interaction, the film area and thickness provide a more targeted look at the bulk liquid film. As a result, when comparing variations in film area, thickness, and mass, small differences should be interpreted with these measurement techniques in mind. This is important to avoid drawing physical conclusions from changes that may actually be numerically influenced due to the post-processing constraint.

Chapter 3

Model Validation

Before the parametric study is conducted, the implemented model is validated to assess its reliability and limits. Validation is a necessary step in CFD-based work because the numerical solutions not only depend on the governing equations but also on modeling assumptions, discretizations, boundary conditions, and limitations of the used models. The validation procedure in this Chapter compares the simulation outputs with available experimental data from Zhang et al. [36]. The aim of this validation study is not only to evaluate the similarities but also to identify differences. These differences will be used to examine the model's limitations and to discuss potential ways to further improve it. This way, the validation study serves both as validation of the model and as a guideline for future model development.

3.1 Description Experimental Setup

The experimental study was conducted on an optical spray-impingement platform to capture the spray evolution and the film development. The setup, seen in Figure 3.1 consisted of two subsystems: a fuel injection system and a high-speed optical imaging system.

A low-pressure PFI injector with 14 nozzles (diameter 0.26 mm) was used to inject pure methanol. The injection pressure was varied between 300 kPa and 500 kPa. The spray was directed vertically downward onto a quartz glass plate. This plate was heated to preset temperatures between 293 K and 423 K using a resistance furnace. After heating, the plate was transferred to the setup. The temperature variation during transfer was monitored with a high precision thermocouple and only changed in the range of $\pm 2^\circ\text{C}$.

Two optical measurement systems were used. Diffuse back-illumination (DBI) with a LED source was used to capture the spray development with a high speed camera. Secondly, the fuel-film properties were obtained with a refractive-index-matching (RIM) method. A camera captured the top view of the liquid film on the quartz plate by using a mirror at a 45° angle. The full calibration of this method is described in [36].

It is important to mention that the RIM method is sensitive to different factors such as refractive index matching, optical calibration, and surface roughness. Due to these constraints, RIM has not been widely used in wall wetting experiments. Small deviations in refractive index between the thin liquid film and the solid wall could introduce optical distortions. The results from this method should thus be interpreted with caution.

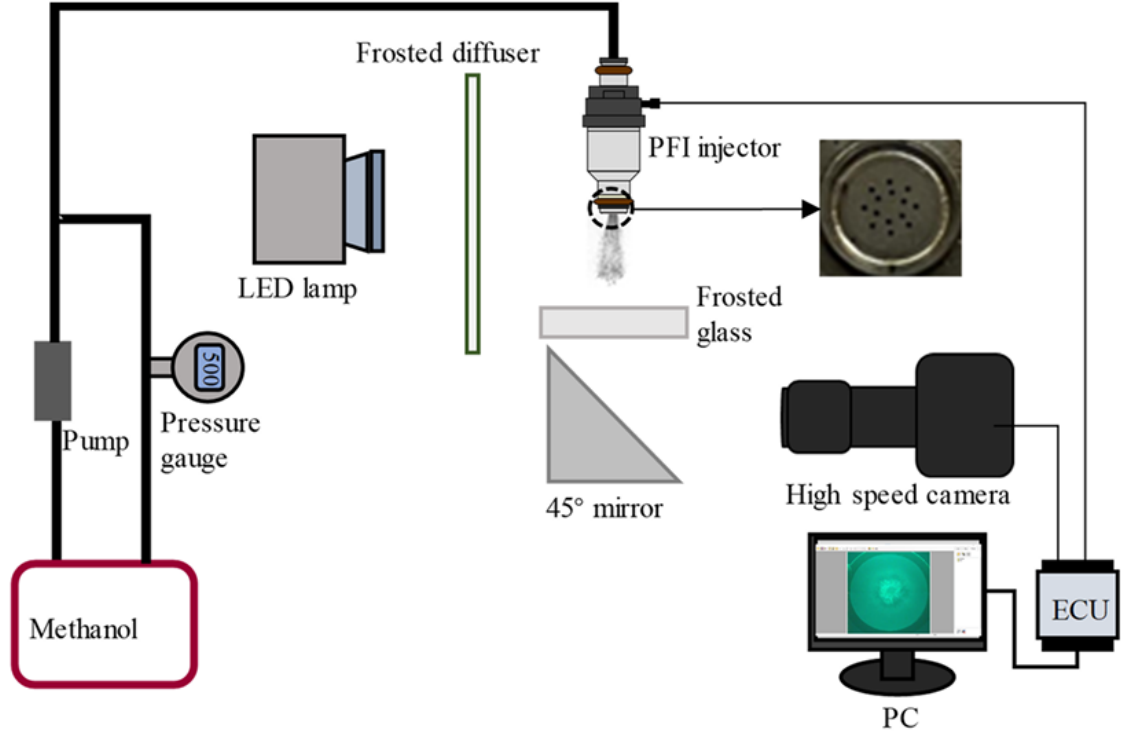


Figure 3.1: Schematic overview of the experimental setup extracted from [36].

Despite these uncertainties, the study by Zhang et al. was selected as the validation reference for this thesis, for several reasons. It is the most recent experimental study on wall wetting for methanol sprays under PFI conditions that clearly reports boundary conditions and injection parameters. Another recent experimental study on methanol film formation is published in 2025 [68]. They used a similar RIM method to measure the methanol film thickness on quartz glass and reported measurements in the same order of magnitude. Other experimental studies on wall wetting are done primarily for gasoline, iso-octane, and diesel fuels. However, methanol's properties are different from the conventional hydrocarbon fuels due to its lower surface tension and higher latent heat of vaporization. As a result, it is not straightforward to directly extrapolate validation data from gasoline or diesel studies.

A second consideration was accessibility. The experimental setup by Zhang et al. uses cost effective measurement techniques. The RIM method combined with DBI is a simpler method than advanced laser-based setups. Techniques such as laser-induced fluorescence (LIF) and phase Doppler interferometry require high-power lasers and complex setups. The RIM method could thus be a potentially accessible experimental approach for future studies on wall wetting. One of the long-term motivations of this thesis was to explore whether numerical models could be validated against such a simplified experimental methodology and whether this experimental approach could be used in future experimental research.

With these considerations in mind, the numerical model was initially implemented to closely reproduce the experiment. The well documented injector geometry, injection pressure, wall temperature, impingement distance, and ambient conditions were adopted in the model. The implemented sub-models are widely used and validated in literature. The expectation was therefore that the model would be capable of reproducing the experimental observations.

3.2 Description Numerical Model

The numerical simulations were performed using CONVERGE software. A full description of the implemented models and meshing is given in Chapter 2. Table 3.1 gives a structured overview of the major sub-models.

Table 3.1: Summary of models and methods used in spray simulation.

Category	Model / Method	Purpose
Multiphase Framework	Lagrangian–Eulerian coupling	Liquid droplets tracked as parcels, gas solved as continuum
	Lagrangian parcels	Represents spray droplets as parcels
	Eulerian Navier–Stokes	Accounts for momentum, energy, and mass exchange with spray
Turbulence	RANS with RNG k – ε model	Captures averaged turbulent behavior
Injector Model	Blob injection model	Introduces droplets equal to nozzle diameter
Breakup Models	KH–RT model	Predicts primary (KH) and secondary (RT) droplet breakup and atomization
Evaporation	Frössling correlation	Captures convective–diffusive evaporation
Spray–Wall Interaction	Bai–Gosman impingement model	Determines whether droplets stick, spread, splash, rebound, or merge with films
Heat Transfer	Conjugate Heat Transfer (CHT)	Solves transient conduction in solid and convection/evaporation in gas
Mesh Strategy	Cartesian base mesh with fixed embedding + AMR	Combines coarse base grid with refined spray region and adaptive refinement for gradients

3.3 Validation Strategy

The validation strategy in this thesis focuses on comparing the fuel film thickness T_f and the fuel film area A_f . The validation is divided into two parameter sweeps to isolate the effects of mechanical droplet impingement and thermal evaporation.

First, at a constant wall temperature of 293 K, the injection pressure is varied from 300 kPa to 500 kPa. This can validate the implementation of the Bai-Gosman impingement model and the KH-RT breakup model, as higher pressures lead to higher droplet Weber numbers and different splashing/sticking ratios.

In the experiment, different pressures were realized using a low-pressure methanol injector. To replicate this behavior numerically, the discharge coefficient of the injector model was calibrated to match the pressure levels for the given injection pulse width and injected mass. Table 3.2 gives the used values for the different pressure set points.

Second, at a constant injection pressure of 500 kPa, the wall temperature is varied from 293 K to 423 K. This stage tests the Conjugate Heat Transfer (CHT) and evaporation models. A summary of the boundary conditions used for this validation is presented in Table 3.3.

Table 3.2: Injection parameters at different pressure setpoints.

	300 kPa	400 kPa	500 kPa
Injection Duration	3 ms	3 ms	3 ms
Injected Mass	20 mg	24 mg	25 mg
Discharge Coefficient	0.411683	0.428	0.398611

Table 3.3: Spray parameters and boundary conditions.

Parameter	Value(s)
Impingement distance D_{imp}	62 mm
Wall temperature T_{wall}	293 K, 323 K, 373 K, 423 K
Injection pressure P_{inj}	300 kPa, 400 kPa, 500 kPa
Injection pulse width T_{inj}	3 ms
Ambient temperature	20 °C
Ambient pressure	1013 kPa
Fuel	Methanol (M100)
Injector	14-hole, 0.26 mm diameter

3.4 Results

3.4.1 Analysis of Experimental Methodology and Numerical Model

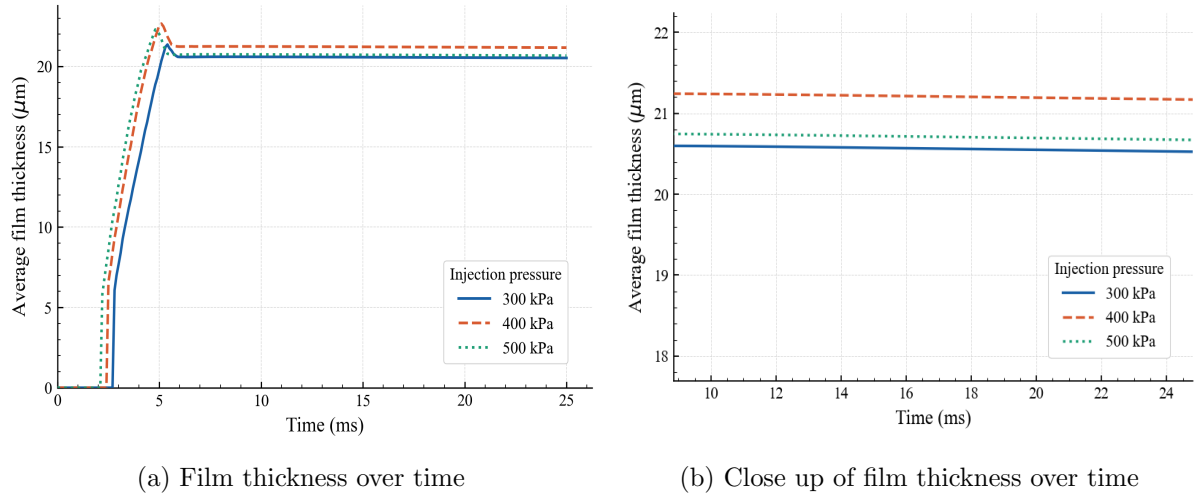


Figure 3.2: Numerical results of the fuel film thickness over time at varying injection pressures.

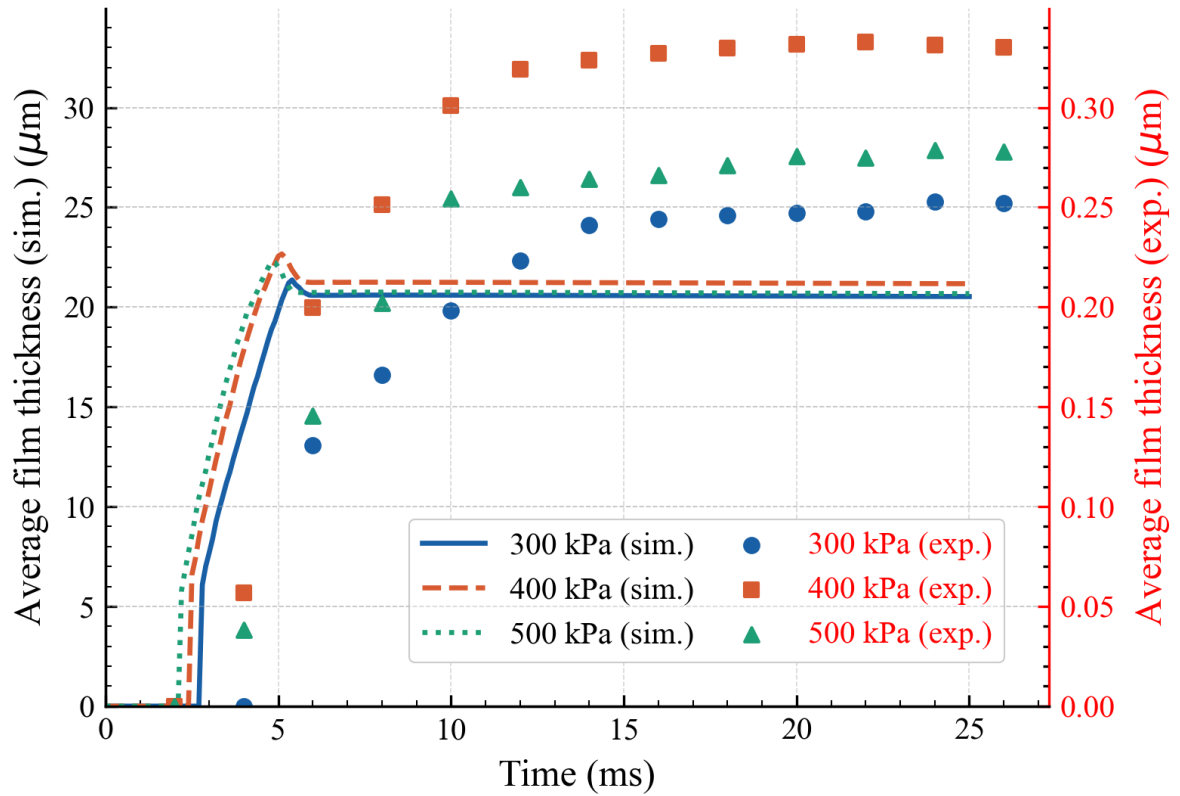


Figure 3.3: Comparison between experimental and numerical fuel film thickness on the wall for varying injection pressures.

From Figure 3.3, it is immediately clear that the model predicts significantly thicker films on the wall compared to the experimental data. The numerical model results in wall wetting that is 100 times larger than the experimental measurements. As an initial step to investigate this difference, a sensitivity analysis of the model parameters was conducted. A range of model parameters was systematically varied to investigate whether this difference was a modeling mistake and could be reduced.

- **Weber number:** The Weber rebound number was first set to the commonly used value of 5. It was then varied over a range from 5 to 50, following the recommendation from the CONVERGE manual. From this variation, no real significant difference was visible in the outcome. This insensitivity can be explained by the dominance of splashing under the investigated operating conditions. Since the impinging droplets carry sufficient energy to splash upon impact, they remain well above both the rebound and spreading regimes. As a result, the Weber rebound threshold has no influence on the simulation outcome.
- **KH-RT breakup model:** The sensitivity of different parameter from the KH-RT breakup model were examined. The breakup time constant, model size constant, and breakup length were all extensively varied. However, the predicted film thickness changed only by a few micrometers. This indicates that the breakup model may have an important effect when the error is in this range. However, the large mismatch with the experimental data is not due to this model.
- **Number of injected parcels:** No straightforward consensus exists on the number of parcels that need to be modeled per nozzle. For common practices the typical range is somewhere between 5 000 and 50 000 parcels. Some studies report values exceeding 200 000. In this validation study, the number of injected parcels was fixed at 15 000 parcels per nozzle to limit the computational cost. While the number of parcels can influence numerical smoothness and convergence, it does not explain a difference of this magnitude between the model and experimental data.
- **Spray cone angle:** One of the parameters that heavily influences the outcome of the spray is the spray cone angle as described in section 2.8. To better understand its impact on the obtained result, a short comparison study was done. At an injection pressure of 300 kPa, the spray cone angle was set at 20° and 45°. Figure 3.4 shows the resulting film thickness and area.

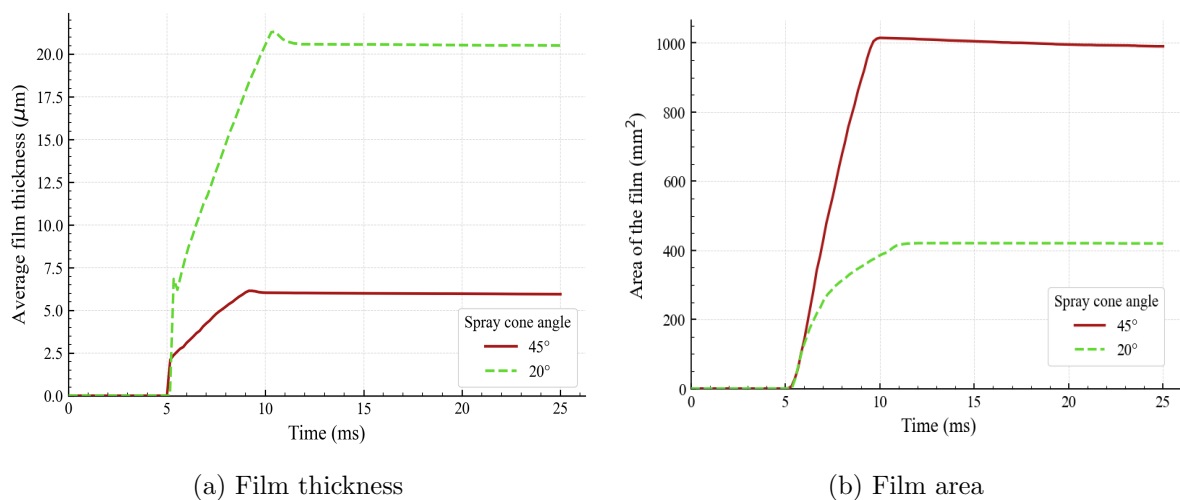


Figure 3.4: Comparison of the liquid film for different spray cone angles at 300 kPa.

A wider spray cone angle results in a larger wetted area and reduced film thickness. At 45° , the film thickness is 4 times thinner. However, this result is still overestimated by more than an order of magnitude compared to the experimental data. The spray cone angle was kept at 20° throughout the study as a baseline, rather than tuned aggressively to fit the data set.

Overall the sensitivity analysis suggest that none of the tested parameters can account for the large deviation. In light of the limitations outlined in Section 3.1, a more critical examination of the experimental data itself was necessary.

Zhang et al. used the DBI and RIM method with a reflecting mirror. This technique is very sensitive to calibration and index matching. A study by Ding et al. [69] states that constant calibration is needed for how the signal intensity relates to the liquid thickness. A small deviation can introduce significant errors. Another study by Henkel et al. [70] reports that RIM only gives accurate measurements up to a film thickness of $0.9\text{ }\mu\text{m}$. Beyond this thickness, the relation between scattered light intensity and film thickness becomes weak, nonlinear, or extrapolated. Thicker films can thus only be estimated. Furthermore, a study published in 2012 by Zheng et al. [71] already raised questions on the limitations of the RIM technique. From this literature, it is clear that using RIM to measure film thickness is not a commonly validated method.

Three experimental studies using the RIM method, all reported values of the measured film thickness in the same order of magnitude. While [36] and [68] investigated methanol injection, [71] focused on gasoline direct injection. Despite the different fuels used, all studies reported average wall-film thicknesses below $1\text{ }\mu\text{m}$. However, the older experimental studies, using laser-based measurements, reported much thicker wall films. Kiura et al.[72] and Senda et al.[73] used gasoline in a controlled intake-port. They reported average film thicknesses around $20\text{ }\mu\text{m}$, depending on gas velocity and wall temperature. Hentschel et al. [74] performed experiments in the intake manifold of a standard SI engine using iso-octane as a fuel. They reported an average film thickness in the range of $20\text{--}30\text{ }\mu\text{m}$ along the manifold wall. Directly under the spray, the local thickness was even measured to be several hundred micrometers. Although the geometries and fuels are different between these studies, both report film thicknesses in the order of tens of micrometers. This suggests that the sub-micrometer film thicknesses for methanol reported by Zhang et al.[36] may be obtained from an underdeveloped measuring technique.

In addition, the limited numerical data on methanol wall wetting further supports the experimental studies using LIF. The master's thesis by Kontkanen reports on film thicknesses in the range of $5\text{--}100\text{ }\mu\text{m}$ [35]. They examined wall wetting using methanol PFI in OpenFOAM with a compressible wall film model. Lien et al. [75] combined the experimental visualization of the methanol spray and film footprint with a CFD simulation in OpenFOAM. Their reported film thickness are also well above the sub-micrometer range. Together, these numerical studies reinforce the view that the experimentally reported film thicknesses below $1\text{ }\mu\text{m}$ are likely underestimations.

However, this does not imply that the experimental trends observed by Zhang et al. [36] are invalid. Despite uncertainties in absolute magnitude, the experimental data clearly shows systematic changes in wall wetting with changing injection pressure and wall temperature. These relative changes are physically meaningful and are also reproduced by the numerical model. The experimental data by Zhang et al. is thus not used as strict quantitative benchmark, but rather as a qualitative reference. The experimental and numerical results are plotted on separate y-axes with independently scaled ranges to focus on their relative behavior.

3.4.2 Results for Varying Injection Pressure

Figure 3.5 shows the scaled comparison of the wall film thickness at different injection pressures. In all cases, the film thickness increases sharply at 2 ms ASOI when the spray first hits the wall and film formation begins. After this initial phase, the growth rate of the film decreases and the film thickness evolves more gradually. It is clear that the numerical model reproduces the same relative trend as the experimental data. With increasing the injection pressure from 300 kPa to 400 kPa, the thickness of the film also increases. Further increasing the pressure to 500 kPa reduces the film thickness.

Figure 3.6 shows the colored images of the film thickness for different injection pressures at 3 time steps (5 ms, 10 ms and 15 ms). From these images it is clear that over time the area of wall wetting increases slightly. This trend is in line with the observations from the experimental data.

Figure 3.8 visualizes the normalized remaining liquid in the domain. It uses the sum of the suspended droplets and the liquid film. From this graph it can be deduced that about 15% of the injected mass is evaporated 25 ms ASOI. Figure 3.7 shows the total film mass over time. The film thickness is formed primarily when the droplets first impinge on the surface. Afterwards the film mass steadily increases. This suggests that the secondary droplets fall back down more rapidly than the liquid film evaporates from the wall. This increase in total film mass is in line with the trend from the experimental data. In the numerical results, the film mass obtained at an injection pressure of 500 kPa is larger than that of 400 kPa even though the film thickness is thinner. This observation is explained by the increasing film area at 500 kPa, as visualized in Figure 3.6.

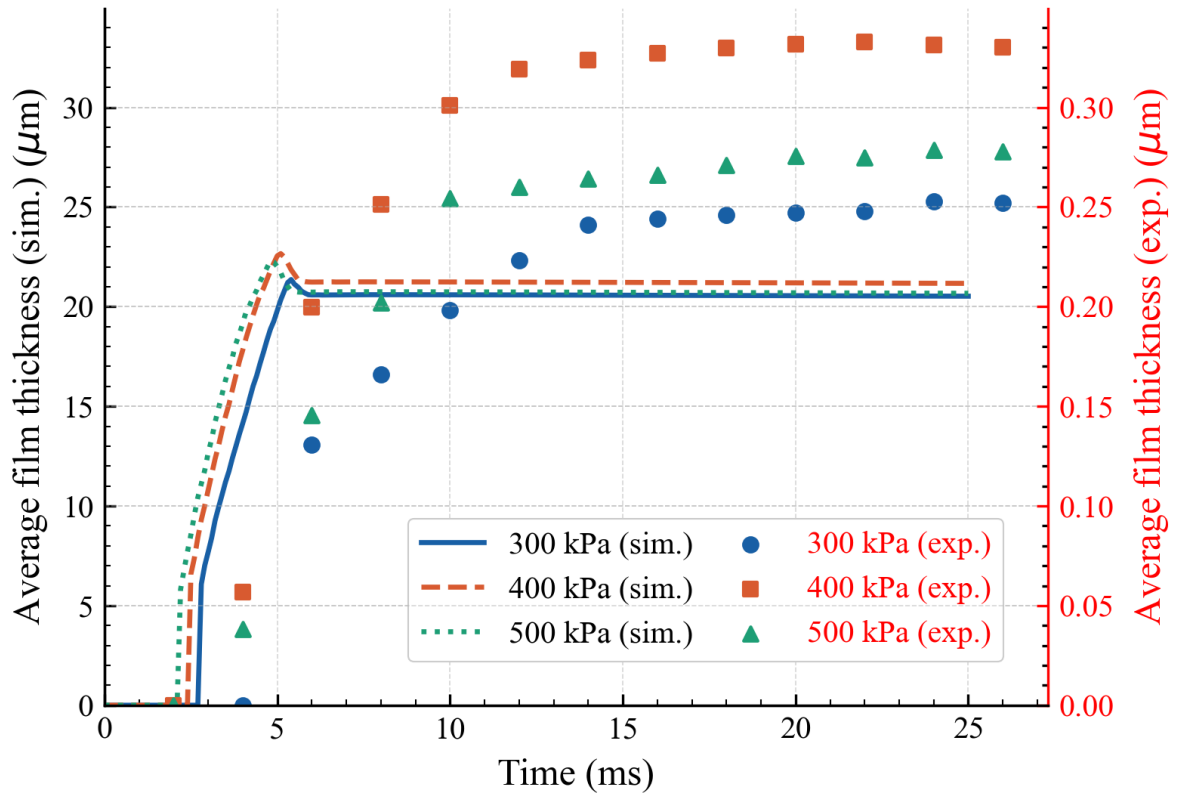


Figure 3.5: Comparison between experimental and numerical fuel film thickness on the wall for varying injection pressures.

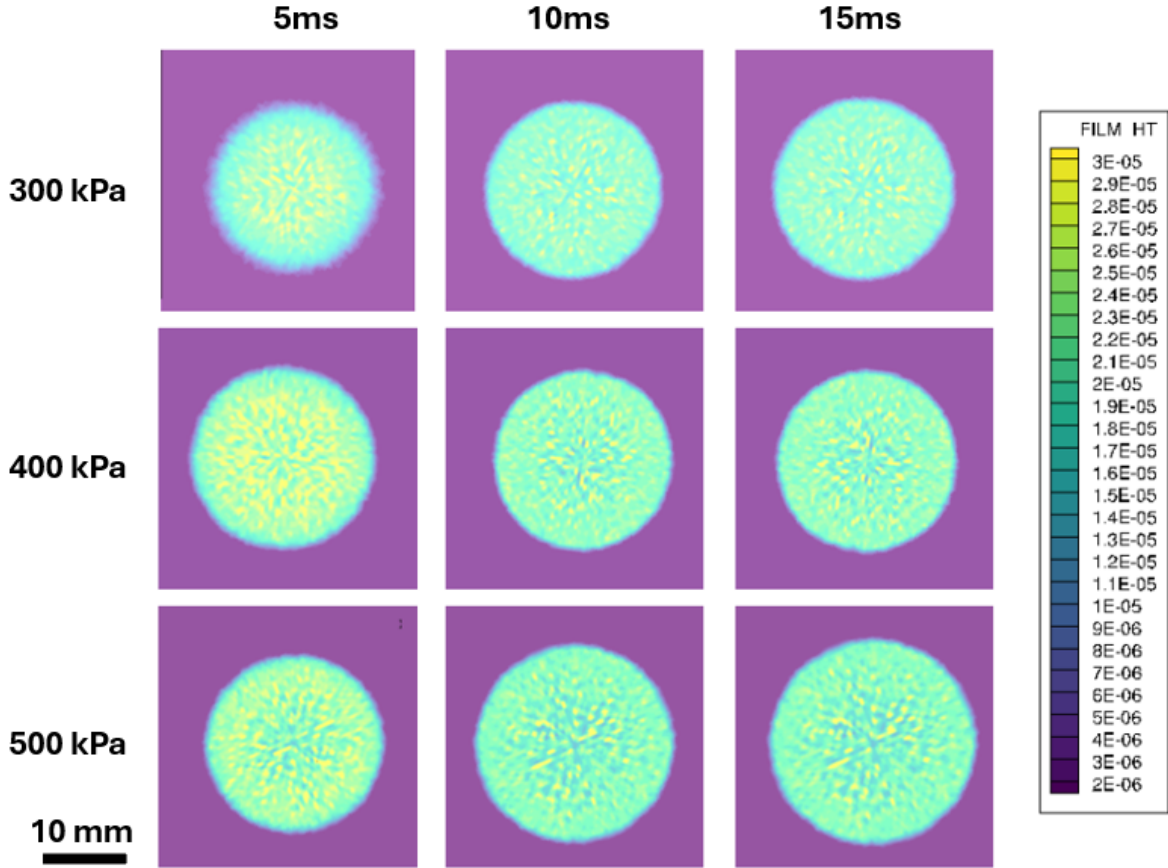


Figure 3.6: Color images of the simulated fuel films for varying injection pressures at different timesteps ASOI.

A remark can be made regarding the film mass measurements from the experimental data. At 25 ms ASOI and an injection pressure of 300 kPa, Zhang et al. reported a wall film mass of approximately 0.2 mg. The total injected mass for 300 kPa was set to 20 mg. This implies that in the experimental setup only 1% of the total injected methanol deposits onto the wall and that 99% is either evaporated or remains suspended as liquid droplets. Such a low fraction of wall wetting is not in line with established knowledge on methanol properties and methanol wall wetting. This observation therefore reinforces the concerns regarding the accuracy of the experimental measurements discussed in Section 3.4.1. In contrast, the numerical model calculated that around 35% of the total injected mass is deposited on to the wall. When interpreting this result, it is important to consider a potential limitation of the Bai-Gosman model. The threshold parameters governing the splashing regime are not validated or fine-tuned for methanol injection. The model may thus overestimate splashing, which would artificially reduce the film fraction. This limitation is further discussed in Section 3.5.1.

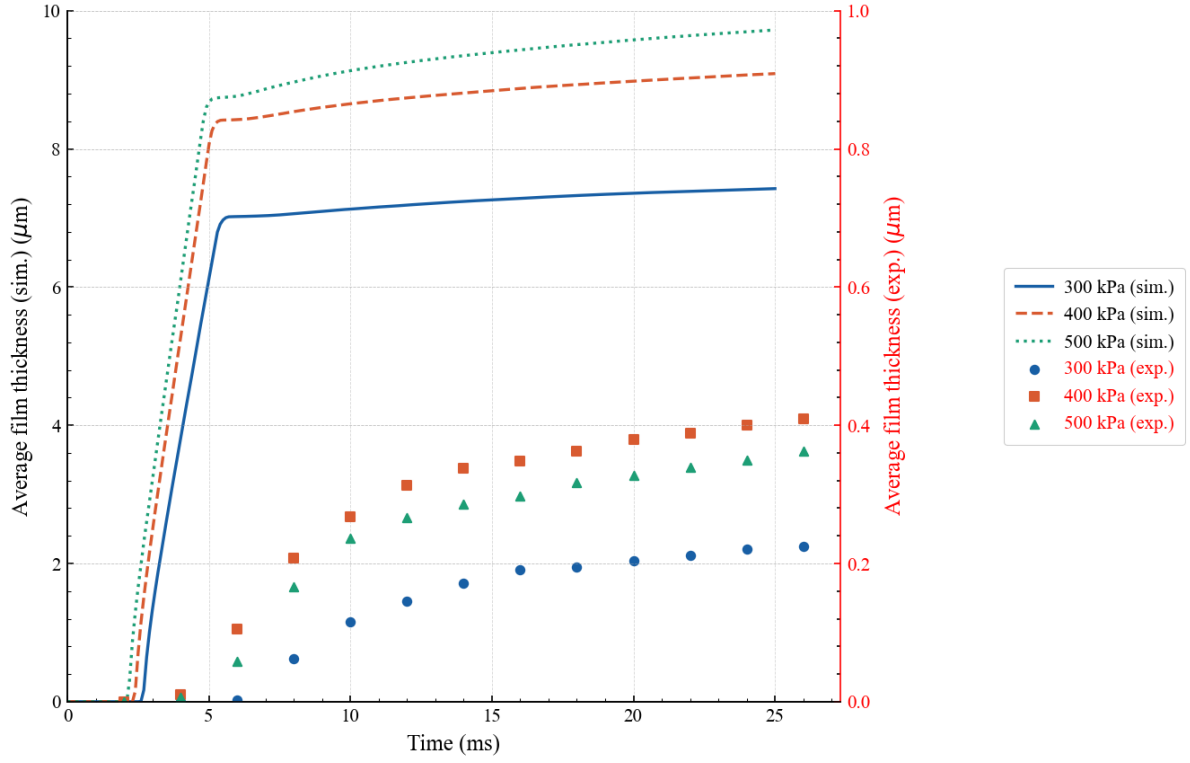


Figure 3.7: Comparison of the numerical and experimental liquid film mass at different injection pressures.

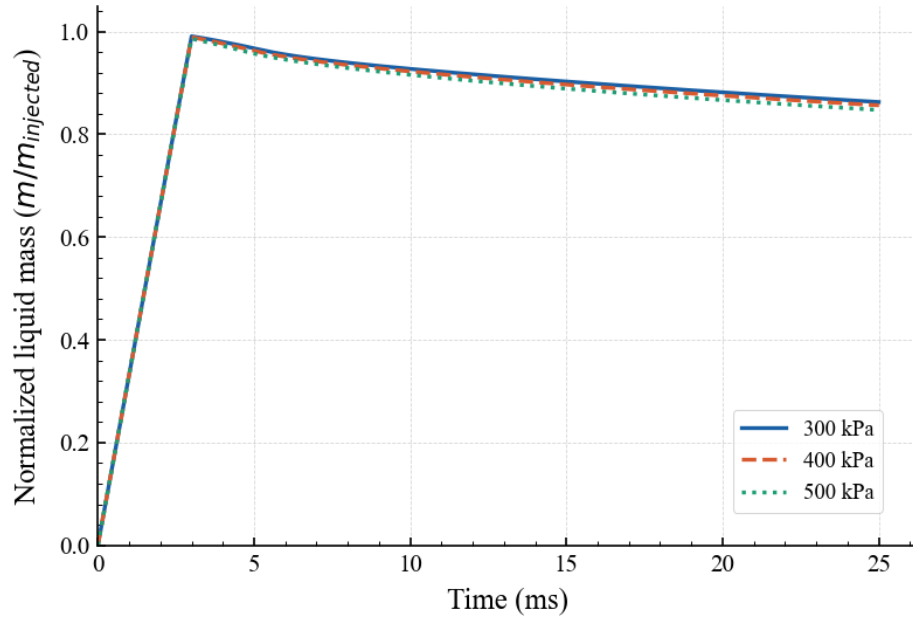


Figure 3.8: Normalized mass of liquid CH_3OH in the domain for different injection pressures.

3.4.3 Results for Varying Wall Temperature

Figure 3.9 shows a comparison of the wall film thickness for different temperatures of the wall. The experimental data is scaled in a way that the trends can be analyzed rather than the absolute values. From the graph it is clear that by increasing the wall temperature from 293 K to 373 K, the film thickness reduces due to faster evaporation in both the experimental and numerical set up. However, the numerical model shows a sharp decrease in film thickness when increasing the wall temperature from 323 K to 373 K.

For a wall at 423 K, the numerical model behaves differently from what was measured in the experimental data. At 423 K, the numerical model simulates even more increased evaporation as the film thickness dries out after a few milliseconds. In contrast, the experimental data observed the Leidenfrost effect, where the vapor layer hindered the evaporation and thus the liquid film increased.

The trends from Figure 3.9 are visualized in Figure 3.10. For a wall at lower temperatures, the fuel film remains stable. As the temperature increases to 373 K, a clear transition occurs. The fuel film becomes substantially thinner by 10 ms ASOI. At 15 ms ASOI the film has nearly completely vaporized. From a wall temperature of 423 K, the initial film formation is minimal and quickly evaporates.

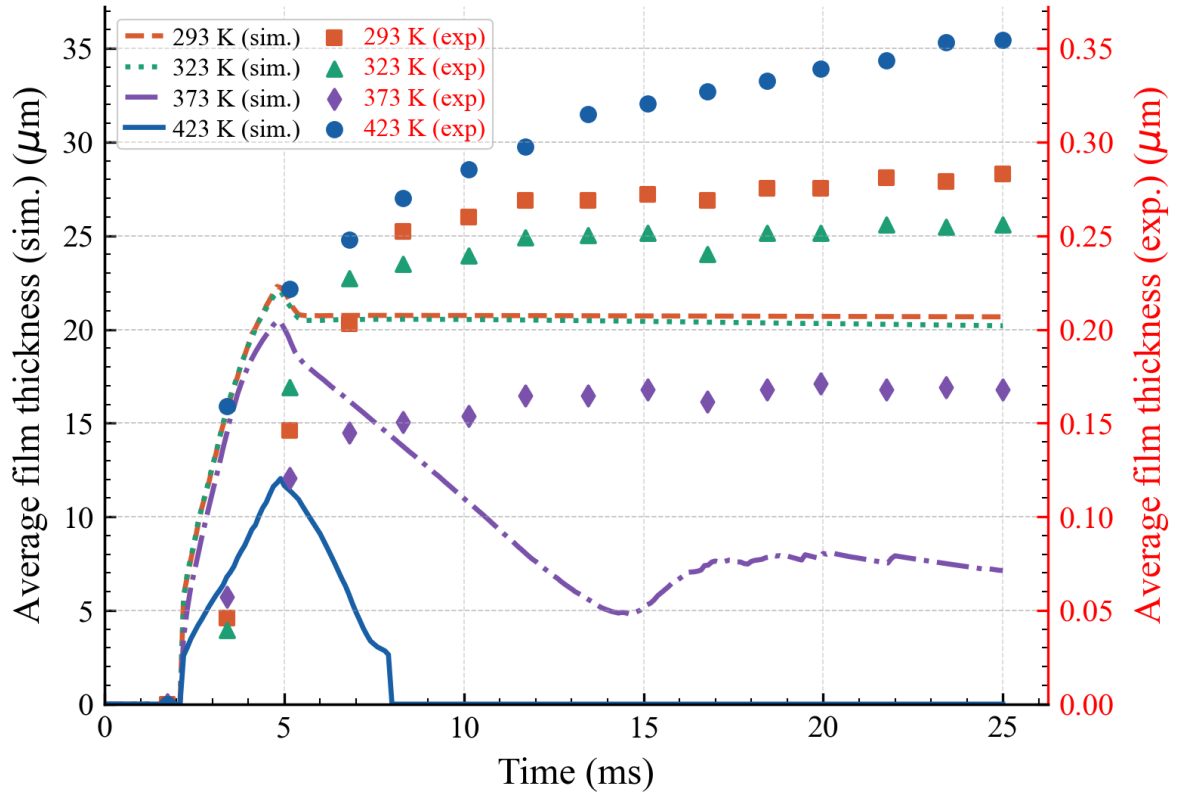


Figure 3.9: Comparison between experimental and numerical fuel film thickness on the wall for varying wall temperatures.

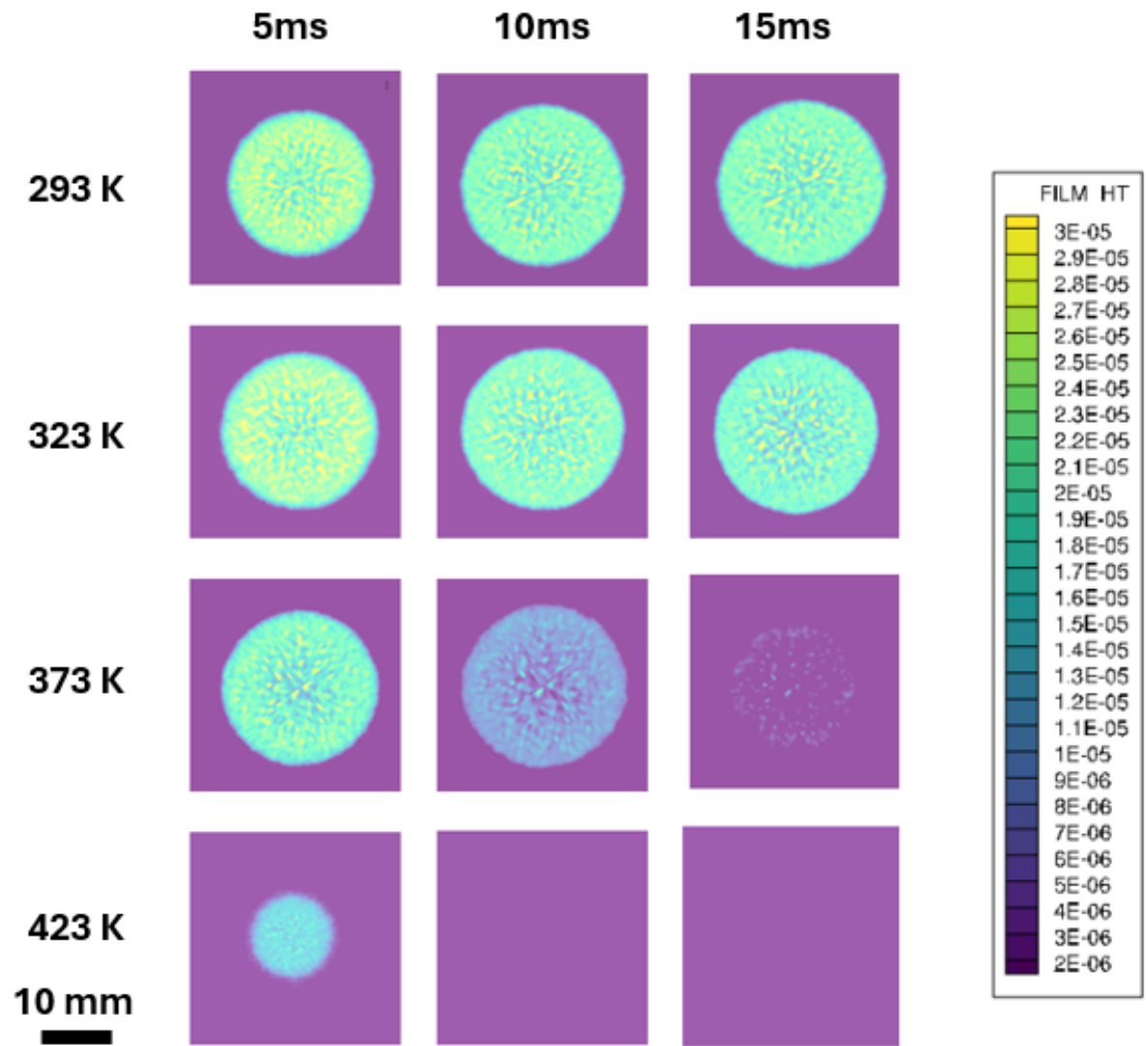


Figure 3.10: Color images of the simulated fuel films for varying wall temperatures different timesteps ASOI.

The graphs below show the dynamic relationship between the wall temperature and the evaporation characteristics of the methanol fuel films. Figure 3.11 shows that at lower temperatures (293 K and 323 K), the wall film mass increases sharply during the injection phase and remains high. The liquid fuel adheres to the wall surface and there is almost no evaporation. In contrast, the peak film mass is reduced for higher temperatures and declines steadily. At 423 K, the film mass is only about 25% of the low temperature cases. The evaporation rate in Figure 3.11 shows a sharp increase when droplets first hit the wall, followed by a sharp decrease when the liquid film has dried out. A more gradual behavior is visible for the simulation with wall temperature 373 K. However, the dry-out is also visible as a sudden decrease in evaporation. Figure 3.13 shows the film formation rate. A negative rate means that more droplets impinge than that are evaporated. A positive value shows that evaporation is dominant.

Figure 3.12 shows the normalized total liquid mass in the domain. At lower temperatures, around 90% of the total injected mass remains liquid throughout the 25 ms simulation. Higher wall temperature helps the transition into the gas phase. Interestingly, the 373 K curve eventually shows a lower normalized liquid mass than the 423 K curve.

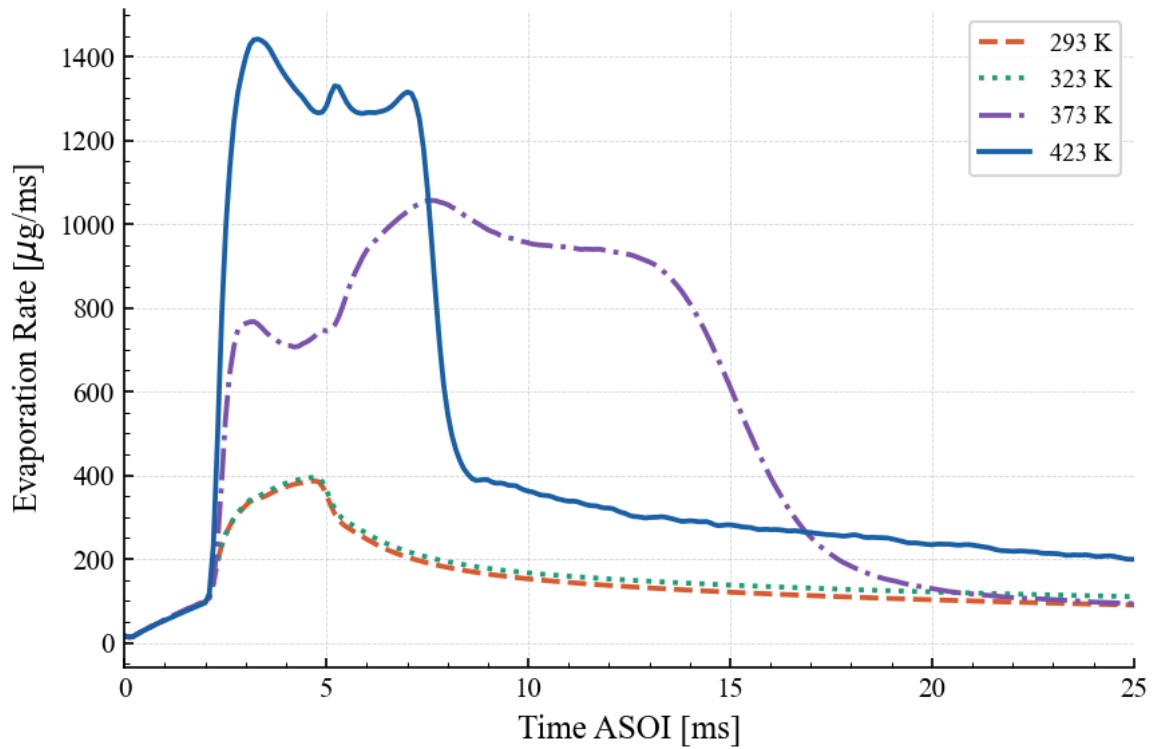


Figure 3.11: Evaporation rate over time of CH_3OH at different wall temperatures.

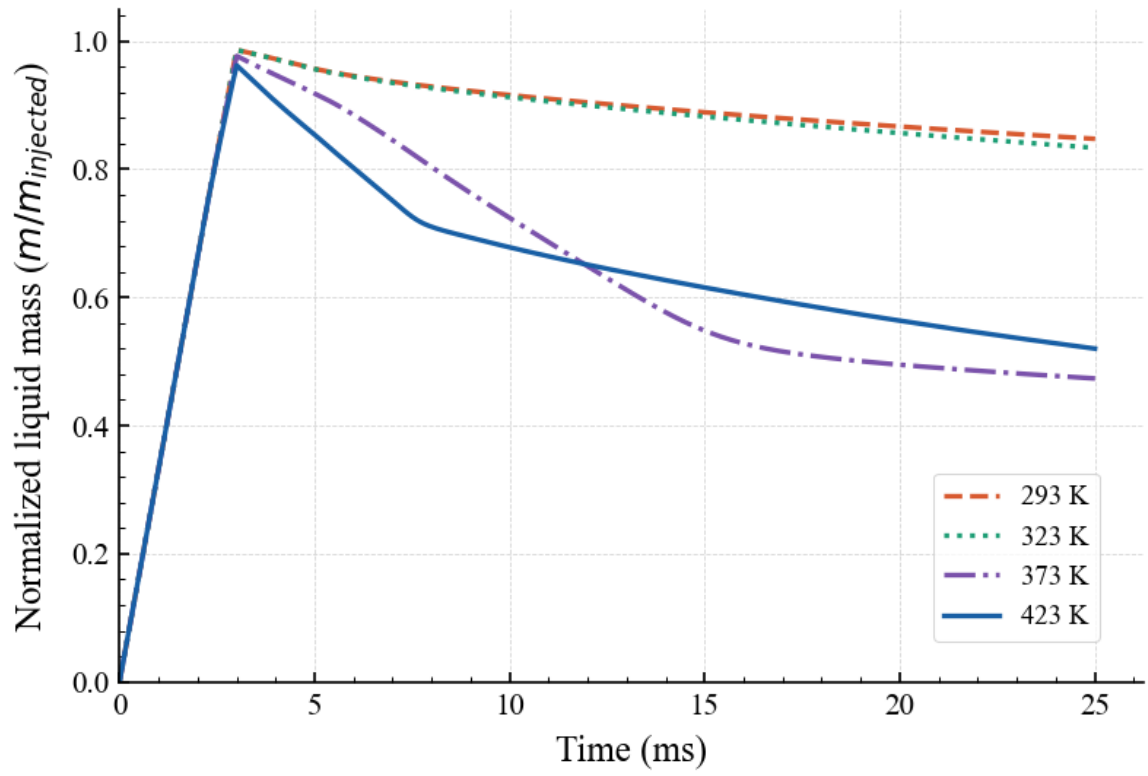


Figure 3.12: Normalized mass of liquid CH_3OH in the domain at different wall temperatures.

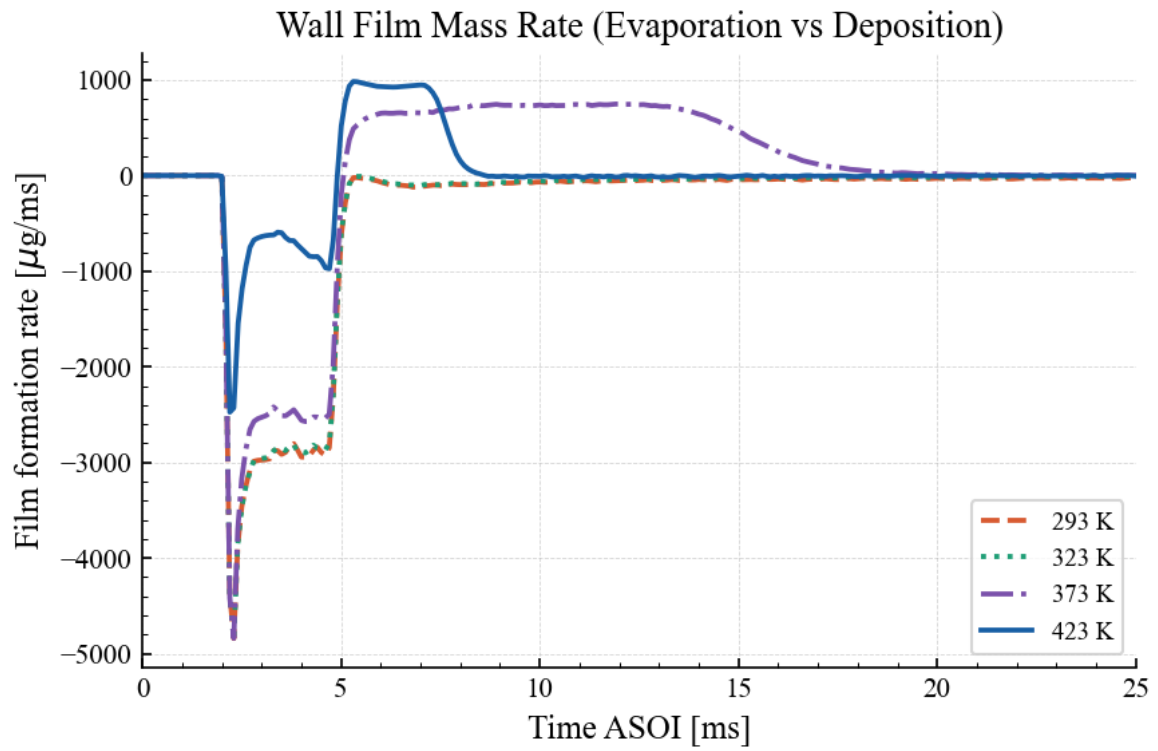


Figure 3.13: Film formation rate of the wall film over time at different wall temperatures.

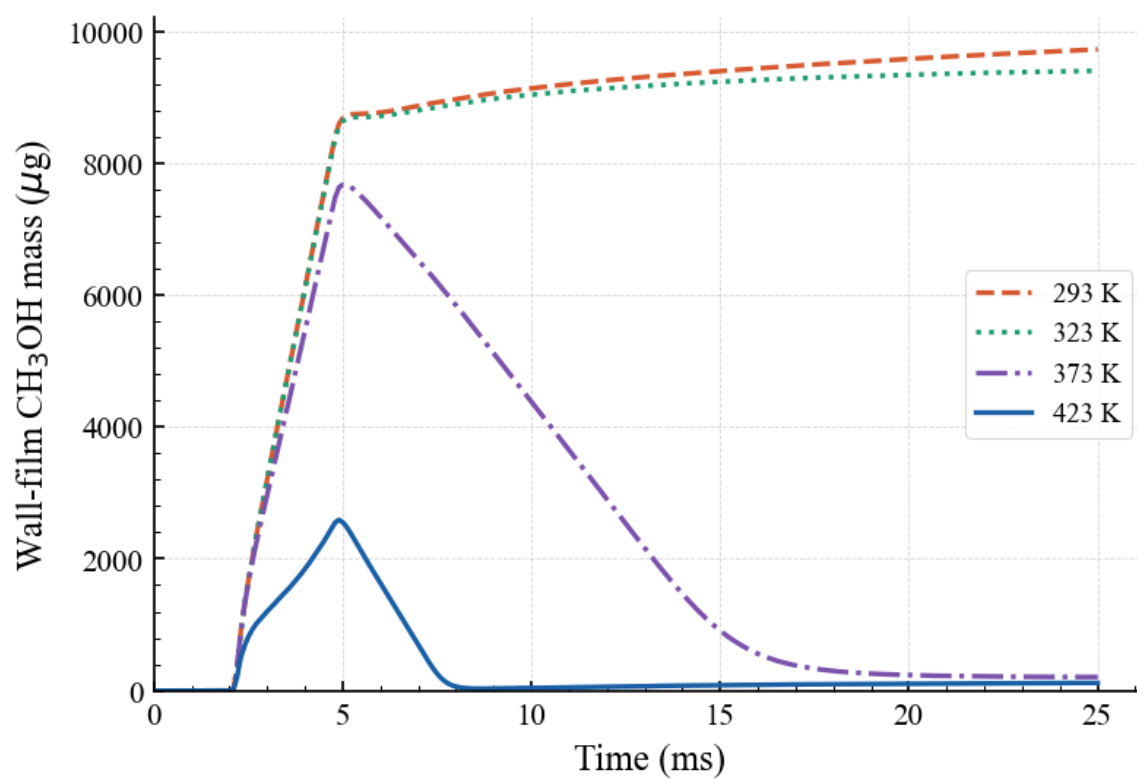


Figure 3.14: Film mass over time for different wall temperatures.

3.5 Discussion

The implemented spray-wall interaction model predicts a film thickness that is two orders of magnitude greater than that observed in the experiment. Figure 3.3 shows that for varying injection pressures, the simulated film thickness ranges from 20 μm to 22 μm , compared with the experimental values that range from 0.24 μm to 0.32 μm . Both the experimental data and numerical data show that increasing the injector pressure initially increases the film thickness, but when increased even more, the film thickness becomes thinner. The numerical model is thus capable of following this physical trend observed in the experiment by Zhang et al. This indicates that the combination of RANS, KH-RT, Bai-Gosman, Frössling, and CHT model can capture the dominant transport and phase-change mechanisms in a qualitative manner.

At the same time, the results reveal that there is a systematic difference. The model film thickness is 100 times thicker and the area about half the size of the experimental data. This difference is primarily assumed to come from the uncertainty and errors in the measured data. However, even in the relative trend a difference is notable. Across different injection pressures, the numerical simulation results are relatively closer to one another than the experimentally measured average film thickness values. Secondly, at very high wall temperature, the numerical model deviates from the experimental behavior. This suggests that a deep analysis is needed to evaluate the implemented model. In the following subsections, possible model limitations are discussed and explicitly linked to the observed behavior in the simulation results from Section 3.4.

3.5.1 Limitations on the Impingement of the Droplets

Figure 3.3 shows that there is only a small separation between the numerical film thickness curves for different injection pressures. How the droplets interact with the wall is determined primarily by the wall treatment and the impingement criteria from the Bai-Gosman model.

Wall Roughness

First, the wall roughness from the quartz glass and the wall treatment in the numerical set-up may influence the numerical outcome. As discussed before, the RIM method requires a roughened quartz surface to create a measurable contrast for film thickness extraction. The roughness of the quartz glass is set to 10.31 μm . The microscopic surface structure cannot be fully resolved in the current mesh. The required orders of refinement to resolve this would not be computationally feasible.

In the numerical setup, roughness is represented through the standard RANS near-wall treatment using an equivalent roughness height K_s and a roughness constant r_s . As a consequence, the roughness is treated as a subgrid correction through the log-law wall function rather than as an explicitly solved geometric element. This means that the model can reproduce the average roughness effect, but not the local peaks and valleys of the surface. For thin methanol films, those unresolved small scale features may still affect the result of sticking, spreading, rebound, or splashing. The wall treatment can capture the mean roughness effect on the flow, but not necessarily the detailed response of an impinging droplet.

The wall function also does not resolve the viscous sub-layer explicitly. It relies on an assumed near-wall velocity profile and empirical correlations. As a result, the detailed velocity gradients and viscous stresses very close to the wall are not directly resolved but are approximated. Since the evolution of the wall film strongly depends on these near-wall interaction, the model may not fully reproduce the balance between film spreading and resistance.

Bai-Gosman Model

A second possible limitation in the numerical model are the thresholds set in the Bai-Gosman model. The outcome of an impinging droplet is determined by empirical regimes, as described in Section 2.8.1. The spray visualization over time in Figure 3.15 shows that a lot of the impinging droplets are splashed and break up into smaller secondary droplets. In this thesis a splash fraction of 0.7 was used. This implies that an impinging droplet in the splashing criterion will generate a smaller secondary droplet and the remainder will stick to the wall.

The splashing threshold is given by the energy parameter E^2 , with a critical value E_{crit}^2 which is set to 3300. This value is a standard empirical correlation for many spray-wall interaction models. However, this parameter is linked to the energy balance between droplet inertia and surface tension. Since the surface tension of methanol (22.5 mN/m) is significantly lower than that of diesel or water, the methanol droplets may be more prone to deformation, breakup, and splashing. Wall roughness causes the energy of the impinging spray to dissipate more and increase the wall wetting. The use of the universal $E_{crit}^2 = 3300$ may not fully take this lower surface tension or the wall roughness into account.

As discussed in Section 3.4.1 the rebound Weber number was set to the common value of 5 and did not show a direct impact on the model in the sensitivity study. However no such study was done for E_{crit}^2 .

In conclusion, it is possible that the implemented Bai-Gosman model over-predicts splashing. If too much mass of the impinging droplets is broken up into smaller secondary droplet, the sensitivity to the varying injection pressure may be damped. This could explain why the numerical film thickness curves lie so close together. In the future, a parameter study regarding the Bai-Gosman model for methanol splashing is necessary to further examine this.

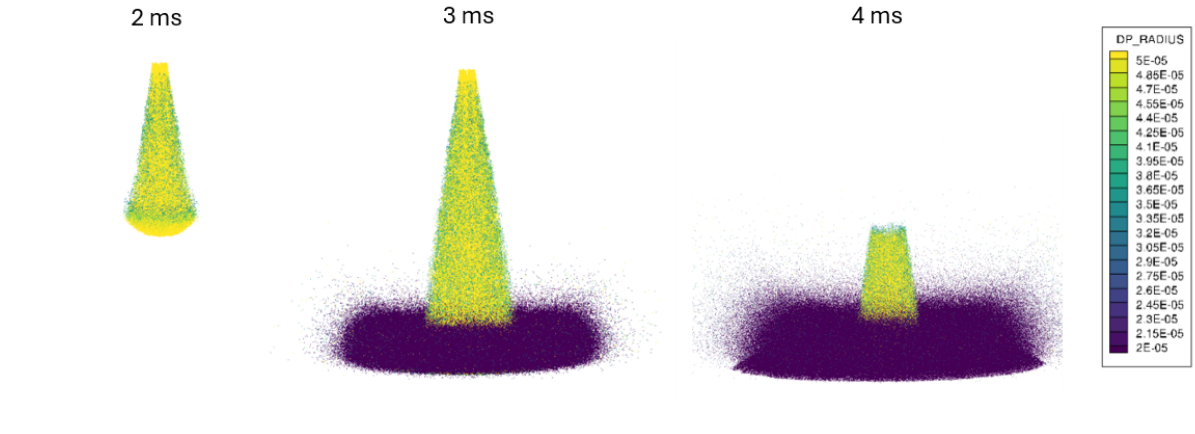


Figure 3.15: Visualization of the spray over time.

3.5.2 Strong Film Evaporation at High Wall Temperatures

Another possible shortcoming of the model lies in the evaporation model and the coupling of it with the CHT. From Figure 3.9 it is clear that with increasing wall temperature, the film thickness decreases. In this context, the model reproduces the expected trend regarding the temperature effect. However, the film thickness in the numerical model dries out faster than in the experiment. This response is especially pronounced for temperatures above 373 K. This suggests that the model may be too sensitive to the wall temperature or that it transfers too much wall heat into evaporation of the liquid film. An additional source of overestimation may lie in the evaporation model itself. In CONVERGE's Lagrangian parcel framework, the film is not fully resolved. The uniform film temperature neglects any thermal gradient across the film thickness. As a result, the vaporization may be overestimated.

In a coupled heat-transfer problem, the film behavior is determined by the evaporation correlation, the thermal response of the solid wall, the interface temperature at the film, and the boiling-regime criterion. The temperature at the contact point of the liquid film and the solid wall is not a constant prescribed setting. It depends on the conduction in the solid, heat extraction by the fluid, and the thermal inertia. If the coupling deviates too much from the reality, the interface temperature of the model can remain higher than that in reality. The evaporation model would predict a temperature that is hotter than it should be, and the evaporation is overestimated. This coupling is an important limitation of the model because the properties of the implemented quartz are assumed to be constant. As described in Section 2.9.3, the implemented properties are obtained from a separate source as they are not described in the experimental paper. Although quartz glass is highly stable, its specific heat and thermal conductivity increase with increasing temperature. This mismatch could explain why the interface stays hotter and evaporates more liquid than reality.

Figure 3.16 shows the temperature distribution across part of the domain when the wall temperature set to 323 K at 15 ms ASOI. The impinging spray produces minimal cooling of the solid wall, which is consistent with the liquid film that forms. Since limited evaporation has occurred, relatively little heat has been extracted from the wall. In contrast, in Figure 3.17, the wall temperature is set to 373 K. At 15 ms ASOI the heated vaporated vapor layer is visibly present above the wall and the wall itself has started to cool down a bit more. The relative difference in temperature distribution between the two walls shows that the amount of film evaporation affects the wall temperature over time. Higher evaporation rates produce more significant wall cooling. However, the temperature gradient is very steep in Figure 3.17 as only the grid cells closest to the edge have cooled down. This suggests that the CHT transfer in the solid region may not be fully resolved. For this reason, the wall temperature will not be included as a parameter in the following simulation matrix. In future work the CHT should be elaborated on further to really capture the cooling interaction of the impinging spray, the liquid film, and the wall.

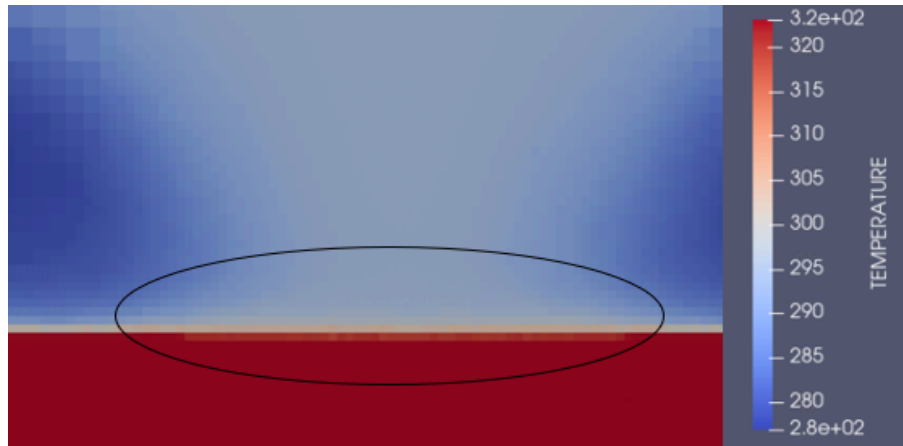


Figure 3.16: Temperature distribution for wall at 323 K at 15 ms ASOI.

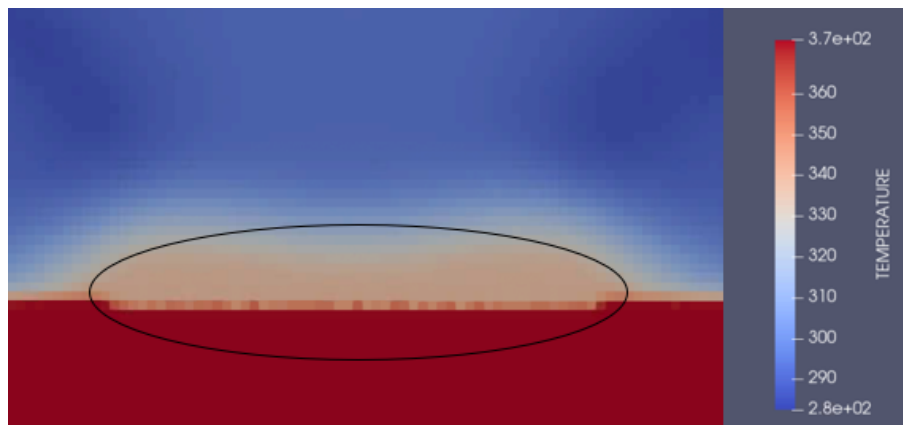


Figure 3.17: Temperature distribution for wall at 373 K at 15 ms ASOI.

3.5.3 Liquid Edge

Lastly, a small discussion is required regarding the film edge transition and the Lagrangian parcel representation. The transition at the film edge in the numerical simulation is not smooth, but discretized into different levels. This is a direct consequence of how the liquid phase in this simulation is represented. In a Lagrangian parcel based model, the wall film is not described as a continuous fluid layer. Instead, it is made up of discrete parcels that stick to the wall, where each parcel represents a small liquid volume. The film is reconstructed from the properties of all parcels attached to a given region on the surface. In this approach, the incoming parcels can easily transition to a wall-film parcel in the same numerical framework.

However, this comes with some serious modeling simplifications. A real liquid film is a continuous volume and is governed by film equations that describe the mass, momentum, and energy conservation. In particular, the film edge is in reality an important interaction between capillary forces, wetting dynamics, surface tension, and viscous forces. The Lagrangian parcel film does not resolve this directly. It cannot represent a contact line or angle, because it does not solve the film equations. Instead, the film boundary is determined by the existence of parcels at a certain place. If the mesh is too fine, there may be too few parcels per cell to resolve physical effects. However, if the mesh is too coarse, boundaries could remain unresolved. As noted in the CONVERGE manual, the film height is calculated based on the number of parcels located in the near-wall cells. This implies that the grid size and orientation directly dictate the calculated film height and that the film boundary is determined by the discrete mass points.

As a consequence of this abrupt edge, the evaporation of the liquid film could be affected. The artificial steps in the simulation causes steeper temperature and fluid concentration gradients than in reality. Models like the Frössling correlation are sensitive to these gradients and thus the evaporation rates and wall heat flux near the edge may be affected. This effect is likely increased by the use of Lagrangian particles. The discrete parcels that evaporate are removed abruptly and causes the film thickness to decrease in a stepwise manner. The redistribution of the liquid is not explicitly resolved, which can make the edge of the liquid film appear sharper than in reality.

Future studies could address this limitation using the Eulerian approach for the liquid film. In the Eulerian approach, the film is treated as continuum and is represented by equations for mass and momentum across the thickness of the film.

3.6 Conclusion of the Validation Study

Overall, the validation study shows that the numerical model is capable of reproducing the spray impingement and wall film formation for methanol. The comparison with the experimental data only uses the relative trend because the absolute values obtained with the RIM method likely have a significant measurement uncertainty. The model captures the changing film thickness trend with varying injection pressures. The model also captures the increased evaporation trend with increasing wall temperature. However, the model may overestimate the evaporation rate due to the simplified CHT and liquid interaction. Several aspects have been identified that could further improve the accuracy of the numerical model: the implementation of more representative wall-roughness correlations, calibration of the Bai–Gosman model specifically for methanol sprays, implementation of an Eulerian liquid-film formulation, and enhancement of the thermal coupling between evaporation and the CHT model.

With the result of this validation study, the rest of the thesis can confidently examine the wall film behavior under varying boundary conditions to identify relative trends.

Chapter 4

Simulation Campaign

4.1 Simulation Strategy

The numerical study on the wall-wetting characteristics of methanol is realized as a design-of-experiments (DoE) study in which operating parameters are varied systematically using the discrete Latin Hypercube Sampling (dLHS) approach. The dLHS is a sampling method that selects discrete values for several parameters in a way that the full range of possible combinations is well represented in the experiment. It ensures that the samples are spread across the entire range of each parameter and that non-linear interactions are captured. Using discrete levels for the values, makes it easier to use as a reference for future experimental work [76].

The simulation workflow follows a fixed sequence for every validation simulation and test case. Firstly, the computational domain, mesh, boundary conditions, and initial conditions are prepared consistently across all runs. Secondly, the specific parameter set from the validation case or from the dLHS design is implemented. Thirdly, each case is solved using the same solver settings, numerical tolerances, and post-processing routines. By following these strict guidelines, changes in the numerical procedure are avoided and the results can be compared correctly. After each simulation the wall wetting parameters are extracted and processed. All extracted data is processed using Python to make clear plots and interpretation. Finally, the results are presented and discussed.

4.2 Case Definition and Introduction

The test cases are designed using the dLHS method to systematically investigate methanol wall wetting under different conditions. The goal of this chapter is to identify how different parameters affect the film formation, the film evolution, and the film evaporation. The test matrix for this study is based on three independent variables: the ambient temperature, the injection pressure, and the fuel temperature. These parameters can directly influence the spray behavior, the film formation and the film evaporation.

The ambient temperature T_{amb} ranges from 5 to 45°C. This covers cold conditions as well as higher temperatures that occur in marine engine environments [77]. The injection pressure p_{inj} is varied from 5 to 20 bar. This is representative for the range of recent injector systems on the market [78]. The fuel temperature T_{fuel} is varied between 20 and 60°C to capture the effect of possible preheating of the fuel. These parameters and values are selected based on available literature, while also taking into account the limitations of the numerical model.

4.3 Geometry and Boundary Conditions

In the parameter study, the same geometry and mesh configuration are used as in the validation setup. The wall is also modeled as quartz glass to ensure that the limitations and assumptions identified during the validation study remain consistent. As a reminder, Figure 4.1 shows the geometry, Figure 4.2 the injector, and Table 4.1 the boundary conditions.

Table 4.1: Boundary conditions

Item	Value
Ambient pressure [bar]	1.013
Wall temperature [K]	293
Injection duration [ms]	3
Nozzle diameter [mm]	0.26
Number of nozzles	14

Table 4.2: Total injected mass

Injection pressure [bar]	Injected mass [mg]
5	25
8	32.7
10	36.6
15	44.8
20	51.8

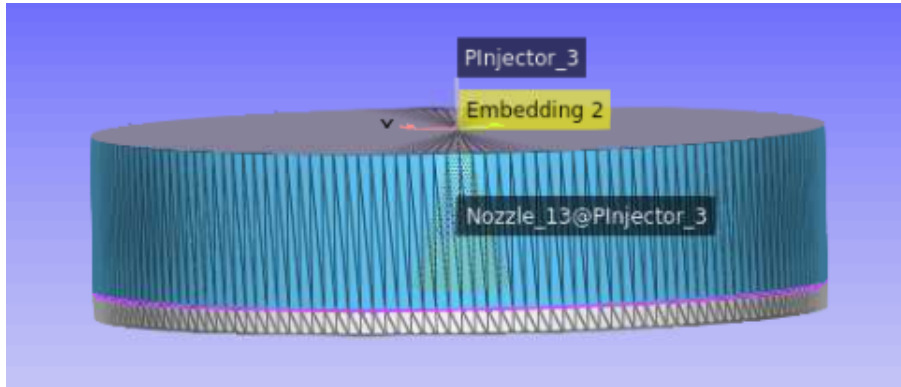


Figure 4.1: Visualization of the geometry.

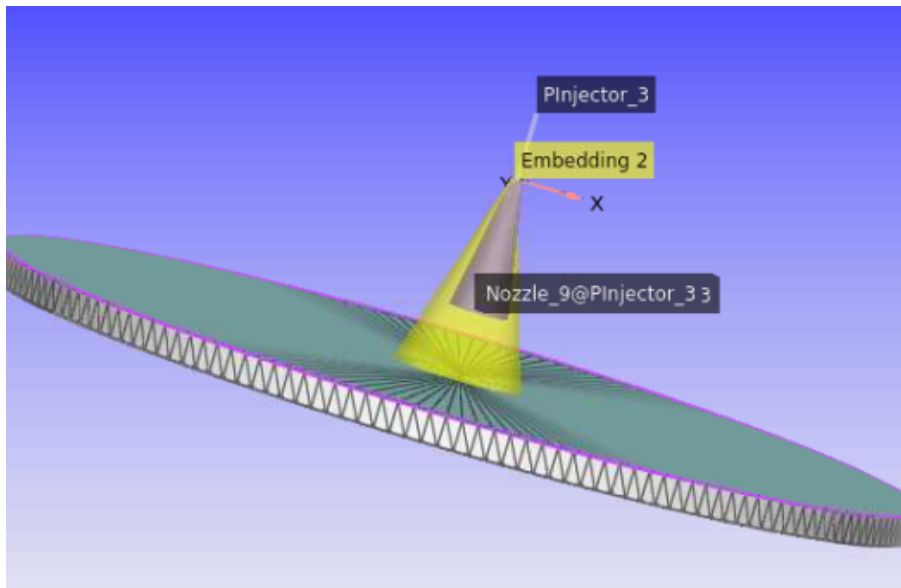


Figure 4.2: Visualization of the injector, fixed embedding and wall.

4.4 Parameter Variations

The experimental matrix in this study is defined by the following parameter levels.

- **Ambient temperature (T_{amb}):** 5, 15, 20, 25, 35, 45 °C.
- **Injection pressure (P_{inj}):** 5, 8, 10, 15, 20 bar.
- **Fuel temperature (T_{fuel}):** 20, 40, 60 °C.

The interaction between these variables is critical for understanding methanol wall wetting. Table 4.3 gives an overview of the 20 selected samples. The matrix is broad enough to identify trends, threshold regions, and interaction effects. The resulting data on the film mass, film area, and film thickness for all these simulations is given in Appendix A.

The results of the simulation campaign are analyzed in three stages. First, a parametric study examines the individual effects of ambient temperature, fuel temperature, and injection pressure on three wall wetting metrics: average film thickness, wetted surface area, and total deposited film mass. Each parameter is analyzed by isolating pairs of runs where one variable changes while the others remain constant. Secondly, a sensitivity and statistical analysis quantifies the relative importance of each parameter and identifies correlation trends across the full dataset. And lastly, the findings are translated into practical implications for methanol PFI engine design.

Table 4.3: Discrete Latin Hypercube Design for methanol wall wetting analysis.

Run	Ambient Temp (°C)	Fuel Temp (°C)	Injection Pressure (bar)
1	5	20	5
2	5	40	10
3	5	60	15
4	5	20	15
5	15	20	8
6	15	40	20
7	15	60	5
8	20	20	15
9	20	40	8
10	20	60	10
11	25	20	20
12	25	40	5
13	25	60	15
14	35	20	10
15	35	40	15
16	35	60	8
17	45	20	5
18	45	40	10
19	45	60	20
20	45	60	8

4.5 Influence of Key parameters

4.5.1 Influence of Ambient Temperature

The first parameter investigated in this study is the ambient temperature. This effect is illustrated through two distinct operational sets: Run 1 vs. Run 17 (conducted at 5 bar injection pressure and 20°C fuel temperature) and Run 2 vs. Run 18 (conducted at 10 bar and 40°C fuel temperature). These two separate settings allow for a detailed analysis on how ambient temperature behaves under different conditions. First each set is analyzed independently before determining if the other operating parameters change the overall impact of ambient temperature. A critical factor in interpreting these results is the 1 μm threshold applied to the extraction of the thickness and the film area.

In the first set (Run 1 vs. Run 17), increasing the ambient temperature from 5°C to 45°C results in a reduction of the film thickness. While both runs follow a similar evolution over time, at higher ambient temperature the thickness profile is consistently lower. Figure 4.4 shows the film area over time. At an injection pressure of 5 bar and fuel temperature 20°C, the film area is only slightly smaller at higher ambient temperature. Interestingly, the film mass adhered to the wall also remains almost identical between these two conditions. This suggests that the ratio between secondary droplets falling back to the film and the overall evaporation (the liquid film and droplets on the wall) is not influenced by the ambient temperature.

In the second set (Run 2 vs. Run 18), the transition from 5°C to 45°C shows an even smaller difference. While the film thickness again decreases with higher ambient temperature, the absolute difference is slightly smaller than at lower pressure. The film area remains stable and nearly identical for both ambient temperature settings. However, the film mass shows a different evolution. Run 18 ($T_{amb}=45^\circ\text{C}$) accumulates a bit more mass than Run 2 ($T_{amb}=5^\circ\text{C}$) as the simulation progresses. The physical mechanisms underlying this are not fully understood from the data presented above. In Section 4.5.3, this will be discussed further.

Film Thickness

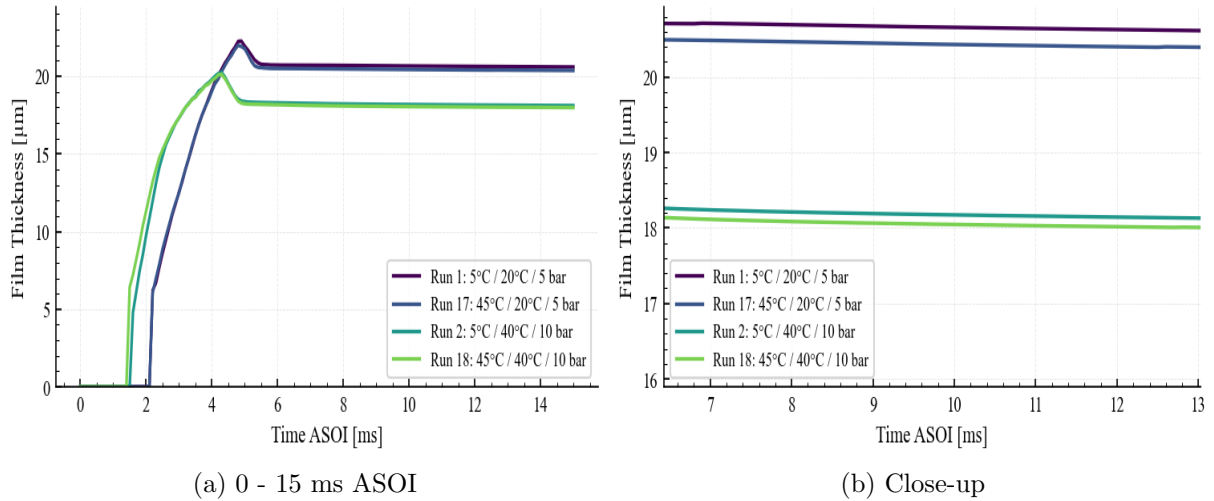


Figure 4.3: Average film thickness over time for four runs representing a 2x2 combination of ambient temperature conditions (5°C vs 45°C) and fuel temperature conditions (20°C vs 40°C).

Film Area

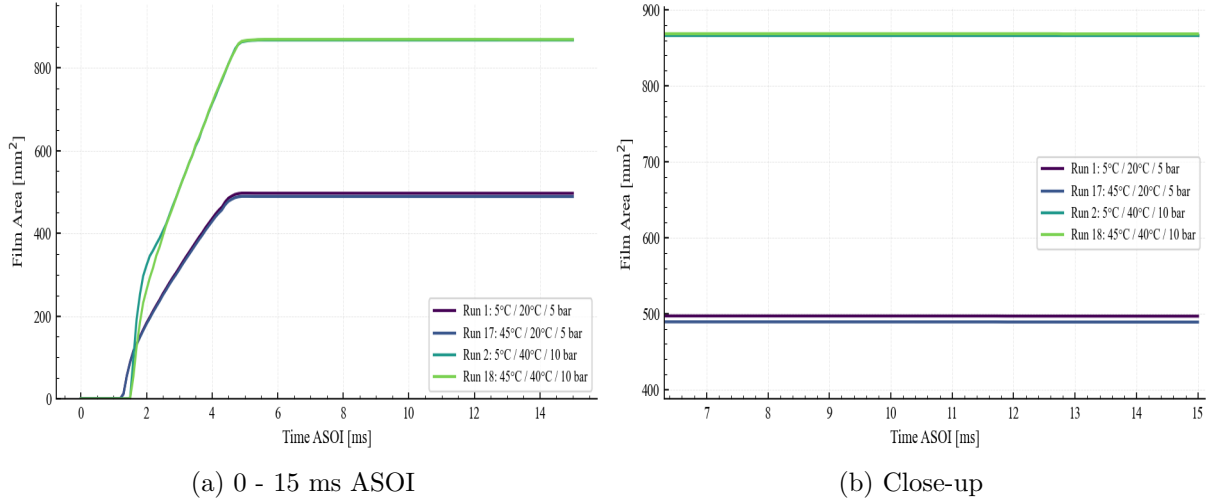


Figure 4.4: Film Area over time showing the influence of ambient temperature.

Film Mass

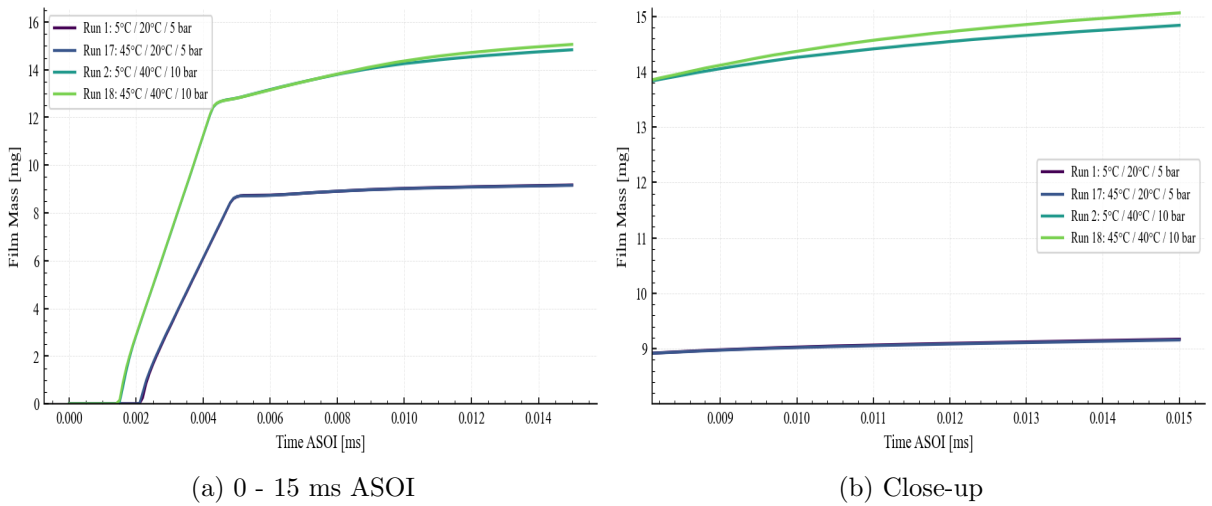


Figure 4.5: Deposited fuel mass over time showing the influence of ambient temperature.

An overview of the influence of the ambient temperature over all simulations is given in Figure 4.6. This bar chart sorts all the resulting film thickness by the ambient temperature. In the same ambient temperature group, they are sorted by increasing fuel temperature. When looking at simulated cases with constant fuel temperature, no clear trend is visible regarding the film thickness. Different sets of constant fuel temperature show different and random increases and decreases in film thickness. A similar bar chart is presented in Figure 4.7 for the fraction of injected fuel adhering to the wall. Again, no clear trend in the influence of ambient temperature on wall wetting is observed. From the comparison graphs and the full simulation matrix in the bar charts, it is clear that the influence of the ambient temperature is minimal.

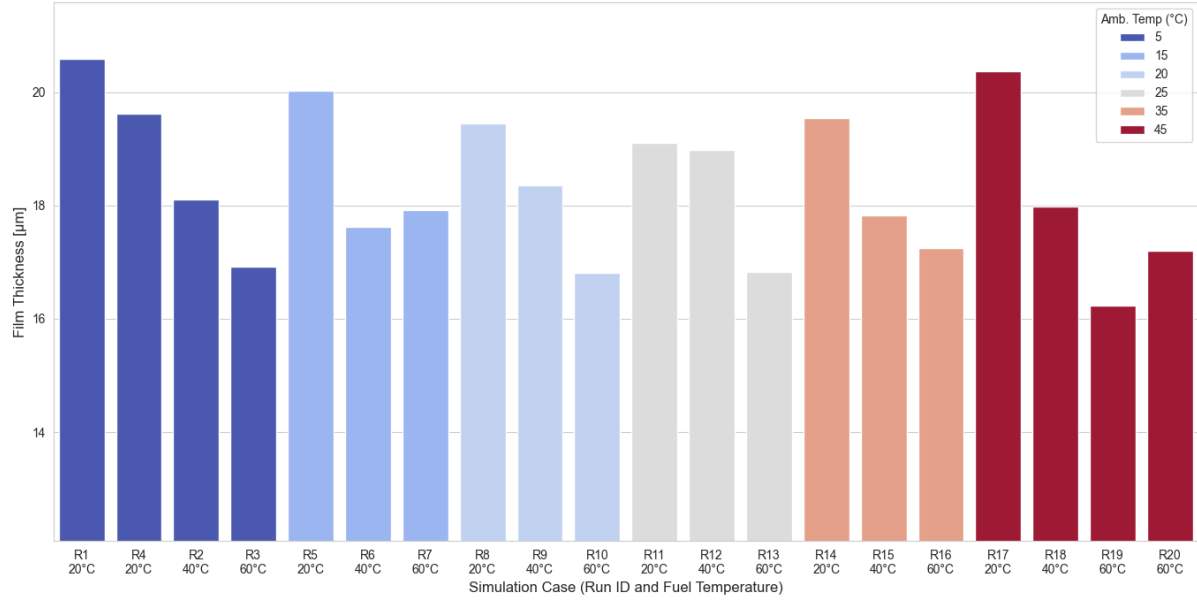


Figure 4.6: Bar chart of the simulated cases showing the methanol film thickness at 15 ms ASOI sorted by ambient temperature and fuel temperature.

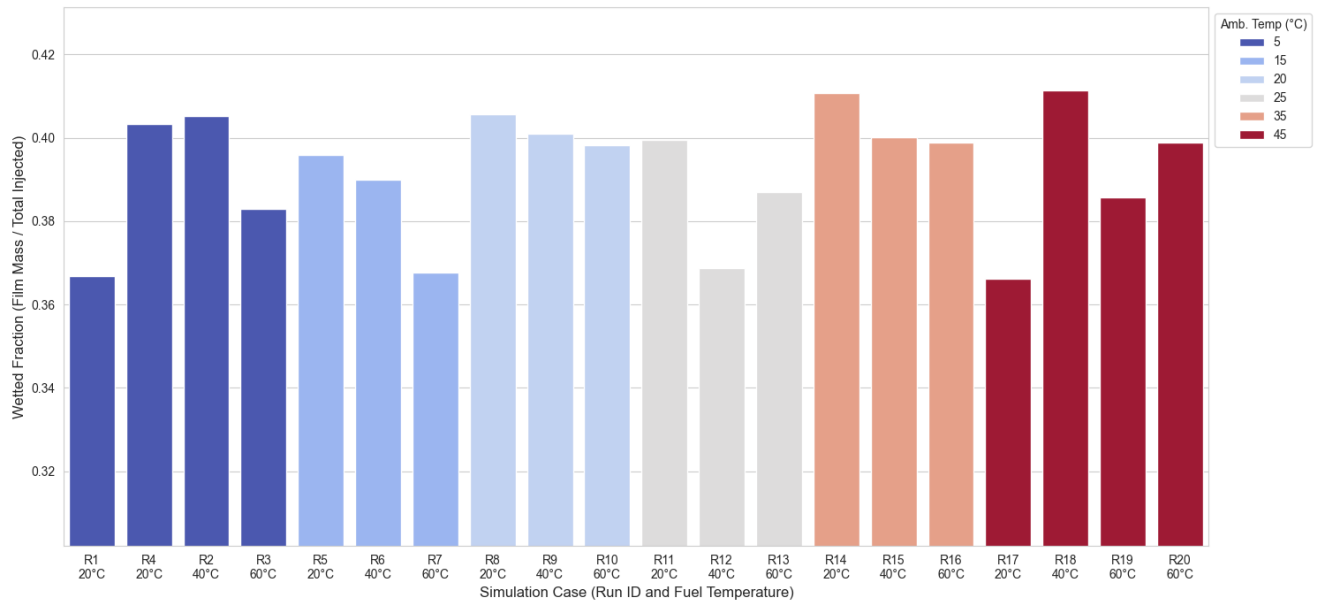


Figure 4.7: Bar chart of the simulated cases showing the normalized film mass methanol at 15 ms ASOI sorted by ambient temperature and fuel temperature.

4.5.2 Influence of Fuel Temperature

Figure 4.8 and Figure 4.9 visualize a clear trend regarding the film thickness and film area. Increasing the fuel temperature leads to a lower average film thickness and a larger film area. Run 14 ($T_{fuel} = 20^\circ\text{C}$) resulted in the smallest area ($\sim 810 \text{ mm}^2$) and the highest thickness ($\sim 19.5 \mu\text{m}$). In contrast, Run 10 ($T_{fuel} = 60^\circ\text{C}$) produces the largest spread out film ($\sim 890 \text{ mm}^2$) and the lowest thickness ($\sim 17 \mu\text{m}$). This trend can be physically explained by looking into the viscosity and surface tension of methanol. Table 4.4 shows these properties at different temperatures. With increasing temperatures, the viscosity and surface tension decreases. This means that when droplets spread on the wall they deform more easily and flow more across the surface. The fuel spreads further out while the thickness decreases.

Table 4.4: Viscosity and surface tension of methanol at different temperatures.

Temperature (K)	Viscosity (Ns/m ²)	Surface tension (N/m)
293	0.00061343	0.022831
313	0.00046043	0.021157
333	0.00035689	0.01947

Film Thickness

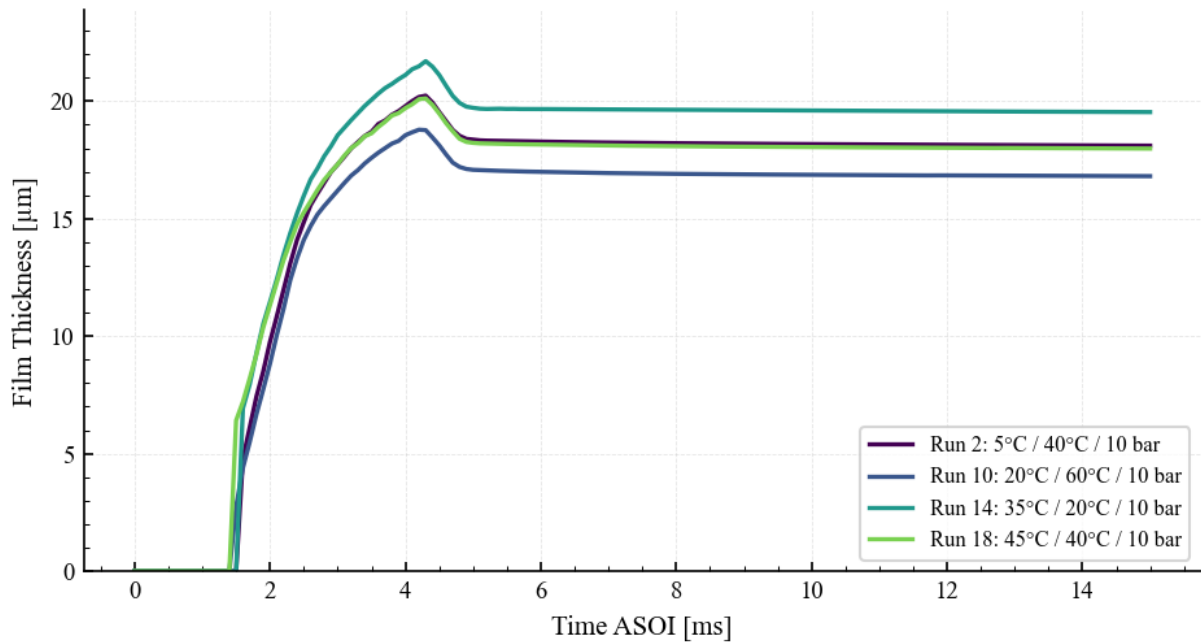


Figure 4.8: Average film thickness over time for four simulated cases at constant injection pressure (10 bar), illustrating the effect of different fuel.

Film Area

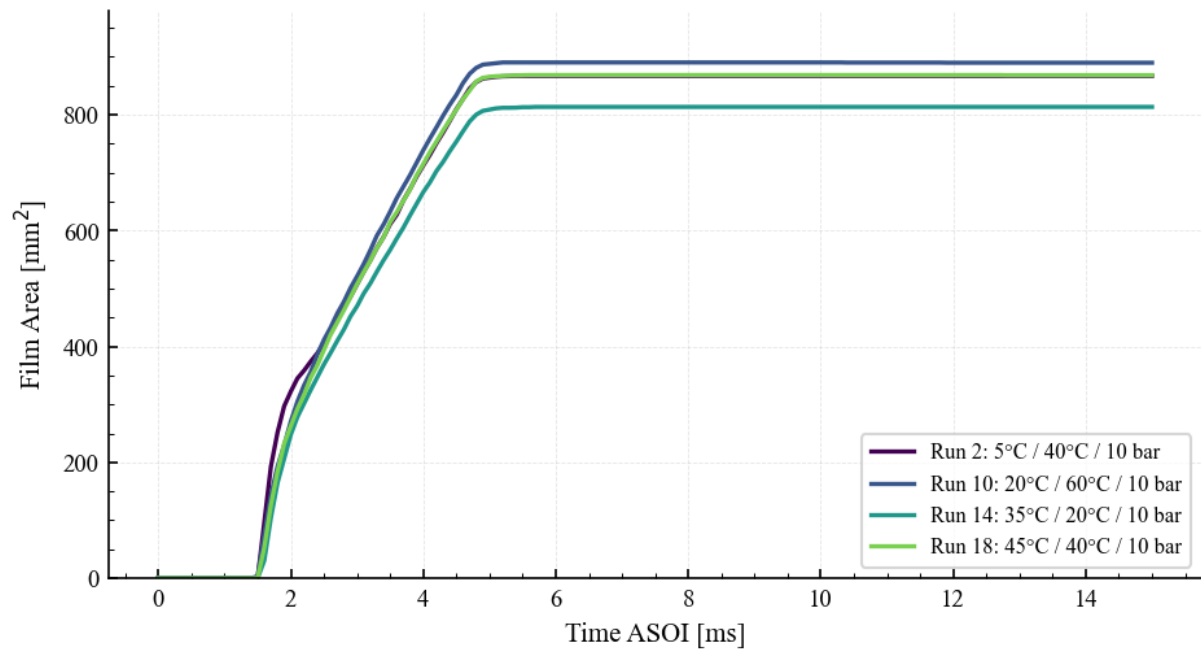
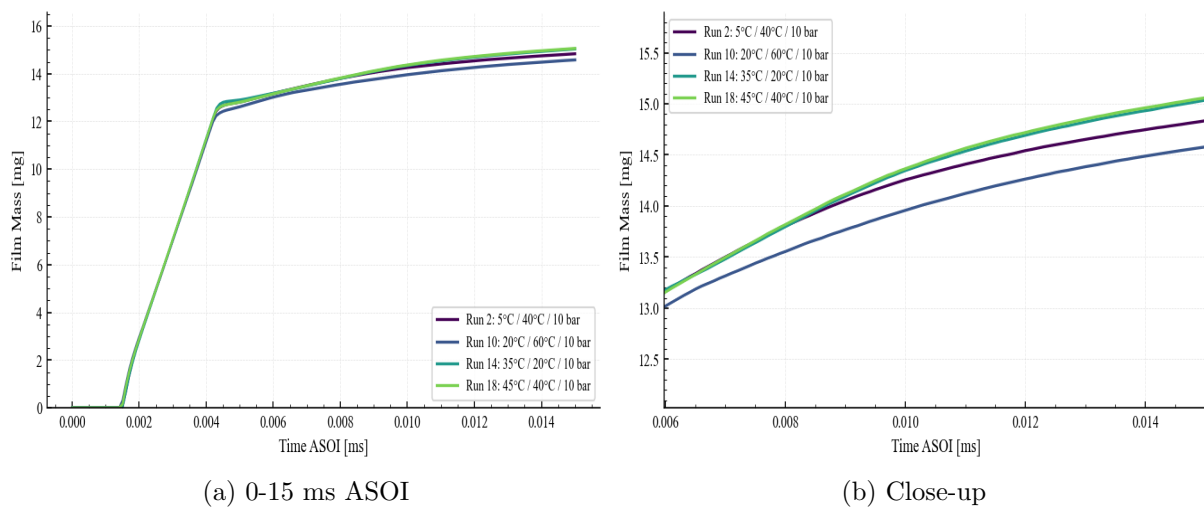


Figure 4.9: Film area over time showcasing the influence of fuel temperature.

Film Mass



(a) 0-15 ms ASOI

(b) Close-up

Figure 4.10: Deposited fuel mass over time showcasing the influence of fuel temperature.

Figure 4.10 shows interesting behavior regarding the accumulated film mass over time. For very high fuel temperature at 60°C the total film mass that adheres to the wall over time is lower than at for lower temperature. In contrast, for fuel temperatures around 20°C and 40°C the behavior is not straightforward. In the beginning of the film formation the film mass for fuel at both temperatures are the same. This suggest that the increased fuel temperature from 20 to 40°C initially does not change the amount of fuel that adheres to the wall. The fuel spreads out more and causes the film thickness to decrease. However, after a few milliseconds this behavior starts to change. Figure 4.10b, shows the deviation where the film mass of run 14 ($T_{fuel}=20^{\circ}\text{C}$ and $T_{amb}=35^{\circ}\text{C}$) and run 18 ($T_{fuel}=40^{\circ}\text{C}$ and $T_{amb}=45^{\circ}\text{C}$) grows larger than for run 5 ($T_{fuel}=40^{\circ}\text{C}$ and $T_{amb}=5^{\circ}\text{C}$). In a first interpretation of this graph, no straightforward physical explanation could be given to this behavior. Therefore a deeper comparison study was done using two extra simulation cases.

The behaviors described above are also visible in 4.6 and 4.7, which summarize film thickness and wetted fraction across all simulation cases. For simulations at the same ambient temperature, the film thickness decreases with increasing fuel temperature. This trend is visible across all ambient temperature groups, though the magnitude of the decrease varies between groups. The wetted fraction chart tells a more nuanced story. There, no prominent trend is visible regarding the influence of the fuel temperature.

4.5.3 Combined Effect of Fuel Temperature and Ambient Temperature

While the above sections describe the overall trend regarding the wall wetting behavior under various ambient and fuel temperatures, some interaction require more attention. To really capture which parameters cause which variations, two more simulations were done. In Run 21, the methanol was injected at 5 bar and 40°C into an atmosphere at 5°C. For Run 22, the ambient atmosphere temperature was raised to 45°C. These results are compared to Run 1 and Run 17 in Figure 4.11. While Figure 4.3 shows a difference in the film thickness reduction between the two sets of which each consists of two runs at different ambient temperatures. This difference in relative behavior could be attributed to either the difference in injection pressure or fuel temperature between the sets. From Figure 4.11a it is clear that the fuel temperature does not affect the observed influence of the ambient temperature. It is thus the increased pressure that causes the effect of the ambient temperature to lessen. From Figure 4.11b it also becomes clear that it is the pressure that suppresses the influence of the ambient temperature on the wall wetting area of the main film and not the fuel temperature.

The film mass evolution shows again interesting behavior. The graph reveals an intersection where the behavior changes. In the initial stages of impingement, the runs with lower fuel temperature show a higher film mass. The resulting graph indicates that it is not the ambient temperature or to relative difference between ambient temperature and fuel temperature that causes this behavior. It is probably the fuel temperature that lies on the basis of this phenomenon. However, the limited extracted data from the simulations is insufficient to formulate a meaningful explanation or hypothesis for the underlying physical mechanism.

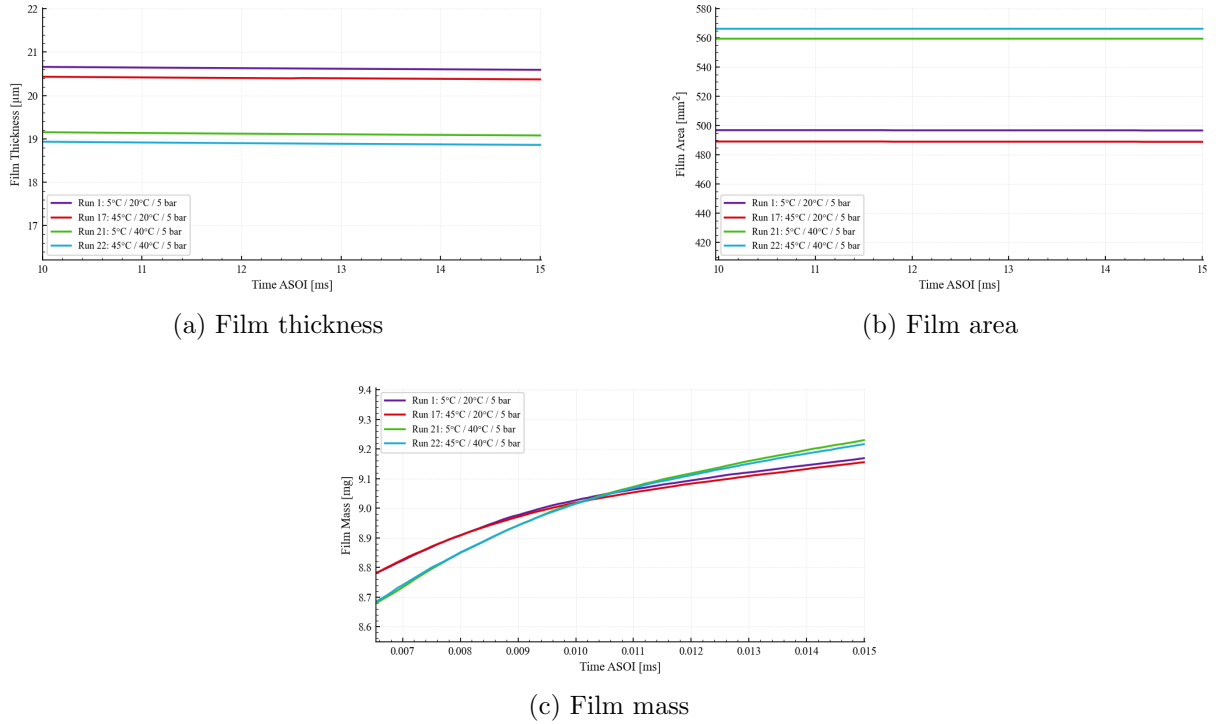


Figure 4.11: Film characteristics over time showing the difference between fuel temperature and ambient temperature.

After examining the influence of temperature on wall-wetting properties, it is also important to analyze how the ambient and film temperatures evolve over time. Figure 4.12 shows the average ambient temperature and film temperature over time. Simulation 1 is considered a cold simulation as the ambient temperature is 5°C and the fuel temperature 20°C. Simulation 20 is considered hot as the ambient temperature starts at 45°C and the injected fuel at 60°C. The small pressure difference between the simulations is neglected in the analysis of the temperature evolution.

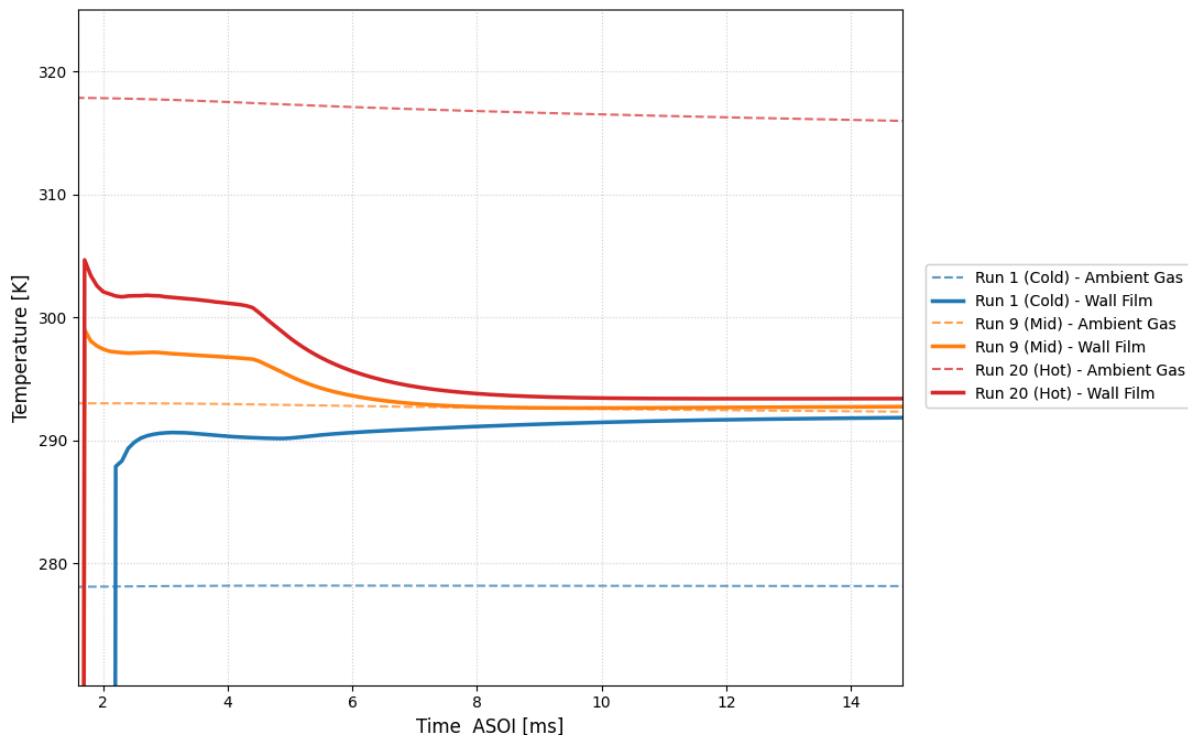


Figure 4.12: Average ambient temperature and film temperature over time.

This graph shows that the film temperature forms a bridge between the initial fuel state and the set wall temperature at 293 K. Fuel injected at temperatures higher than the wall temperature undergoes a rapid cooling phase, and stabilizes just above the wall temperature in approximately 8 ms. When the cooled fuel forms a film on the wall it starts to heat up slowly due to the wall temperature. The initial spike from 0 K in the temperature profiles should be disregarded.

A second observation from Figure 4.12, is the behavior of the average ambient temperature. For the high ambient temperature case, there is a steady decrease in gas temperature over the 15 ms duration. This drop in ambient temperature is a direct result of the vaporization. As fuel droplets evaporate, they extract energy from the surrounding gas. The fact that this cooling is only pronounced in the high-temperature case suggests that evaporation rates increase significantly with ambient and fuel temperature. To support this observation, Figure 4.13 shows the evaporation rate of the droplets for simulation 1, 9, 20.

In this study, the evaporation rate is determined from a combined mass balance of the droplet and wall film phases, and is corrected for the injected mass. Specifically, it is calculated as the negative sum of the time derivatives of the droplet and film masses, with the injection rate subtracted during the injection period. This ensures that only mass transferred to the vapor phase is captured. As a result, the obtained evaporation rate represents the true phase change process throughout the entire time domain, including during injection.

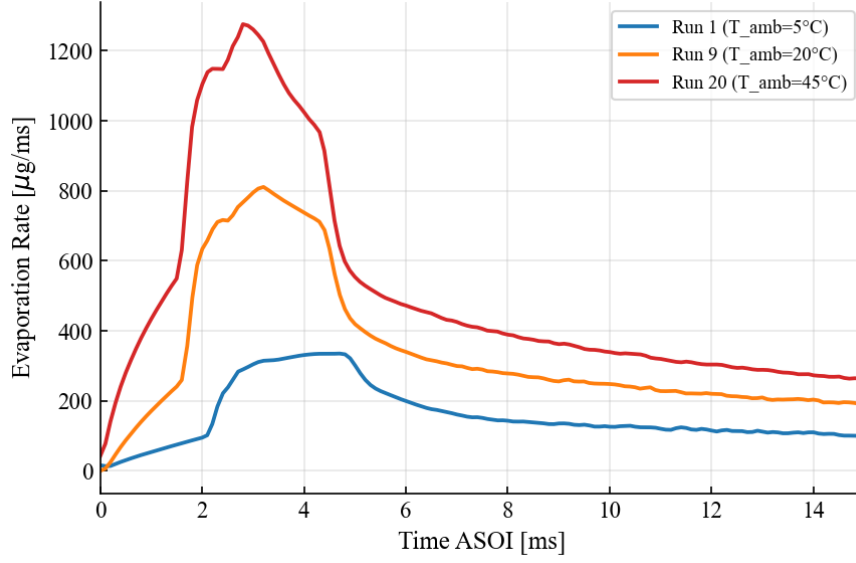


Figure 4.13: Evaporation rate of injected methanol at different temperatures.

The evaporation rate at higher ambient and fuel temperatures is larger than in colder environments. The evaporation rate shown in Figure 4.13 takes both the free-droplet as the wall film evaporation into account. However, due to the observations in Section 4.5.1 that the film thickness, area, and mass are almost identical for varying ambient temperatures, it can be stated that the difference in evaporation rate originates primarily from the faster free droplet evaporation.

This is confirmed by the bar charts in Figure 4.14 and Figure 4.15. The bar charts show the distribution of the total injected mass at 15 ms ASOI. From these, it is clear that both the increase in ambient temperature and the increase in fuel temperature have a significant impact on how much of the droplets is evaporated. The evaporated fraction grows considerably as either temperature increases, with the highest evaporated fractions observed at 60°C fuel temperature and 45°C ambient temperature. In contrast, the film fraction deposited on the wall remains stable across all runs, hovering consistently around 37–42% of the injected mass. The suspended droplet fraction consequently decreases as more mass is evaporated. Comparing both figures, the ambient temperature appears to exert a somewhat stronger influence on the evaporated fraction than the fuel temperature.

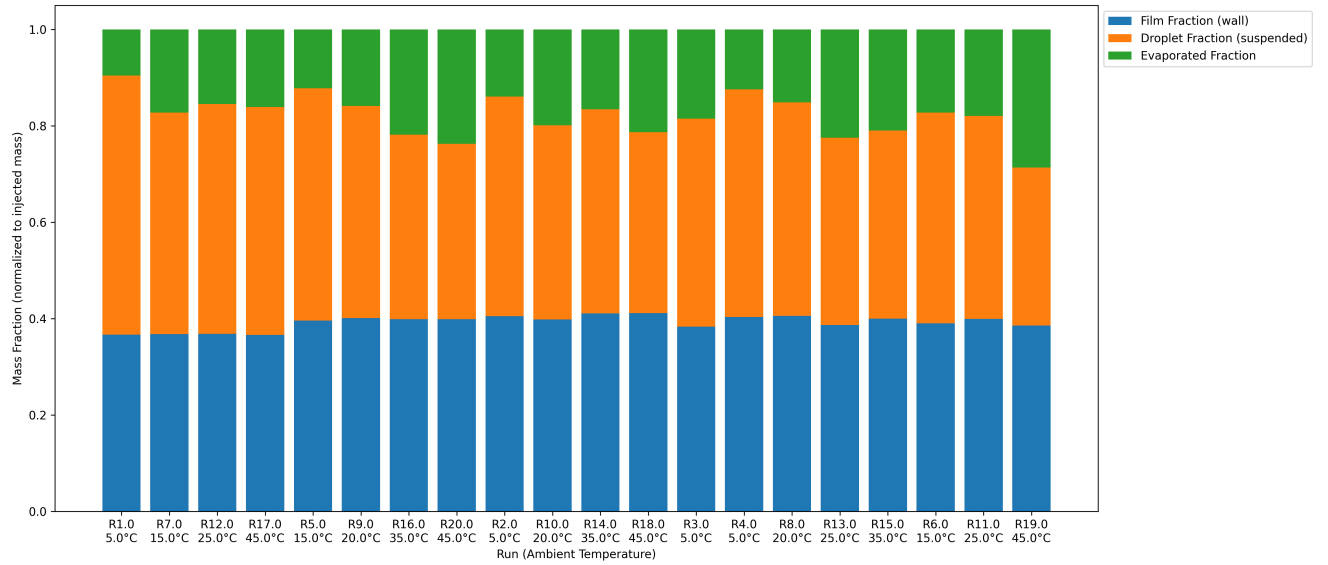


Figure 4.14: Bar chart of simulated cases illustrating the normalized mass fractions distributed among the wall film, suspended droplets, and evaporated phase sorted by injection pressure and ambient temperature.

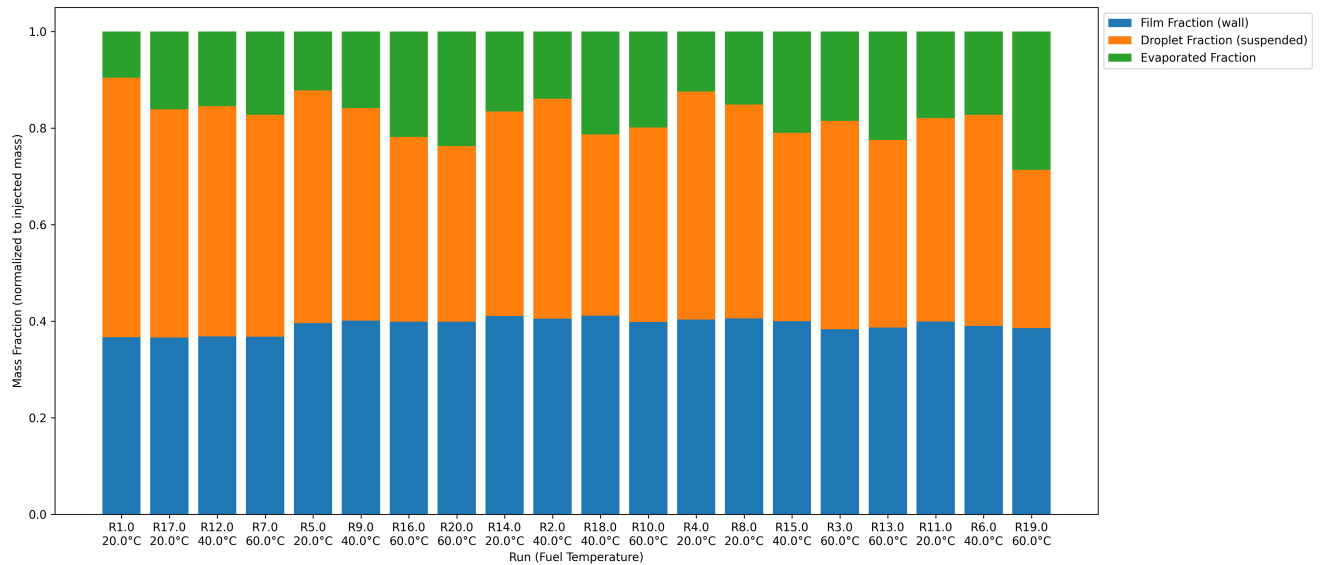


Figure 4.15: Bar chart of simulated cases illustrating the normalized mass fractions distributed among the wall film, suspended droplets, and evaporated phase sorted by injection pressure and fuel temperature.

4.5.4 Influence of Injection Pressure

Finally, the influence of the injection pressure on wall wetting is discussed. In this section the varying ambient temperature is again set aside. From Figure 4.16 it is clear that increasing the injection pressure from 5 bar to 20 bar results in a decrease in the average film thickness. This observation is confirmed over all the simulated cases by the bar chart in Figure 4.20. This bar chart shows the resulting film thickness at 15 ms ASOI for all simulated cases. The decreasing trend is immediately visible when comparing the simulated cases for the same fuel temperature and increasing pressure.

Upon closer examination of the evolution in Figure 4.17, it is clear that the decrease in film thickness is not linear with increasing pressure. This graph shows that the initial increase in injection pressure decreases the film thickness by 1 μm . However, when increasing the injection pressure even further, this decreasing trend diminishes to only a few tenths of a micrometer. Continuing to increase the injection pressure does not automatically translate in a major improvement in the film thickness. However, as described in Section 3.4.1, this trend only appears after the threshold of 4 bar. Before this threshold increasing the injection pressure led to an increase in film thickness. For the film area there is no such threshold. The wetted area grows steadily with increasing pressure because the higher droplet momentum at elevated pressures causes greater spreading upon impact.

These trends can be explained physically by the kinetic energy of the droplets. At lower pressures, the spray is characterized by larger droplets with insufficient kinetic energy to overcome the surface tension of the existing liquid layer. The impinging droplets pool together. This explains why the average film thickness is highest at 5 bar. The fuel lacks the radial momentum required to spread across the wall. With increased pressure droplets become more atomized and possess higher velocities. Upon impact, the kinetic energy is converted into spreading. This physical mechanism is clearly shown in the film area graphs, where the wetted surface grows substantially with pressure. The liquid film is stretched over a larger area and thus reduces the average thickness. Section 4.6.3 shows the visualization of the wall film for all simulations.

Film Thickness

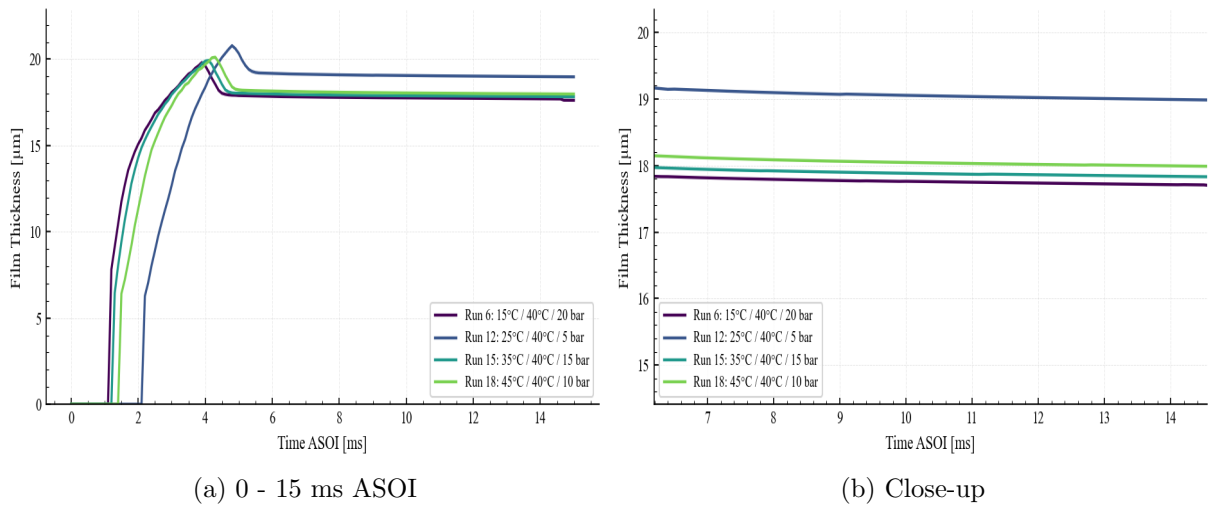


Figure 4.16: Average film thickness over time for four simulations at constant fuel temperature (40°C), illustrating the influence of different injection pressures.

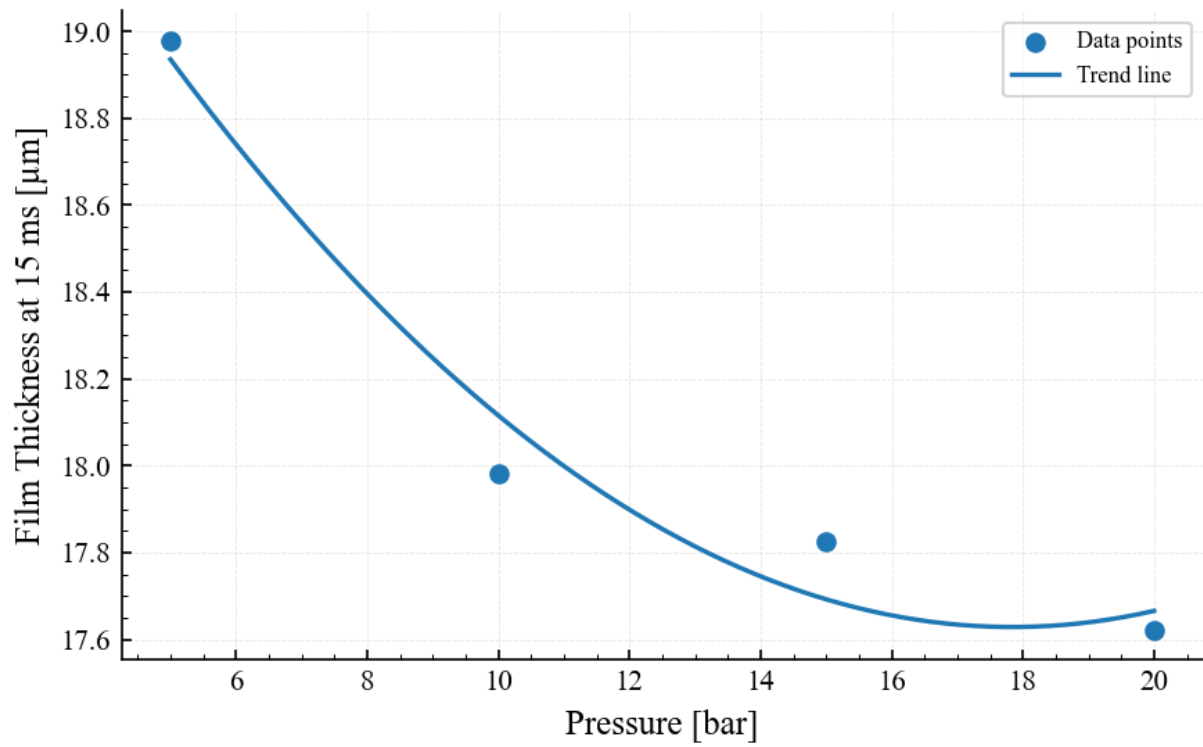


Figure 4.17: Trend in film thickness at 15 ms for increasing the injection pressure.

Film Area

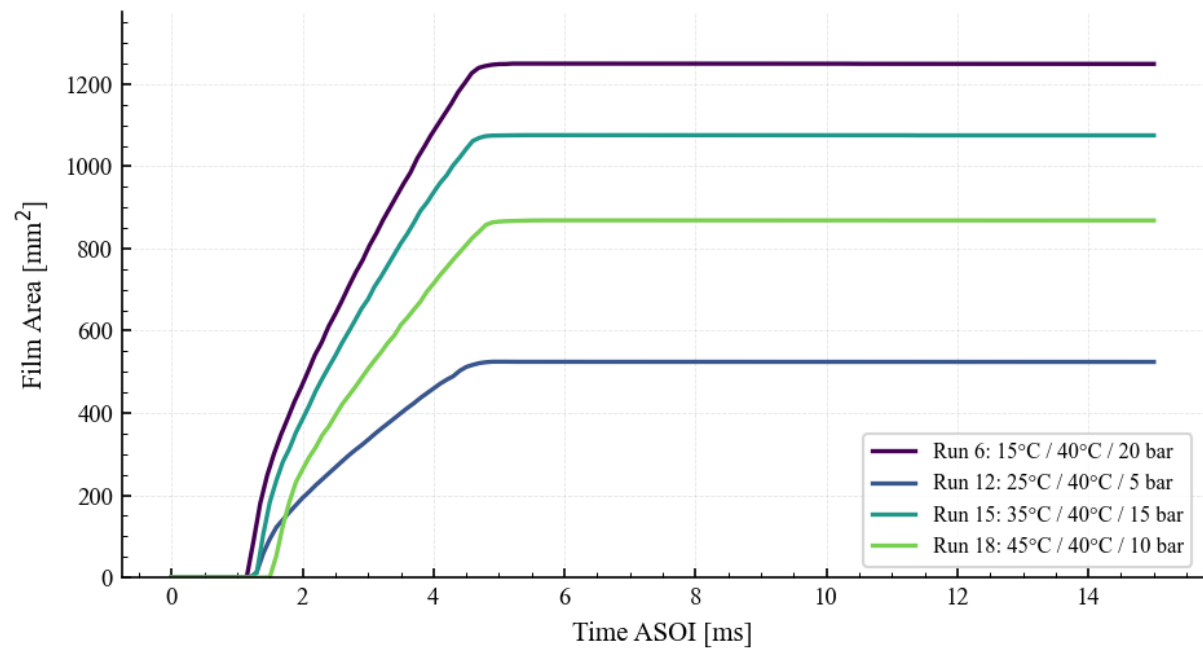


Figure 4.18: Film area over time showcasing influence injection pressure.

Film Mass

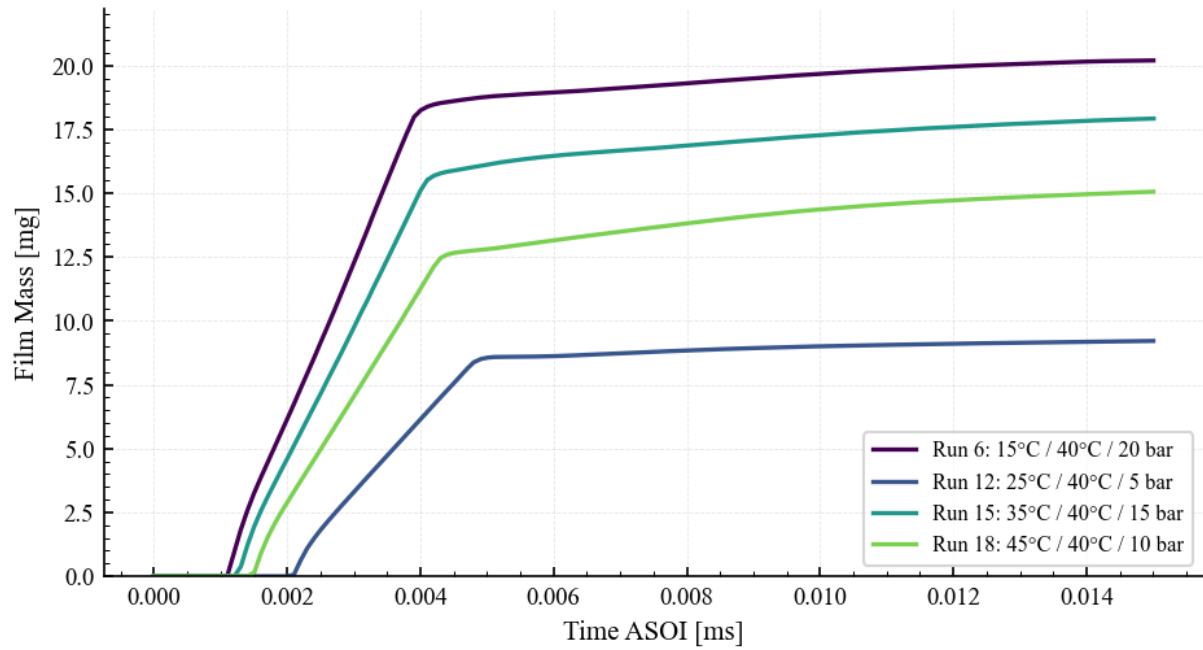


Figure 4.19: Film mass over time showcasing influence injection pressure.

Figure 4.19 shows an interesting behavior regarding the total film mass on the wall. From Run 1 to Run 4 the injection pressure is raised with 10 bar (from 5 bar to 15 bar). The results show that with this pressure increase the total accumulated film mass also increases. This observation is easily explained by the fact that when the injection pressure increases the total amount of fuel also increases as discussed in Section 4.4.

Therefore it is useful to look at the relative amount that sticks to the wall. Figure 4.21 shows the relative fraction that sticks to the wall for all simulated cases sorted in groups of pressure and increasing film temperature. From this graph it can be deduced that a different trend is visible. With increasing pressure the fraction that adheres to the wall increases initially going from 5 bar to 8 bar, and even to 10 bar. However, increasing the pressure even further cause the relative fraction of fuel that adheres to the wall to start decreasing. Therefore, while the reduction in film thickness becomes less pronounced above 10 bar, operating at higher pressures may still be beneficial if maximizing the amount of fuel delivery is the priority.

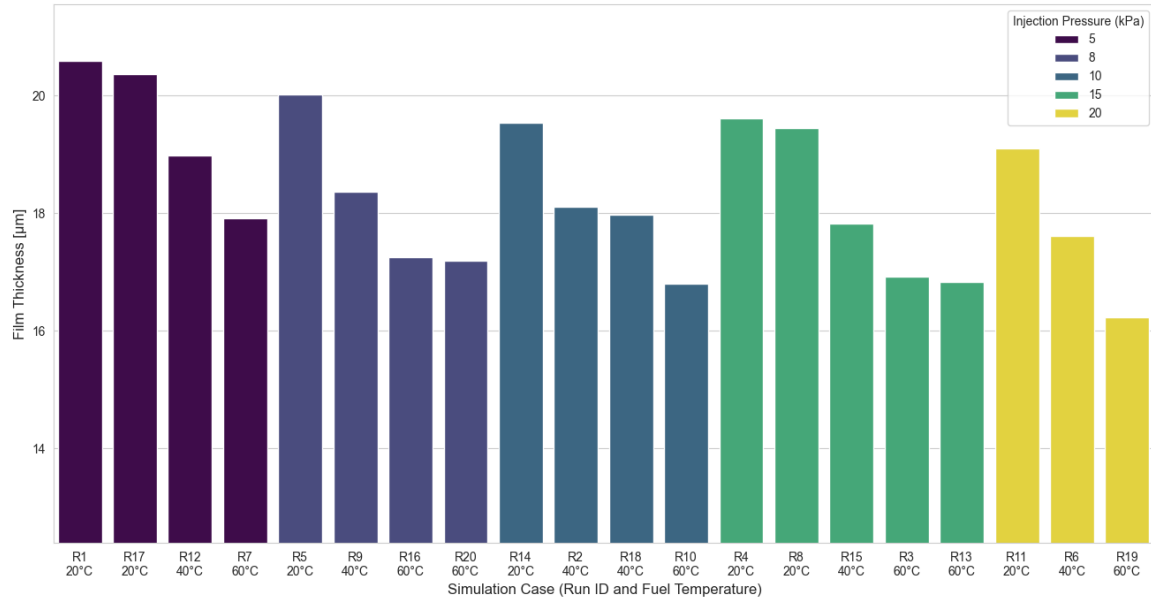


Figure 4.20: Bar chart of the simulated cases showing the methanol film thickness at 15 ms ASOI sorted by injection pressure and fuel temperature.

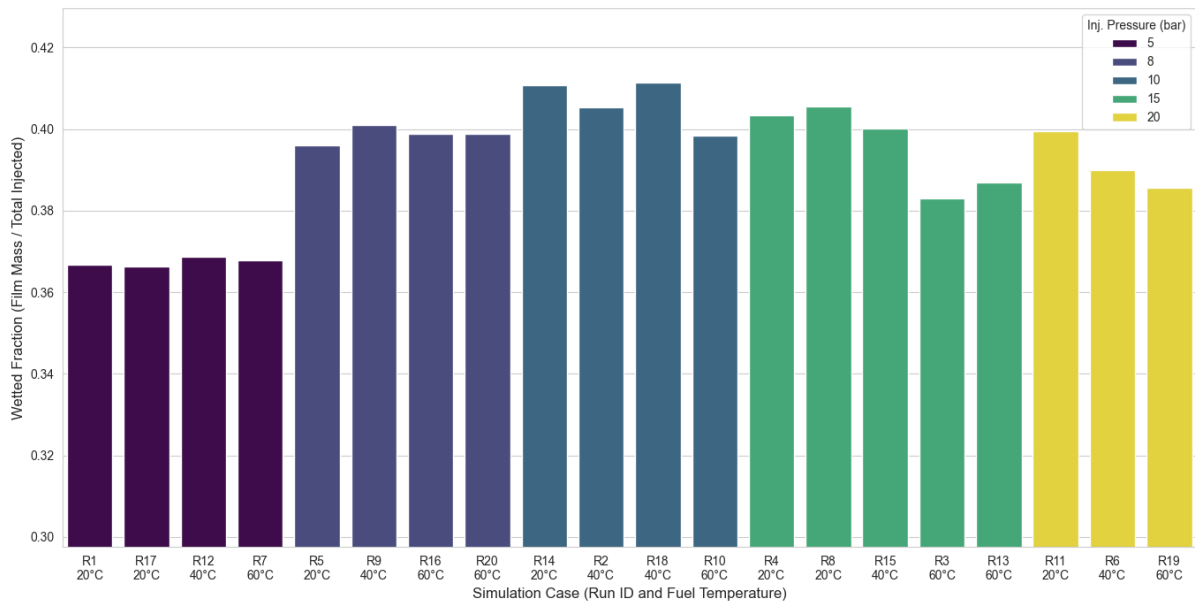


Figure 4.21: Bar chart of the simulated cases showing the normalized film mass methanol at 15 ms ASOI sorted by injection pressure and fuel temperature.

4.6 Interaction Analysis

Now that the individual parameter effects have been discussed, a more in depth analysis can be given of how the fuel temperature, ambient temperature, and injection pressure interact and dictate the wall film formation.

4.6.1 Spearman Correlation Matrix

To quantify the strength and direction of the relationship between input parameters and film characteristics, a Spearman rank correlation matrix was generated from the simulation results. A Spearman correlation matrix is a table that shows the strength and direction of monotonic relationships. It does not assume a linear relationship or normally distributed data. Instead, it is based on ranked values. The Spearman correlation coefficient, r_s is calculated by first ranking the data and then applying the formula in Equation 4.1. Where d_i is the difference between the ranks of each observation and n is the number of observations.

$$r_s = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)} \quad (4.1)$$

The value of the coefficient ranges from -1 to +1. A value of +1 means that as one variable increases, the other one also consistently increases. A value of -1 means that as one increases, the other consistently decreases.

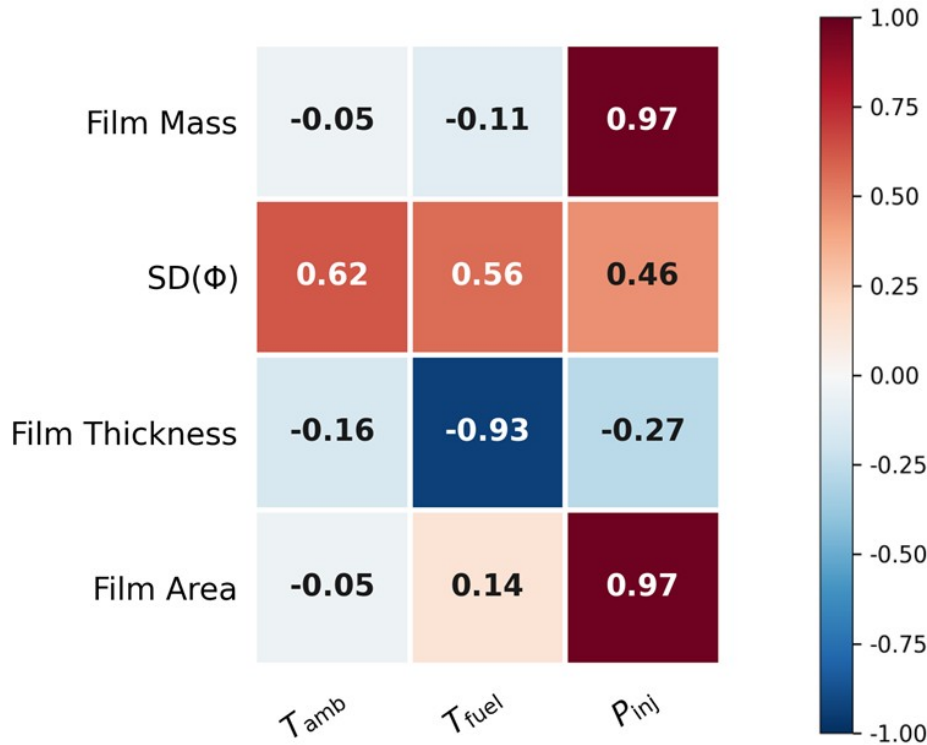


Figure 4.22: Spearman Correlation matrix

Because this thesis focuses on identifying general trends rather than estimating precise correlation coefficients, a smaller sample size is acceptable for the Spearman rank analysis. Previous research has shown that for strong correlations, a reliable Spearman analysis can be performed with sample sizes as low as 16–20 observations [79].

Figure 4.22 shows the Spearman correlation matrix for the 20 simulated cases. It uses the film area, the film thickness, the film mass, and the standard deviation of the equivalence ratio in the domain as output. For each parameter and each simulation the values at 15 ms ASOI are used. ϕ_{dev} is an indicator of localized fuel rich zones (in the gas phase). It is thus a metric of how well the evaporated fuel has been mixed with the air.

One of the strongest correlations in the entire matrix is the negative correlation between fuel temperature and film thickness. This verifies that fuel temperature is the dominant parameter controlling the average film thickness across the investigated operating space. Physically this may be explained by methanol’s high latent heat of vaporization. Warmer fuel carries more thermal energy from the start of injection. This can promote evaporation during injection and upon impingement, which results in a thinner overall deposited film. Secondly, the film with hot fuel spreads out further due to the reduction in viscosity. The matrix also confirms that the film area increases with fuel temperature. However this correlation with the film area is much weaker for increasing fuel temperature than for increasing pressure. So while the reduced viscosity of the fluid is indeed a correlation with the film area, the kinetic energy of the droplets is more influential for the wetted area.

The two other strong correlations observed, involve the injection pressure. While the average thickness decreases with increasing pressure, the total film mass and wetted area both increase strongly. The higher pressure injection deposits fuel over a larger surface area. This produces a film that spreads over a larger area but is thinner. With an increase in injection pressure also comes an increase in the total injected mass. This mass increase translate to an absolute increase in the film mass that adheres to the wall.

The ambient temperature consistently shows the weakest correlations across all output metrics. This statistically confirms that within the 5-45°C range, the ambient temperature is only a second order parameter for methanol’s wall wetting under PFI conditions.

The $SD(\phi)$ output parameter is the standard deviation of the equivalence ratio. This parameter can offer an interesting insight in the distribution of the vaporized methanol. Higher values indicate the presence of richer fuel vapor pockets within the domain. Even though this study did not focus on the homogeneity of the vapor mixture, this parameter may support the hypothesis in Section 4.5.3. In this study the absolute values do not have a significant meaning. However, it could be interesting to see how the input parameters influence the homogeneity of the gas mixture in the domain. The Spearman correlation shows that the increasing ambient temperature, the fuel temperature and the fuel pressure all increase the presence of rich gaseous zones. Interestingly, the ambient temperature has the strongest correlation. In contrast, the ambient temperature has only a weak influence on the average film thickness. This supports the observation that the ambient temperature does not significantly affect how much fuel deposits on the wall. However, it has a significant impact on where and how uniformly the evaporated fuel is distributed throughout the domain.

4.6.2 Fuel Temperature and Injection Pressure Compensation

The results discussed in Section 4.5.2 and Section 4.5.4 show that increasing fuel temperature and increasing fuel pressure both reduce film thickness, but through different mechanisms. Therefore, an interesting question to ask is whether it is possible to achieve the same film thickness at low pressure by raising the fuel temperature, and vice versa. To visualize this an iso-contour plot is made of the film thickness in the pressure-temperature space. Figure 4.23 presents a surface map of the film thickness at 15 ms ASOI across the fuel temperature and injection pressure parameter range.

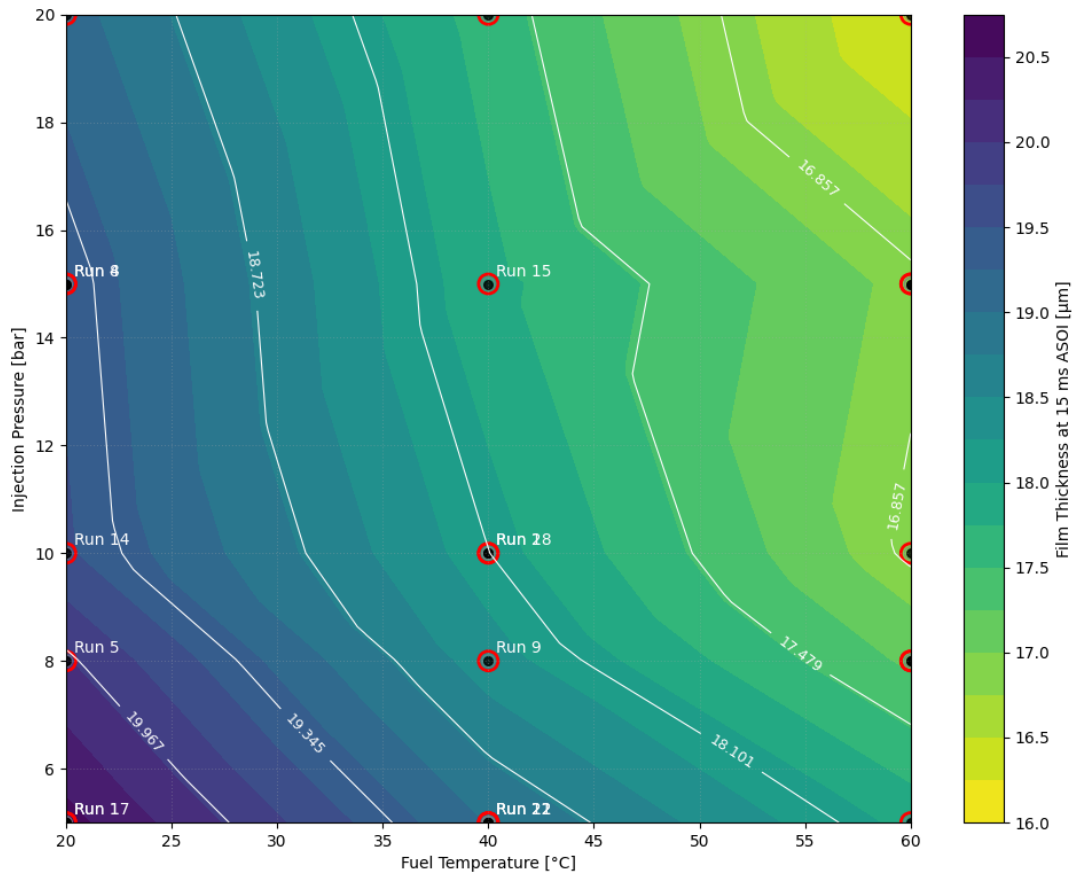


Figure 4.23: Iso-contours of the pressure-temperature space.

The contour lines run predominately vertically across the graph. This indicates visually what the Spearman Correlation showed mathematically, that increasing the fuel temperature is the dominant factor in reducing the film thickness. Moving from 20°C to 60°C fuel temperature introduces a reduction of 3-4 μm in film thickness across all pressure levels. The near-uniform pattern across all pressure levels and fuel temperatures shows the robustness of the fuel temperature effect.

By contrast, increasing the pressure produces a smaller but still visible reduction in the film thickness. The contour lines curve increasingly toward the low pressure region and are more closely spaced. This reinforces the trend from Figure 4.17. At lower pressures, an increase in pressure has a more pronounced effect than at already high pressures. In high-pressure regions, the contours become more vertical. This indicates that further pressure increases only result in limited additional improvement in film thinning.

The lower-left corner of the map corresponds to the thickest films in the data set. Figure 4.20 visualizes this in a bar chart that corresponds to Run 1 and Run 17. These simulations were carried out at the lowest injection pressure and fuel temperature of the entire simulation matrix. Both factors simultaneously contribute to poor atomization and limited evaporation, which leads to maximum wall-film accumulation. The upper-left corner of the map in Figure 4.23 shows the simulations at high injection pressure and low temperature. There the film thickness lies in the region of 19 μm . At high injection pressures, more fuel is injected. However, the better atomization of high injection pressure does not increase evaporation enough to compensate for the increased fuel amount, so more fuel ends up as a film.

The iso-contour lines reveals that the combinations of fuel temperature and injection pressure result in the same film thickness. These lines have a slightly negative slope, which indicates that a reduction in fuel temperature can partially be compensated by an increase in injection pressure to maintain the film thickness. The other way around, for a decrease in pressure it is always possible to compensate by increasing the fuel temperature within the studied range. For example, An injection at 20 bar with a 20°C fuel temperature can be replaced by an injection at 5 bar and 40°C.

Finally, the spatial distribution of the data points across the map is reasonably uniform, which is a direct consequence of the design of the simulation matrix using the dLHS method. However, the upper-right region exhibits some irregular contour curvature that is likely an artifact of interpolation rather than a genuine physical trend. This region should therefore be interpreted with caution.

4.6.3 Visualization of the Wall Film

This section provides a visual overview of all simulated cases for reference. Each simulation is represented at three timesteps (5, 10, and 15 ms ASOI) and illustrate the film area and film thickness. The color scale values are given in meters.

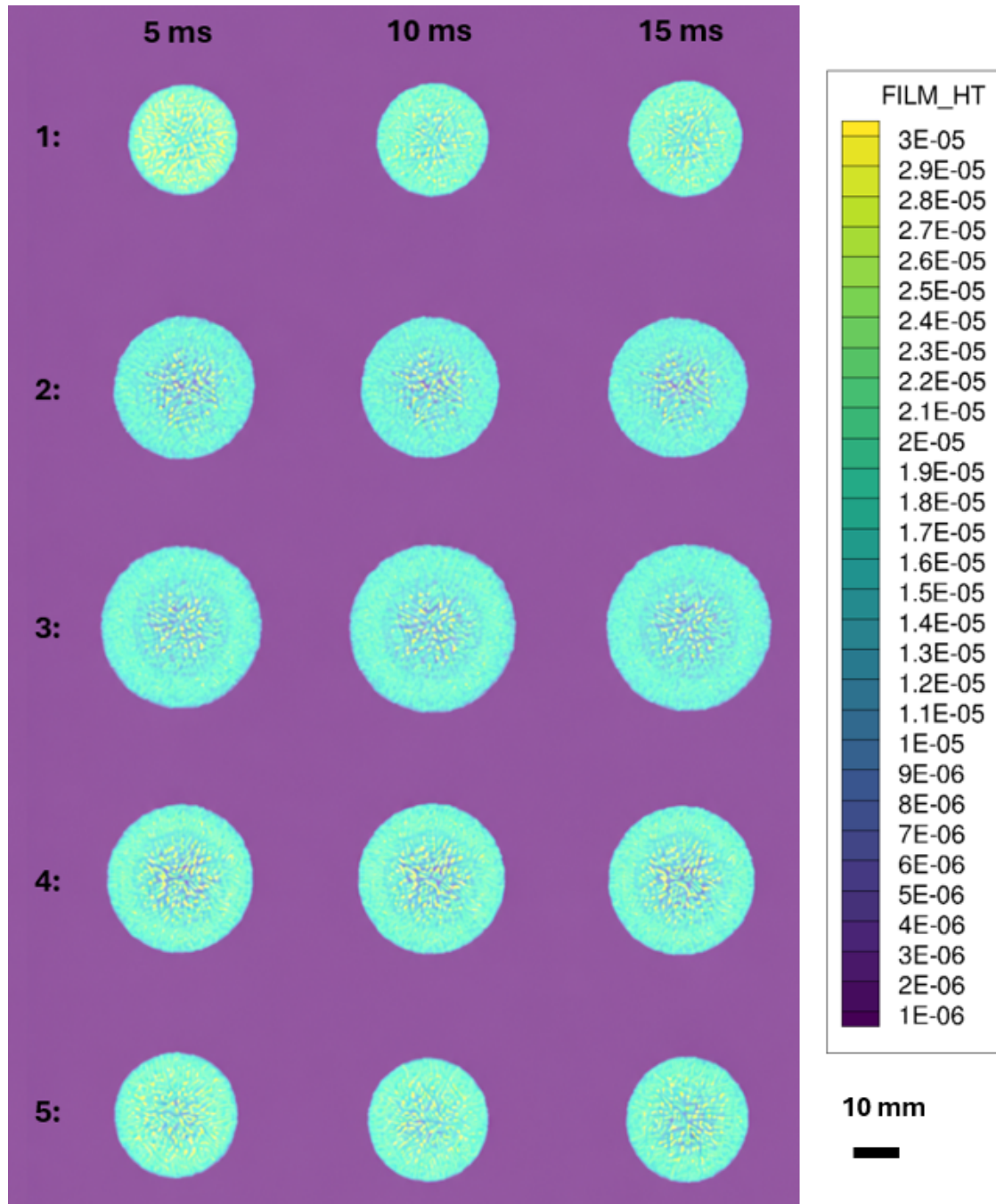


Figure 4.24: Visualization of the film thickness and area simulation 1 - 5.

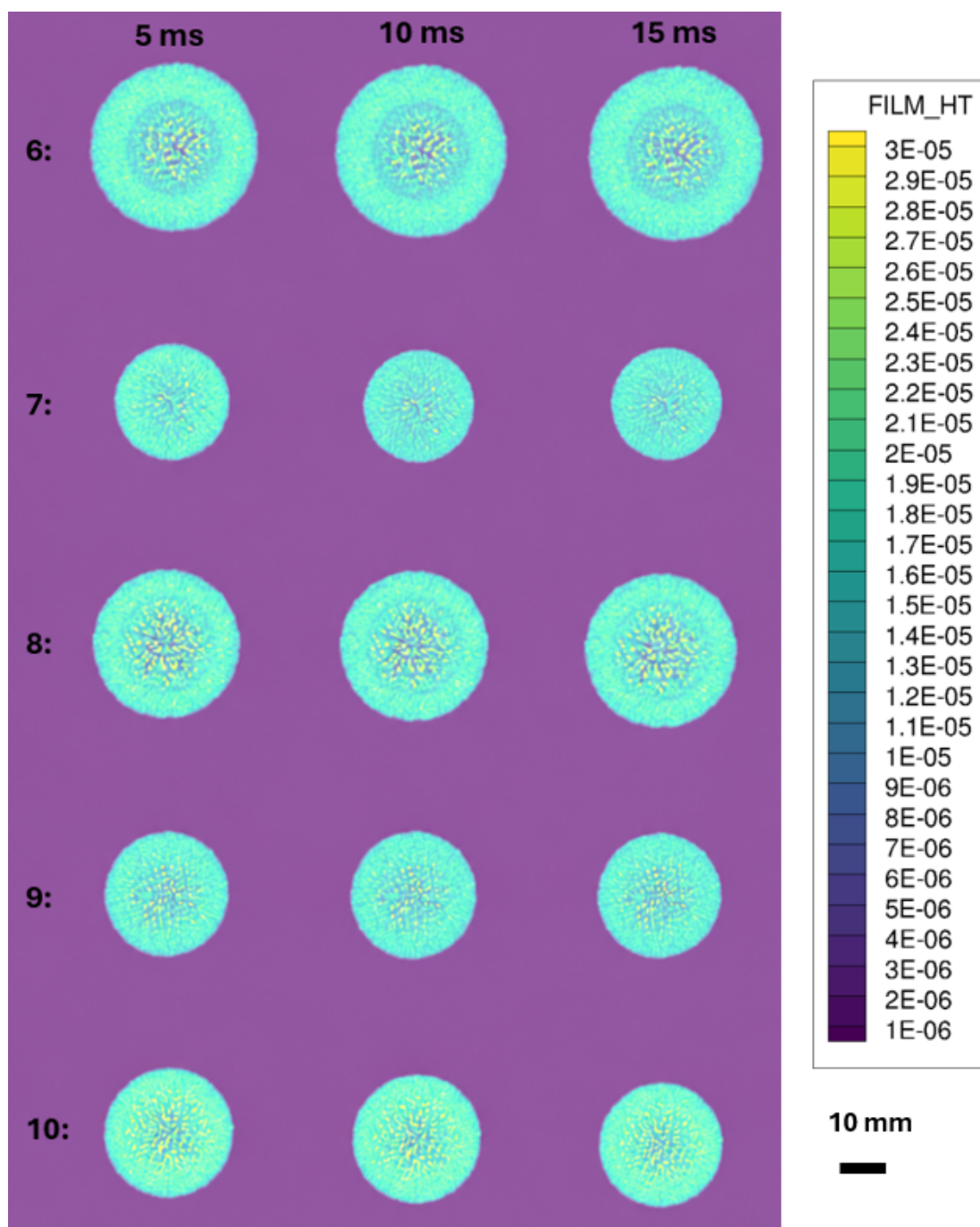


Figure 4.25: Visualization of the film thickness and area simulation 6 - 10.

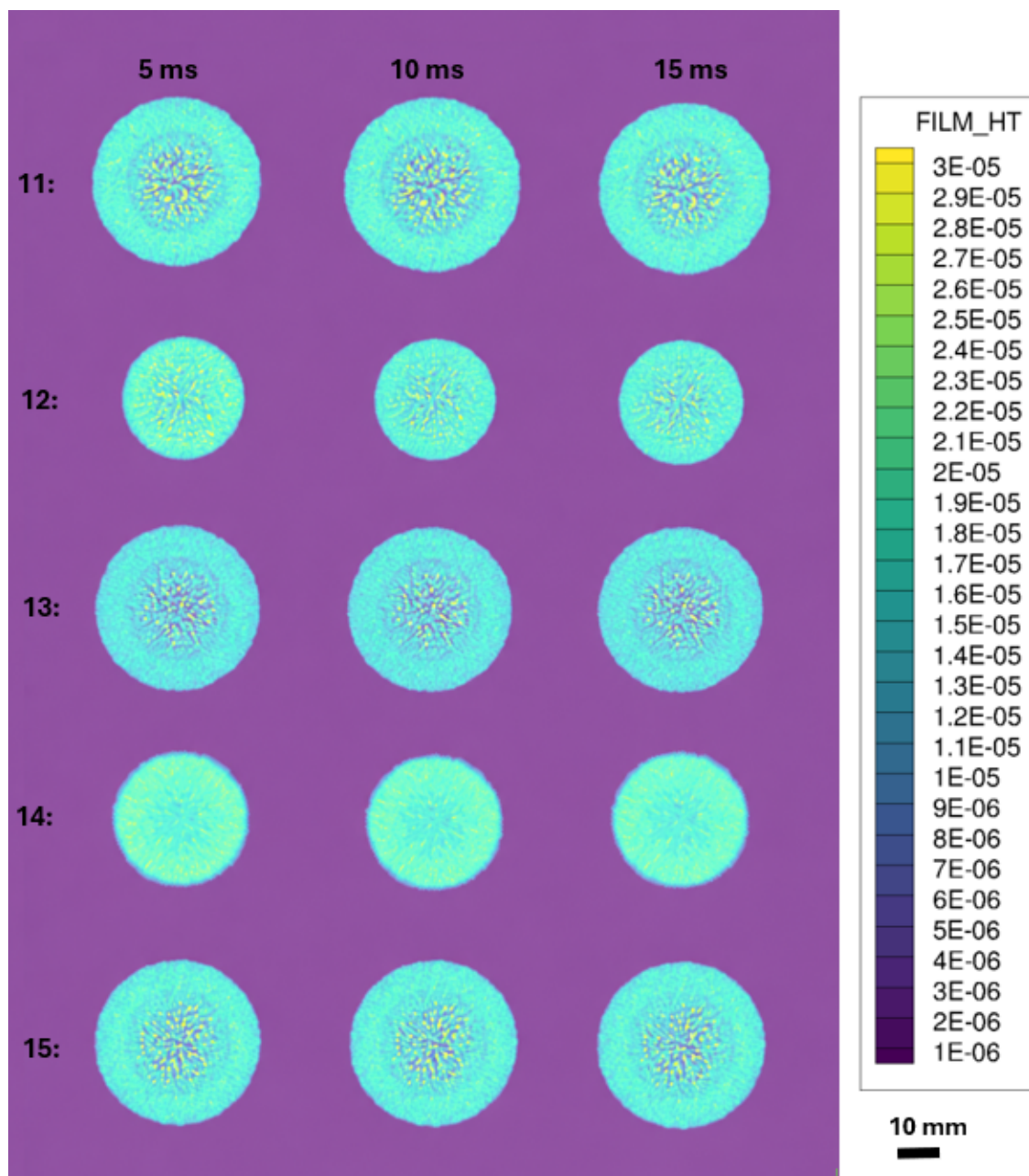


Figure 4.26: Visualization of the film thickness and area simulation 11 - 15.

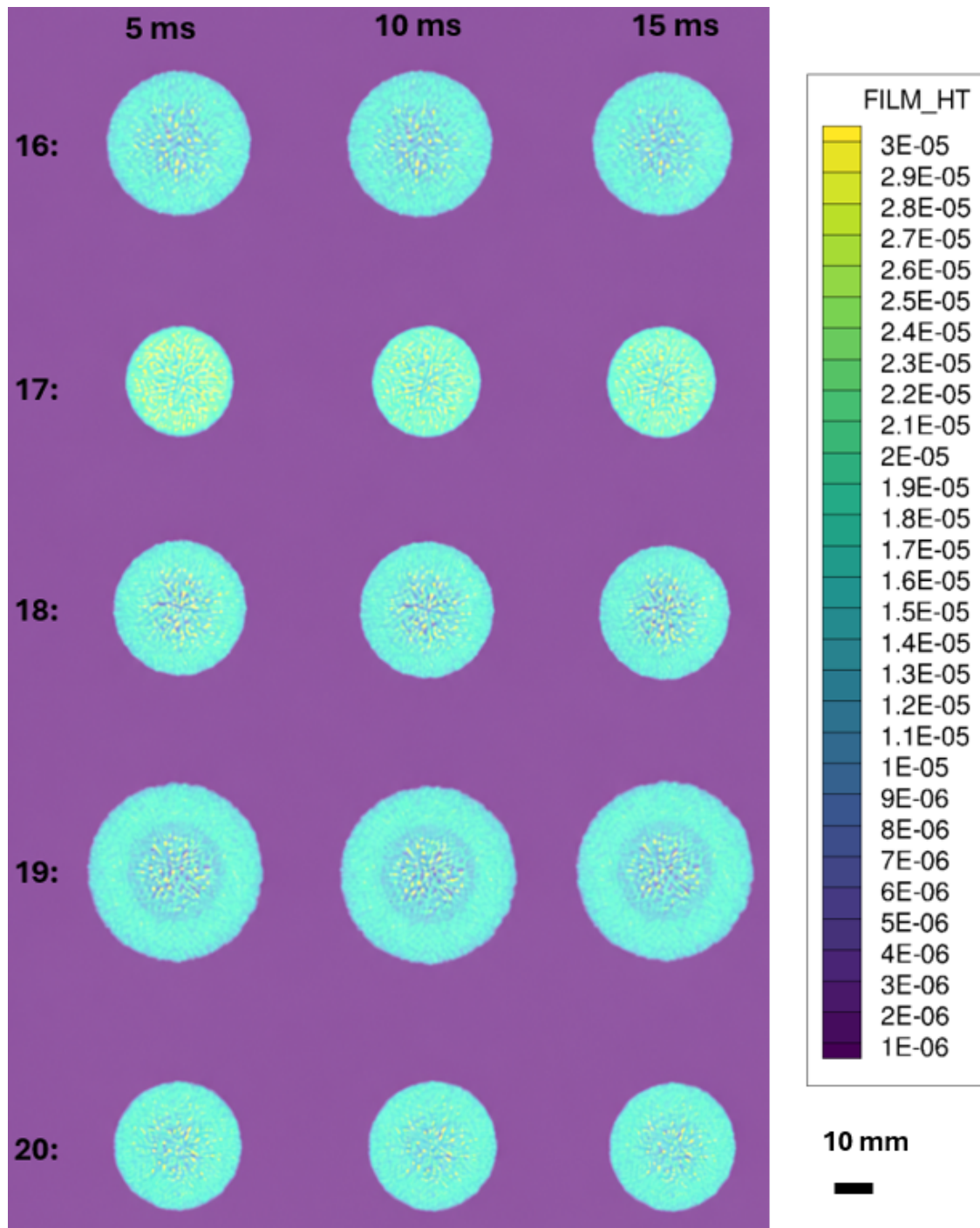


Figure 4.27: Visualization of the film thickness and area simulation 16 - 20.

4.7 Translation to Real Engine Design

While the above described analysis focuses on the methanol film formation on a frosted quartz glass disc, this section connects the findings to the more complex real PFI engine environments.

One of the strongest findings in the Spearman matrix is the strong correlation between fuel temperature and film thickness. This carries a direct implication for real engine design. In methanol PFI engines, active fuel preheating prior to injection could meaningfully reduce wall wetting without requiring fundamental changes to the injection hardware itself. This is particularly relevant during cold starts, where wall temperature and ambient temperature are at their lowest and wall wetting will therefore be the most severe. Excessive wall wetting during cold start is a known contributor to unburned hydrocarbon emissions and poor combustion efficiency in the first engine cycles [80].

The pressure analysis in Section 4.5.4 revealed a non-linear relationship between the injection pressure and the film thickness. Furthermore, it was observed that there is a threshold region for the fuel fraction that sticks to the wall. First, with increasing pressure, the fraction of fuel that adheres to the wall increases. Increasing the injection pressure above 10 bar stabilizes and even slightly decreases this fuel fraction. This can suggest that the zone of 5-10 bar may be an unfavorable operating window in engine calibration. Operating either below this range where less fuel is injected overall, or above it where improved atomization begins to offset the greater fuel mass, may result in less wall wetting. Higher injection pressure also results in a larger film area. In a real engine, this matters because the port geometry can be complex. A more distributed film improves fuel evaporation, air-fuel mixing, and combustion efficiency.

The findings in this study indicate that ambient temperature has an almost negligible influence on wall film formation for methanol injection. This is a significant difference from gasoline and diesel spray dynamics. In gasoline engines, an increase in the ambient temperature correlates with a noticeable reduction in wall wetting [75]. Furthermore, the temperature sensitivity of emissions in gasoline engines has been well documented. Recent studies, show that lower ambient temperatures can cause emission increases ranging from 14% to 284 % [81]. The relative insensitivity of methanol wall wetting to ambient temperature is likely rooted in methanol's exceptionally high latent heat of vaporization. This could suggest that increasing the intake air temperature may be less effective for improving overall engine operation than it is in gasoline engines.

The simulation study in this thesis has adopted simplifications which are also important to take into account in the translation to real engine design.

The first difference between the numerical setup and a real intake port is the wall material that was used in this study. The simulation uses quartz glass to match the experimental validation setup. However, quartz glass has very different thermal properties from stainless steel intake ports, such as lower thermal conductivity and lower thermal diffusivity. In a real engine, the intake runner walls conduct heat more rapidly, which will cause the wall temperature to be more dynamic and influence the film evolution. The change to aluminum alloy walls could therefore change the trends and how the investigated parameters influence film formation.

Secondly, in a real PFI engine, the intake port has a strong airflow during the intake stroke. This airflow has two important effects that the model in this study does not capture. First, the aerodynamic drag on the spray will change the trajectory of the droplets and influence their interaction with the wall. Second, the airflow over the wall film will influence the convective behavior of the film.

Next, the geometry is also simplified to an injector perpendicular to a flat plate. In a real engine, the injector is positioned at a certain angle and directed at a three dimensional port geometry with curved walls and valves. The position (closer or further from hot regions) and the angle of the injection will also drastically determine the outcome of the wall wetting film. However, even though the absolute value and shape of the film may strongly vary, the trends observed in this study remain physically meaningful.

Finally, this study only simulates the results of a single injection over the duration of 15 ms. In a real engine, multiple injection cycles follow one another, determined by the engine speed. The residual film from one cycle serves as the initial conditions for the next. Over multiple cycles, the film will behave differently from this single injection study.

Chapter 5

Conclusions

International regulations push the maritime sector towards more sustainable operation. Methanol is a promising alternative fuel, but its high latent heat of vaporization and low volatility lead to significant wall wetting in port fuel injection systems.

This thesis successfully implemented and validated a CFD-based framework in CONVERGE v5.0 for simulating methanol wall wetting under PFI conditions. The model was validated against the experiments by Zhang et al. [36]. The validation study highlighted, not only the model limitations, but also revealed the limitations of the experimental RIM method. A systematic DoE study was conducted to investigate the influence of fuel temperature, ambient temperature, and injection pressure on methanol wall film characteristics. This chapter summarizes the key findings, evaluates the strengths and limitations of the model, and proposes directions for future work.

5.1 Model Strengths and Weaknesses

The validation study showed that the numerical model successfully captures the experimentally observed trends with respect to the injection pressure. Secondly, the experimental trend of decreasing film thickness is also noticeable when the wall temperature is increased from 293 K to 373 K. However, at high temperatures, the model predicts stronger evaporation than observed in the experiment. The possible limitations of the numerical model can be summarized as follows:

- Spray-wall interaction and surface roughness modeling: the Bai-Gosman model relies on empirical regime criteria that may not be fully calibrated for methanol-specific splashing behavior. It is also possible that the unresolved wall roughness has an effect on the resulting liquid film.
- Conjugate heat transfer modeling with quartz glass: the simplified material properties and limited thermal coupling can lead to an overestimation of heat flux into the liquid film and thus cause excessive evaporation.
- Lagrangian wall film representation, in which the discretized film edge limits the resolution of continuous film spreading and evaporation near the contact line.

It was also noted that using the RIM technique to measure fuel wall wetting may not be fully reliable. The reported measurements from this technique severely underestimate the film thickness and adhered mass.

5.2 Key Findings

The main goal of this study was to find which operating parameters strongly influence wall wetting for methanol injection. The first parameter examined was the ambient temperature. The results indicate that this parameter has minimal influence on film formation, in contrast with the behavior observed for gasoline sprays. Compared to the fuel temperature, the influence of the ambient temperature on the film thickness was negligible. The film area and mass were even less influenced by the ambient temperature, especially at pressures above 8 bar.

On the other hand, the fuel temperature was a dominant factor. Higher fuel temperatures showed a reduction in the film thickness (about 3-4 μm) while increasing the wetted area. This area increase can be attributed to the wider spreading of the film due to lower viscosity and surface tension at higher fuel temperatures. It can thus be concluded that it is not the relative difference between ambient and fuel temperature but the absolute value of the fuel temperature that will significantly influence the wall wetting outcome.

The last input parameter that was systematically varied, the injection pressure, showed similar trends to the fuel temperature. With increasing pressure the film thickness decreases, but not linearly. Beyond 10 bar, the rate of thickness reduction diminishes. However, an interesting observation was made regarding the relative fraction of the injected mass. The results showed that increasing the injection pressure from 5-10 bar introduced an increase in the fraction that adhered to the wall. Beyond 10 bar, this effect is reversed.

The statistical importance of the input parameters was examined using the Spearman correlation matrix. It was noted that the injection pressure had the strongest positive correlation on the film area and film mass. Meaning that with increasing pressure the film area and film mass increased strongly. The film thickness is mostly influenced by the fuel temperature. And the correlations of the ambient temperature emphasized that this was only a secondary parameter and has very little influence. Following this correlation, it was examined if it was possible to achieve the same film thickness at low pressure by raising fuel temperature, and vice versa. The iso-contour of the pressure and temperature space revealed that a reduction in fuel temperature can partially be compensated by an increase in injection pressure to maintain the film thickness. The other way around, for a decrease in pressure it is always possible to compensate for the reduced film thickness by increasing the fuel temperature in the examined range.

From these findings, useful elements can be translated to real engine design. The pressure analysis showed that there is a fuel pressure threshold between 10 bar and 15 bar where the film thickness reduction diminishes and the fuel fraction that adhered to the wall stabilizes. This suggests that for real engine design it may not be necessary to increase injection pressure beyond this threshold. Furthermore, the limited influence of the ambient temperature highlights the implications of methanol's high latent heat of vaporization compared to traditional gasoline engines.

However the model simplifications introduced limits to the direct translation to real engine design. The first and foremost limitation is the simplified geometry and use of the quartz wall. The thermal behavior and geometrical shape of this quartz wall will likely have a significant influence on the film formation. This is not taken into account in this study. The model also did not include any airflow as present in a real engine intake port.

5.3 Recommendations for Future Work

This thesis does not only gives more insight into the wall wetting phenomena of methanol, it also provides directions for future studies. During the validation study, it was clear that there are scarce validated or calibrated numerical models for methanol injection. In particular, the Bai-Gosman model, warrants further investigation to determine the threshold values for methanol specific droplet impingement.

The wall temperature analysis highlighted the fact that the coupling between the heat transfer of the wall and the fuel is a critical part in predicting wall wetting. Therefore, future studies should focus on implementing more realistic wall properties as well as better heat transfer coupling. This thesis focused on a single injection in a simple geometry. Future studies should focus on multi-cycle simulations in more realistic geometries to improve the understanding of methanol film formation under PFI conditions.

Finally, this study also highlights the need for more reliable experimental measurements of methanol wall wetting. The limited availability of validated data for low pressure methanol injection is also a limiting factor in the numerical studies. Addressing this gap will be essential for unlocking the full potential of methanol as a sustainable marine fuel.

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Appendix A

Resulting Film Parameters

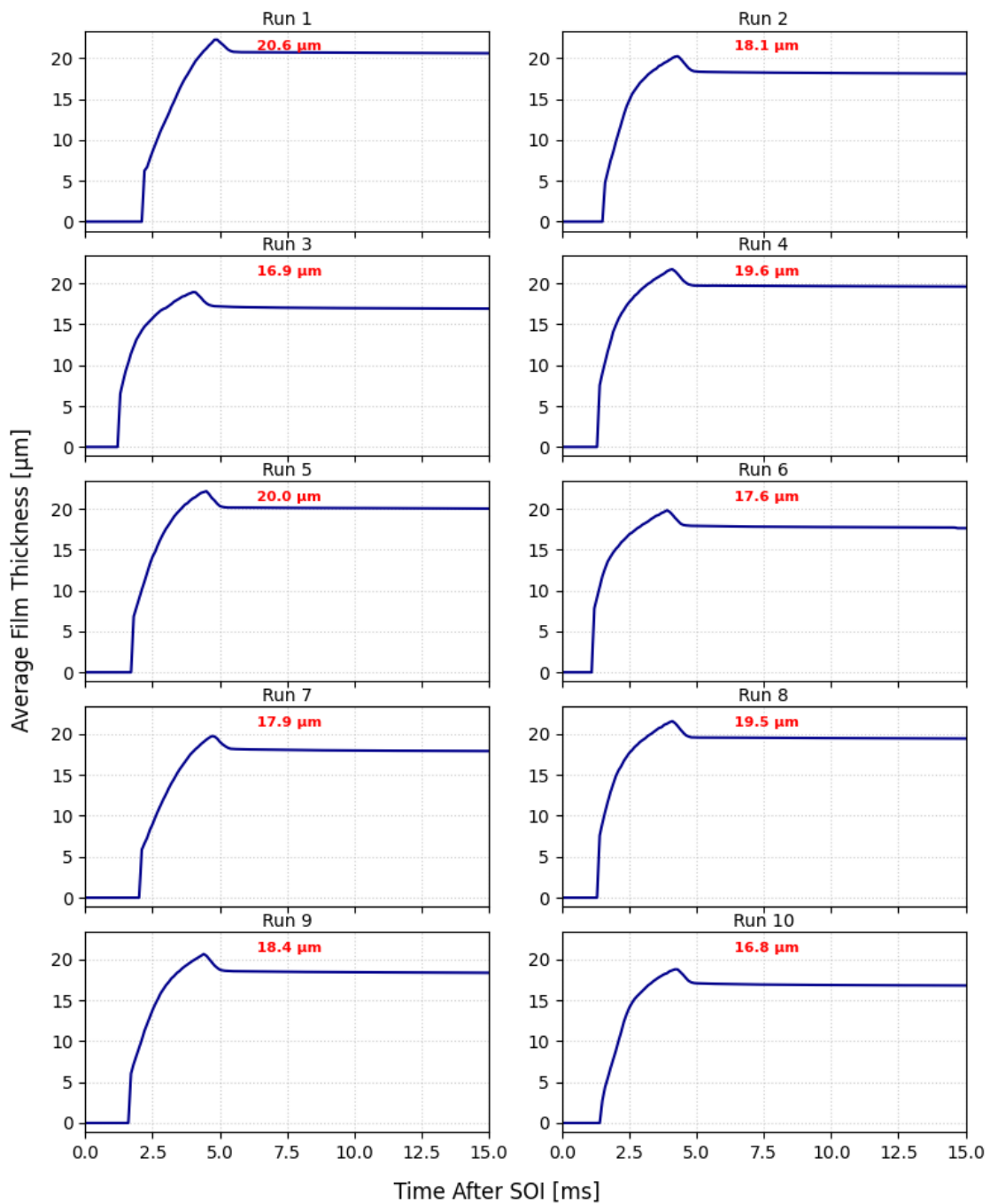


Figure A.1: Average film thickness over time run 1 - 10.

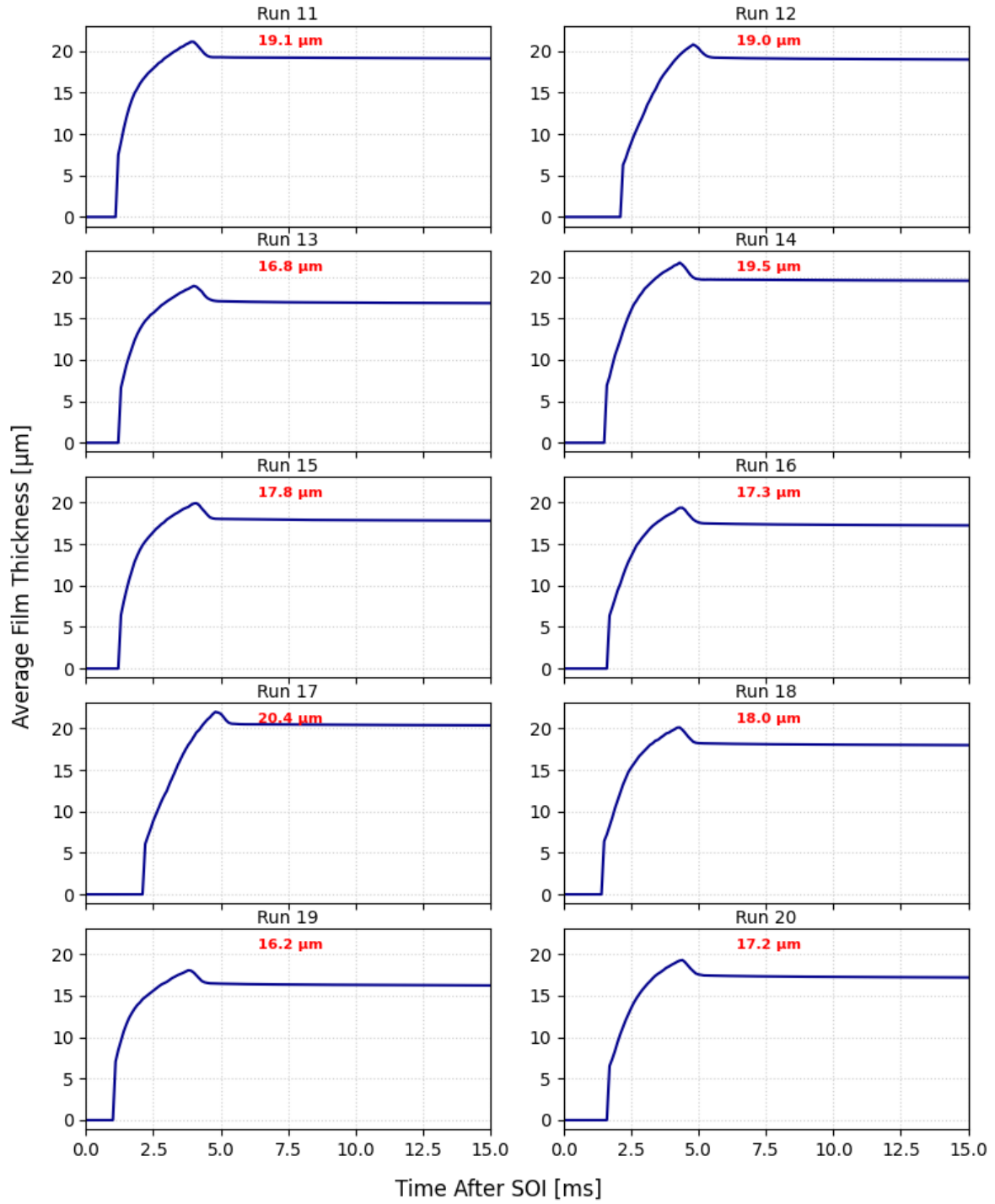


Figure A.2: Average film thickness over time run 11 - 20.

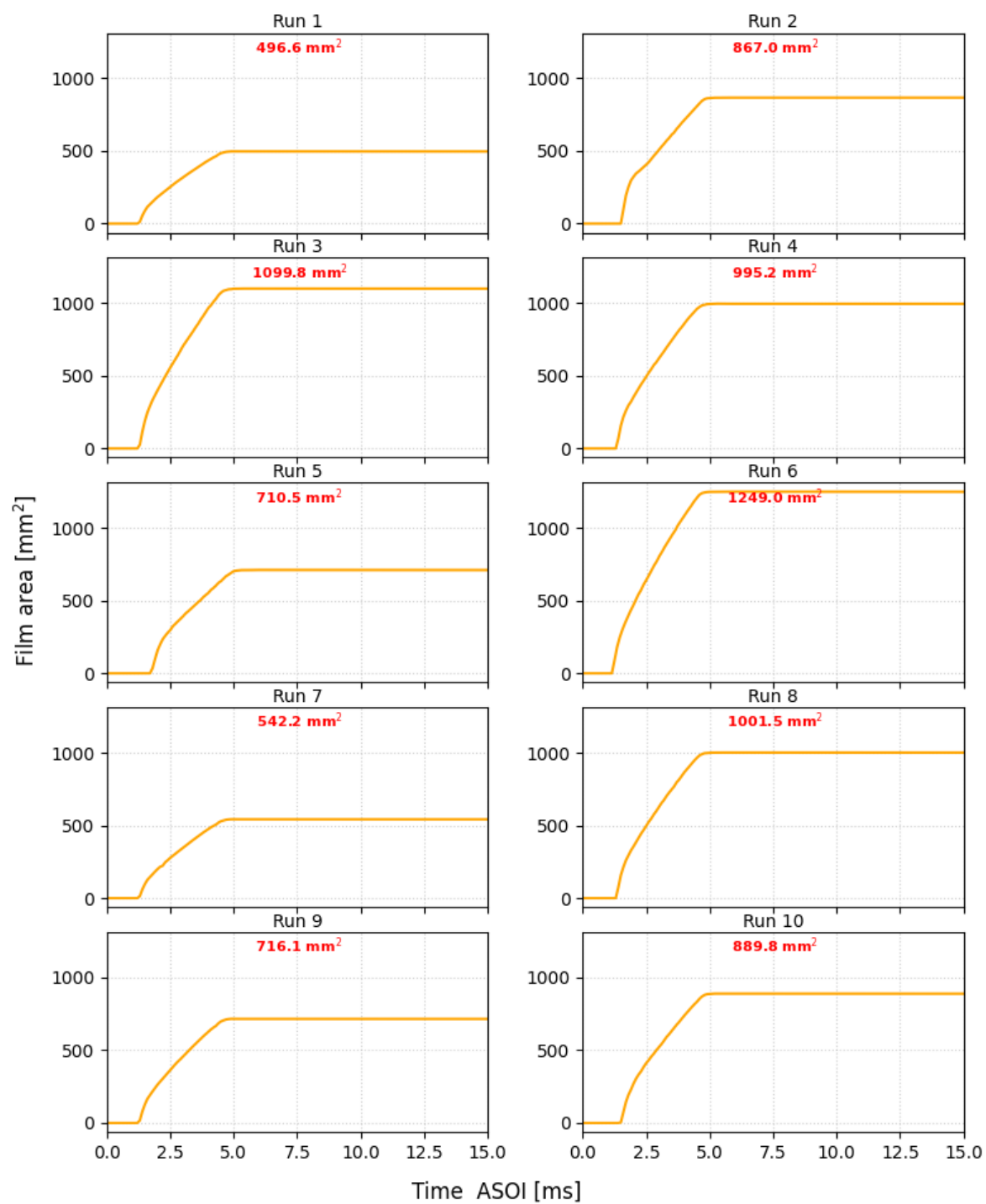


Figure A.3: Average film area over time run 1 - 10.

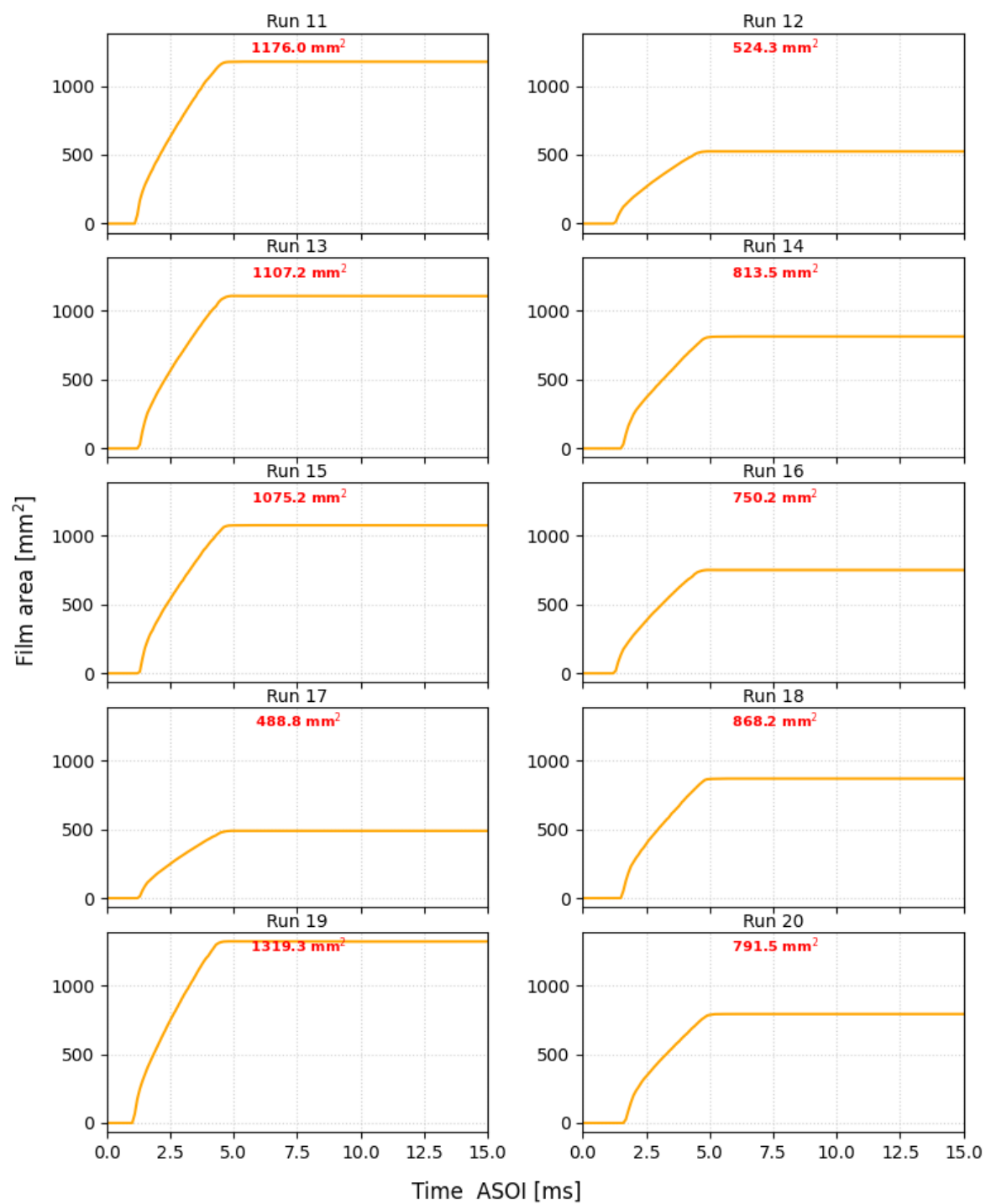


Figure A.4: Average film area over time run 11 - 20.

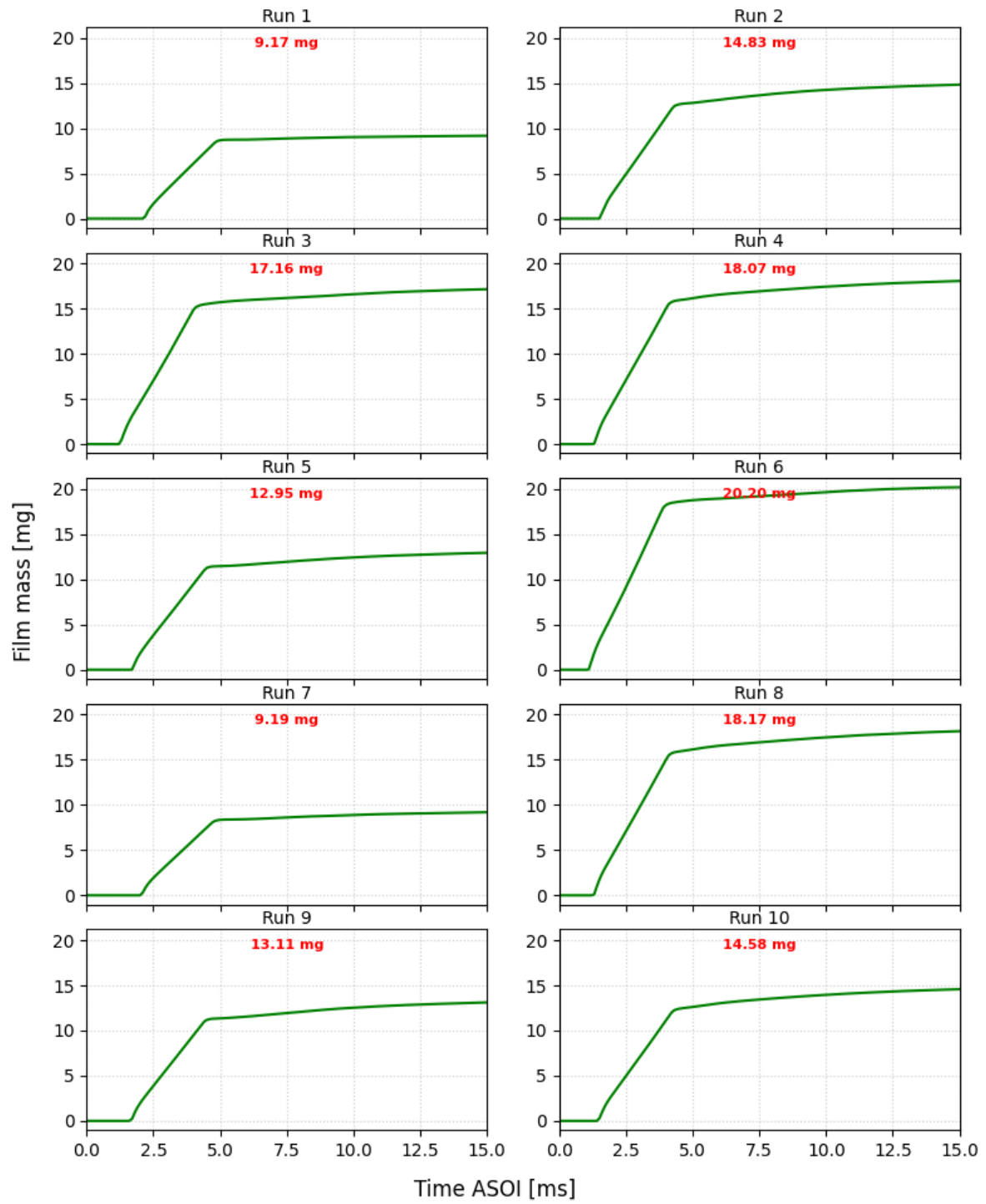


Figure A.5: Average film mass over time run 1 - 10.

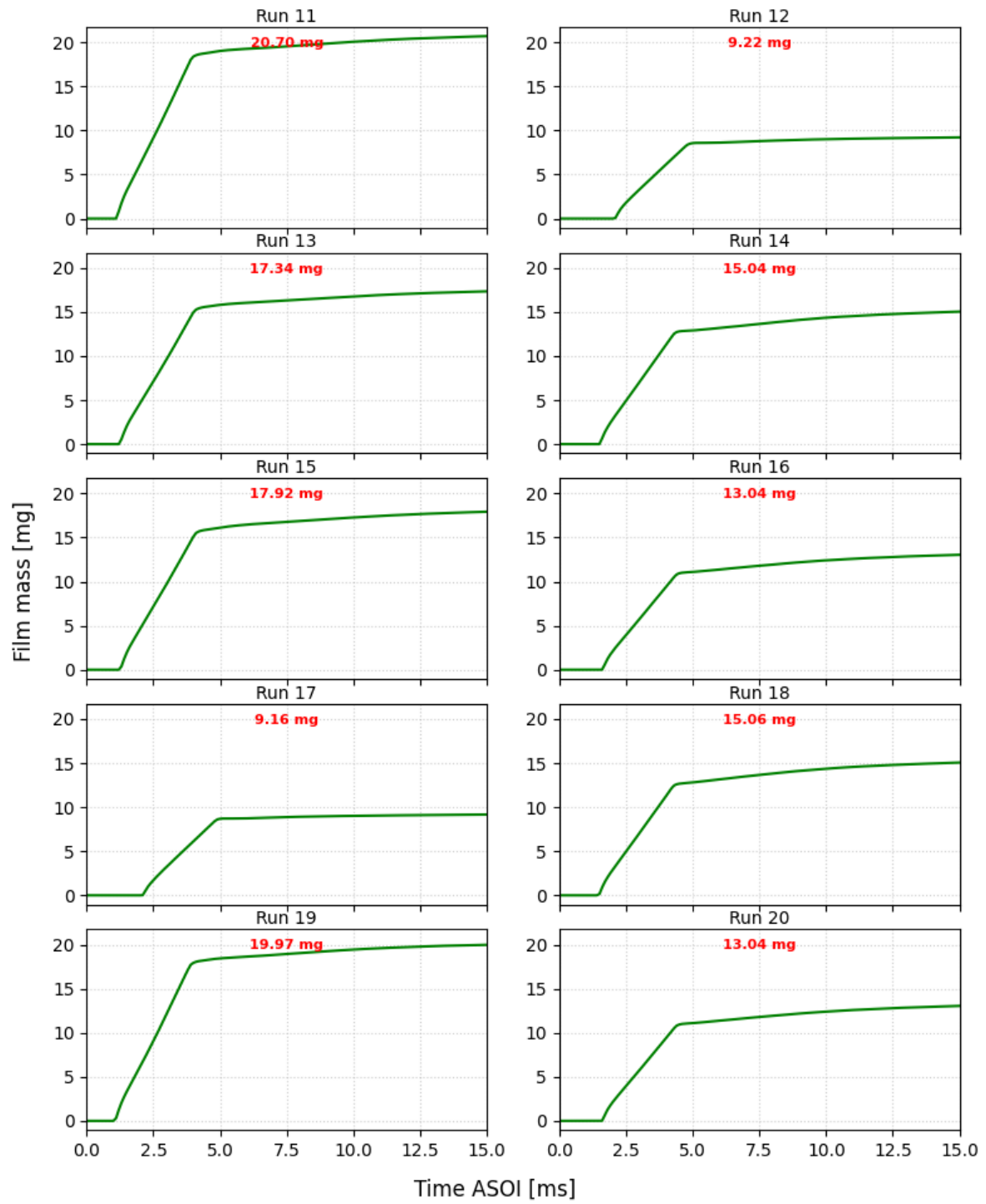


Figure A.6: Average film mass over time run 11 - 20.

