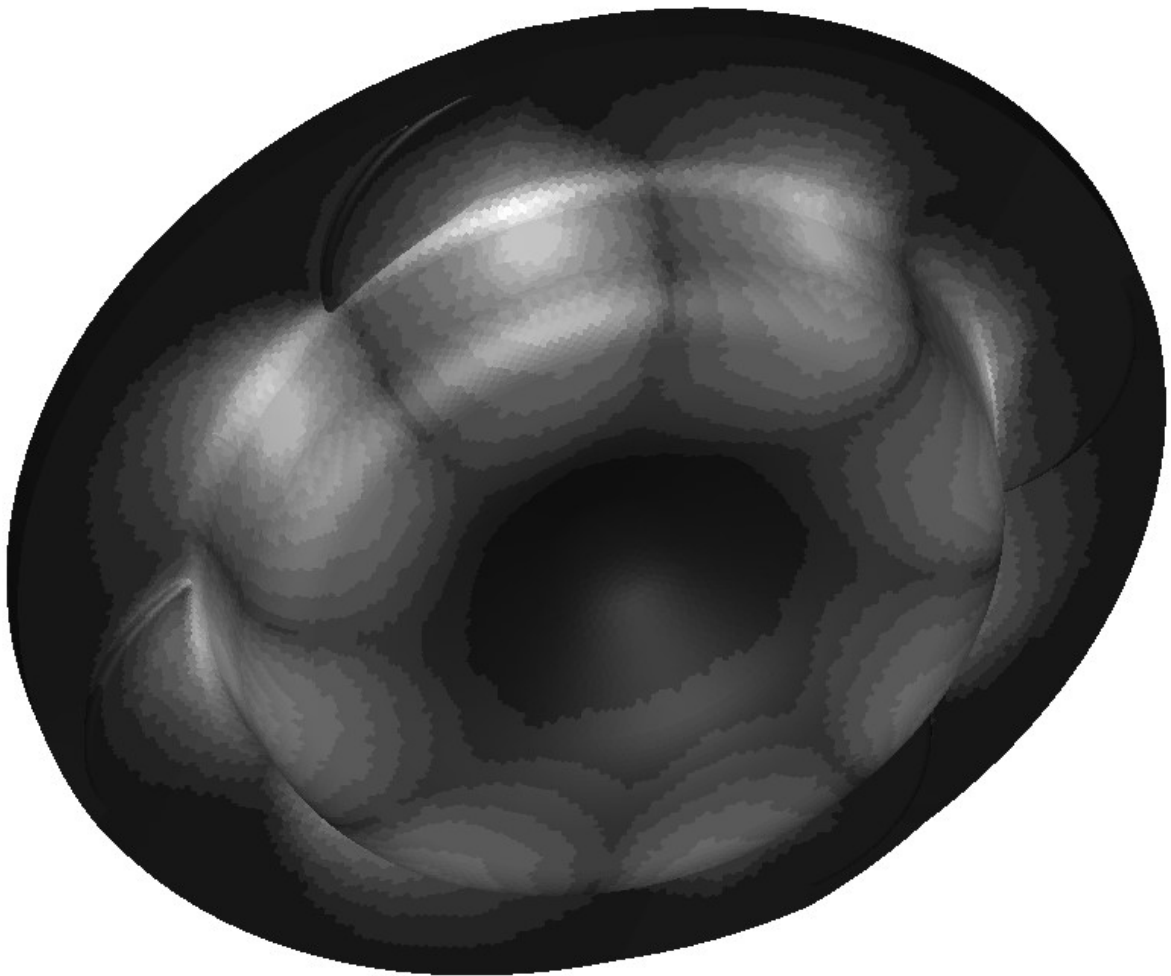




Final report

Efficient Diesel – combustion chamber insulation for improved Diesel efficiency





Date: 12.11.2019

Town: Zürich

Publisher:

Swiss Federal Office of Energy SFOE
Combustion Research Programme
CH-3003 Bern
www.bfe.admin.ch

Co-financed by:

CORNET/FVV Project "Efficient Diesel"

Agent:

ETH Zürich
Institut für Energietechnik
Laboratorium für Aerothermochemie und Verbrennungssysteme
Sonneggstrasse 3
CH-8092 Zürich
<http://www.lav.ethz.ch/>

Authors:

Dr. Karri Keskinen, Aerothermochemistry and combustion systems laboratory, ETH Zürich,
keskinen@lav.mavt.ethz.ch
Dr. Walter Vera-Tudela, Aerothermochemistry and combustion systems laboratory, ETH Zürich,
wveratudela@lav.mavt.ethz.ch
Dr. Sushant Pandurangi, Aerothermochemistry and combustion systems laboratory, ETH Zürich,
sushpa@lav.mavt.ethz.ch
Dr. Yuri M. Wright, Aerothermochemistry and combustion systems laboratory, ETH Zürich,
wright@lav.mavt.ethz.ch
Prof. Konstantinos Boulouchos, Aerothermochemistry and combustion systems laboratory, ETH
Zürich, boulouchos@lav.mavt.ethz.ch

SFOE head of domain: Dr. Carina Alles, Carina.Alles@bfe.admin.ch

SFOE programme manager: Stephan Renz, info@renzconsulting.ch

SFOE contract number: SI/501606-01

The author of this report bears the entire responsibility for the content and for the conclusions drawn therefrom.

Swiss Federal Office of Energy SFOE

Mühlestrasse 4, CH-3063 Ittigen; postal address: CH-3003 Bern
Phone +41 58 462 56 11 · Fax +41 58 463 25 00 · contact@bfe.admin.ch · www.bfe.admin.ch



Zusammenfassung

In diesem Projekt werden Verfahren zur Minderung von Wärmeverlusten in dieselmotorischen Brennräumen untersucht. Im Speziellen wurden sogenannte «thermal swing materials» untersucht, deren Temperatur der Brennraumtemperatur folgt um die Temperaturdifferenz zu verringern. An der ETH Zürich wurde auf die folgenden Punkte fokussiert: (i) Identifikation geeigneter Materialcharakteristiken der Beschichtungen, (ii) Grundlagenversuche in der optisch zugänglichen Hochtemperatur-Hochdruck-Zelle (HTDZ) inkl. Wärmestrommessungen, (iii) 3D CFD Berechnungen für die Zelle sowie für einen PKW Dieselmotor, für welchen an der TU Berlin Messungen durchgeführt wurden. Das Fraunhofer IPK führte Beschichtungen der Proben und Charakterisierung der verwendeten Materialien sowie Oberflächenbeschaffenheiten durch. Die Ergebnisse zeigen, dass «thermal swing» Beschichtungen Potential aufweisen, um Wandwärmeverluste zu verringern. Aufgrund von Nichtidealitäten der untersuchten Materialien kann das volle Reduktionspotential jedoch nicht realisiert werden. In der Zelle wurden Spray-Wandinteraktionen durch optische Verfahren untersucht und Wandwärmeströme gemessen, unterstützt durch numerische Inversionstechniken. Die 3D CFD wurde um aktuelle, in der Literatur dokumentierte Erkenntnisse (Messungen und DNS) ergänzt, um Effekte der Oberflächenrauigkeit abzubilden. Letztere spielt eine Schlüsselrolle und verhindert das Ausschöpfen der Wandwärmeübergangsreduktion. Aufgrund der hohen Oberflächenrauigkeiten waren zur korrekten Modellierung der Wandwärmeübergänge ausserdem Modifikationen der üblicherweise verwendeten Reynolds-Analogie notwendig. Im motorischen Kontext traten bei beschichteten Kolben sowohl in den Messungen an der TU Berlin als auch in den Simulationen an der ETH Unterschiede in den Brennverläufen zutage, welche den Wirkungsgrad negativ beeinflussten. Zukünftige Entwicklungen sollten nebst optimalen Beschichtungseigenschaften insbesondere auch glatte Oberflächen sicherstellen.

Summary

Methods to provide better diesel combustion chamber insulation are investigated in this project. The investigations focus specifically on capabilities of thermal swing materials, which aim to adapt to the temperature of the surrounding gas. The research task of ETH Zürich focuses on (i) determining suitable material characteristics for coatings, (ii) carrying out fundamental optical/heat flux experiments in a high pressure/temperature cell, and (iii) performing 3D CFD simulations for both the cell and an engine for which experiments are carried out in TU Berlin. Fraunhofer IPK carries out coating procedures and provides material and surface characterisations that are employed in both simulations and experiments. Results indicate that thermal swing coatings, here diagnosed primarily by examining a 130 µm porous zirconia coating, show potential for reducing engine heat losses. However, non-ideal factors present in the materials studied prevent the realisation of the full reduction potential. Spray-wall phenomena were examined through optical measurements, heat flux measurements and computational inverse techniques. 3D CFD models were implemented based on state-of-the-art literature (including experiments and direct numerical simulations) of rough-wall flows. It is found that surface roughness is a key non-ideal component that can mitigate the advantages that are gained through thermal swing. Moreover, modelling heat transfer requires modification of the widely adopted strong Reynolds analogy in the case of rough-wall flows. The present zirconia-coated results do not indicate lower instantaneous heat fluxes through walls. In the engine context, combustion phasing differences, noted in both ETH simulations and TU Berlin experiments, appears to be another important contributor to efficiency losses. The findings suggest that, in addition to favourable material properties, future work in coating development should focus on ensuring surface smoothness.



Contents

Zusammenfassung	3
Summary	3
Contents	4
List of abbreviations	6
Symbols	7
1 Diesel combustion chamber insulation: study background	8
1.1 Economic impact and significance for SMEs	8
1.2 Motivation for the investigations	9
1.3 Overview of project work packages	10
1.4 Objectives for work carried out at ETHZ	11
1.5 Synergy between work carried out by ETHZ and the other institutes	12
2 Research Methodology	13
2.1 Planned coating materials to be studied	13
2.2 Basics of heat transfer	14
2.3 WP1: Parameter study to define optimum material properties	17
2.4 WP3: Experimental characterisation of wall heat transfer for coated and uncoated pistons in an optically accessible high pressure and high temperature chamber	18
2.4.1 The high pressure and temperature cell	18
2.4.2 Precombustion and injection	18
2.4.3 Impingement plate and wall heat flux sensor	20
2.4.4 Optical diagnostics: broadband chemiluminescence & OH-chemiluminescence	21
2.4.5 Wall heat flux measurement: processing of coated results	24
2.5 WP4: 3D-CFD with Conjugate Heat Transfer	27
2.5.1 HTDZ: case setup, computational grids and workflow	28
2.5.2 Spray modelling and injector characterisation	30
2.5.3 Combustion modelling	31
2.5.4 Wall treatment	31
2.5.5 Rough wall modelling	33
2.5.6 OM651 computational grid, workflow and case setup	37
3 Results	38
3.1 Computational characterisation of applicable materials	38
3.1.1 1-D CHT simulations to assess insulation materials and configurations	38
3.1.2 Examining the validity of the 1-D CHT assumption in engine conditions	40
3.2 Heat transfer experiments in the high pressure and temperature cell	41
3.2.1 Spray morphology: broadband chemiluminescence	41



3.2.2	Wall heat flux measurements: uncoated case	43
3.2.3	Wall heat flux measurements: coated case	48
3.3	Heat transfer simulations using 3D CFD	51
3.3.1	HTDZ simulations: Spray morphology	52
3.3.2	Wall heat flux trends between models and grids	53
3.3.3	Wall heat transfer in the Zirconia-coated HTDZ simulation	55
3.3.4	Explorative simulations in the OM651 metal engine configuration	59
4	Main accomplishments and conclusions	64
5	National and international collaboration.....	66
6	Dissemination.....	66
7	References.....	66



List of abbreviations

BC	Boundary condition
BDC	Bottom dead centre
BL	Boundary layer
BMEP	Brake mean effective pressure
CA	Crank angle
CFD	Computational fluid dynamics
CHT	Conjugate heat transfer
CMC	Conditional moment closure
CVC	Constant volume chamber
DVS	Deutscher Verband für Schweißen und verwandte Verfahren
ECFM	3-zones extended coherent flame model
ECN	Engine combustion network
EOI	End of injection
FPS	Frames per second
HRR	Heat release rate
HTDZ	Hochtemperaturdruckzelle (high pressure and temperature cell)
HVLP	High velocity low pressure
IC	Internal combustion
LHS	Left hand side
LotW	Law of the wall
LPT	Lagrangian particle tracking
PDF	Probability density function
RA	Reynolds analogy
RANS	Reynolds averaged Navier-Stokes
RHS	Right hand side
RMS	Root-mean-square
SME	Small and medium-sized enterprise
TBC	Thermal barrier coating
TDC	Top dead centre
TUB	Technical University of Berlin
TSM	Thermal swing material
WHT	Wall heat transfer
WM	Wall modelled



Symbols

A	Area
c_p	Heat capacity at constant pressure
C_D	Coefficient of discharge
C_f	Coefficient of friction
C_μ	Eddy-viscosity model constant
d	Diameter
E	Logarithmic law constant
$F_{V,soot}$	Soot volume fraction
h	Heat transfer coefficient
k	Turbulent kinetic energy
L	Characteristic length scale
L_v	Virtual line-of-sight luminosity
m	Mass
Nu	Nusselt number
p	Pressure
Pr	Prandtl number
Pr_t	Turbulent Prandtl number
q	Heat flux
R_a	Average roughness
R_t	Line-averaged peak-to-valley roughness
R_{rms}	Root-mean-square roughness
R_s	Sand grain-equivalent roughness
R_s^+	Scaled sand grain-equivalent roughness
s_R	Skewness of roughness probability density function
t	Time
T	Temperature
u	Velocity
u^+	Scaled velocity
u_τ	Wall shear velocity
x	Distance
y^+	Scaled wall-normal distance
α	Thermal diffusivity
$\delta_{w,v}$	Wall viscous length scale
ΔT	Temperature swing
κ	von Karman constant
λ	Thermal conductivity
μ_t	Turbulent viscosity
ν	Kinematic viscosity
ρ	Density
τ	Shear stress



1 Diesel combustion chamber insulation: study background

1.1 Economic impact and significance for SMEs

The results of the research project will provide potential for innovations, in particular for the manufacturers of vehicles with smaller internal combustion engines. The anticipated research results relate to a large extent to the efficiency of direct injection diesel engines and will therefore be of direct benefit for all manufacturers, developers, and users. The results will also be relevant for the improvement of spark ignition engines.

The research on questions concerning modern diesel engines is in particular of fundamental importance for future innovations and developments by small- and medium-sized enterprises that are involved in the manufacturing of components, or in design and consultancy in this field. This applies above all because as a rule these companies are not able to carry out such demanding investigations themselves at present, as they do not have access to the test beds and measuring equipment required. The results of the project will be used directly by SMEs who use their specialist knowledge to provide services in the field of diesel engine combustion technology, e.g. engineering computation and consultancy services, which are typically provided by small and medium-sized enterprises. Furthermore, SMEs can also benefit from the practical introduction of the prospective research results relating to the extension, upgrading and application of engine process simulation programs. Finally, many manufacturing companies will benefit from the results that will also belong to the group of small- and medium-sized enterprises. These include manufacturers of pistons in development projects as well as companies involved in the development, realisation and application of coating methods. Due to the ongoing dialogue of the SMEs with major manufacturers in the working group and the joint initiation of the project and the practical implementation of the results, the generation of shared know-how will be supported and the position of Germany's suppliers and service-providers will be strengthened.

The market for industrial coating services is dominated by SMEs. The German research institution "Forschungszentrum Jülich" describes this market sector in a way that "in Germany, companies that work with coating or surface technology, are traditionally small or medium sized enterprises" [1] (quote translated). A study from the "DVS – Deutscher Verband für Schweißen und verwandte Verfahren", describes the overall economic impact of coating technology together with joining and separation technologies. With 330,000 employees a total value creation of 18.8 billion euro is reached in this segment [2]. In order to improve competitiveness of these SMEs, it is necessary to find new applications for modern coating systems.

The demands for increased performance and efficiency in internal combustion engines together with a reduction of exhaust emissions calls for an innovative development of all components along the drive train. Particular focus is placed here on the inner-engine measures, since by reducing of the engine-out emissions by adaptations to the exhaust gas treatment system, the back pressure can be lowered and the losses in the work process can be reduced. A large proportion of the difference between the energy of the fuel introduced and the effective work done by the engine is attributable to the thermodynamic cycle. Among other things, this is influenced by the compression ratio, the valve timing, the calorific properties of the intake gas, and the wall heat losses. To reduce the heat loss, it is important to have a suitable bore/stroke ratio, and the geometry of the combustion chamber must also be optimised. A further possibility for optimisation is to reduce the heat losses from the combustion chamber by thermal insulation. However, with a constant wall temperature, the deployment of coated pistons does not



necessarily lead to a better thermal efficiency of the engine. It has been found that with low wall temperatures the heat transfer from the working gas to the wall in the internal combustion cycle is too high, whereas with high wall temperatures the heat transfer from the wall to the working gas increases, reducing the density of the gas and lowering the trapped mass. This disadvantage can be overcome with a rapidly changing wall temperature, which can be achieved if the insulation layer has a low thermal capacity. The use of coated pistons offers considerable potential to reduce the wall heat loss and optimise the combustion. The complexity of the burning processes during combustion and the rapid movement of the piston present major challenges regarding the material properties and the nature of the coating. Since the piston expands as a result of the high temperatures during combustion, the insulation material must also be able to make corresponding geometric changes. In addition to the expansion of the coating material it is also important to take into consideration its mechanical, chemical, and thermal durability. At the same time, both the thermal conductivity and heat capacity of the material should be as low as possible in order to meet the thermodynamic requirements.

Various coating materials will be evaluated systematically in the course of this research project by means of test bench measurements and heat transfer simulations. The results will add to basic knowledge about the durability and applications of coated pistons in the engine, and also provide insights into combustion processes, flame distribution, emission development, and heat transfer in insulated combustion chambers under varying operating conditions. This will be very important for subsequent applications in vehicles and will offer potential for further technological advances in this field.

Since the application of insulation layers to the pistons of diesel engines is known to influence their thermal efficiency, it is expected that further optimisation could lead to considerable improvements in engine efficiency. Solving the engineering challenges involved requires knowledge and expertise which can be gained by basic research on the insulating properties of coatings. One of the ways this project aims to make a significant contribution is by carrying out experiments on a single cylinder engine. This will be used to verify models which are to be developed on the basis of theoretical system analysis. This will generate systematic basic knowledge that can be used directly for the optimisation and further development of diesel engines. The results will have potential for a wide range of subsequent applications by small and medium-sized enterprises. These could typically include service providers involved in engine testing and modelling, or also in the production and testing of coatings.

1.2 Motivation for the investigations

Although extensive research and development on the effects of heat transfer from gas to cylinder wall in combustion engines has been carried out in the past, there are still many open questions. The innovative approach of the proposed project allows new options to improve the combustion engine thermodynamics. SMEs active in research and development will have different ways to use the results from the projects.

- Within the field of component development, the SMEs can optimise technologies such as injection systems, gas exchange valves and others.
- As consultancy companies, SMEs will benefit from the results as they have a perfect database for the validation of simulations with 1D- and 3D-models.

Without the results of the project SMEs will not be able to develop into this direction as measurements are too complex and ambitious without access to the research competences of the involved research consortium.

In order to be competitive, it is also necessary for SMEs in the coating service industry to offer high quality coatings and to apply modern machinery. These SMEs are always in the need of new



applications and increased market volumes for their specialized coating services. Furthermore, these SMEs need high expertise regarding coating durability in different environmental conditions. The project proposal addresses these needs in the following way:

- Different coating materials and layer systems are examined in the combustion chamber. These experiments lead to new knowledge regarding coating materials and durability. SMEs can apply this knowledge for their own coating services.
- The project goal is to increase efficiency of the combustion chamber with new coating systems. This leads to new coating applications and an increased market volume for coating services.

1.3 Overview of project work packages

The investigations will be carried out by three research institutes (TU Berlin, VKM; ETH Zurich, LAV; Fraunhofer IPK), with six work packages, as summarised in Table 1:

Table 1. Summarised description of work packages

WP1	ETH & TUB	Parameter study to define optimum material properties
WP2	IPK	Development of suitable coatings and application processes
WP3	ETH	Experimental characterisation of wall heat transfer for coated and uncoated pistons in an optically accessible high pressure and high temperature chamber (HTDZ)
WP4	ETH	3D-CFD with Conjugate Heat Transfer
WP5	TUB	Characterisation of various coatings in two engine configurations
WP6	all	Synergetic evaluation of findings and documentation of results

Figure 1 shows the timeline of the project on a work package level. It should be noted that a project extension was requested by TU Berlin on the FVV side, which has not influenced the work time budgeting of ETHZ.



Project timeline and work packages

Project duration 01.09.17 – 29.02.20

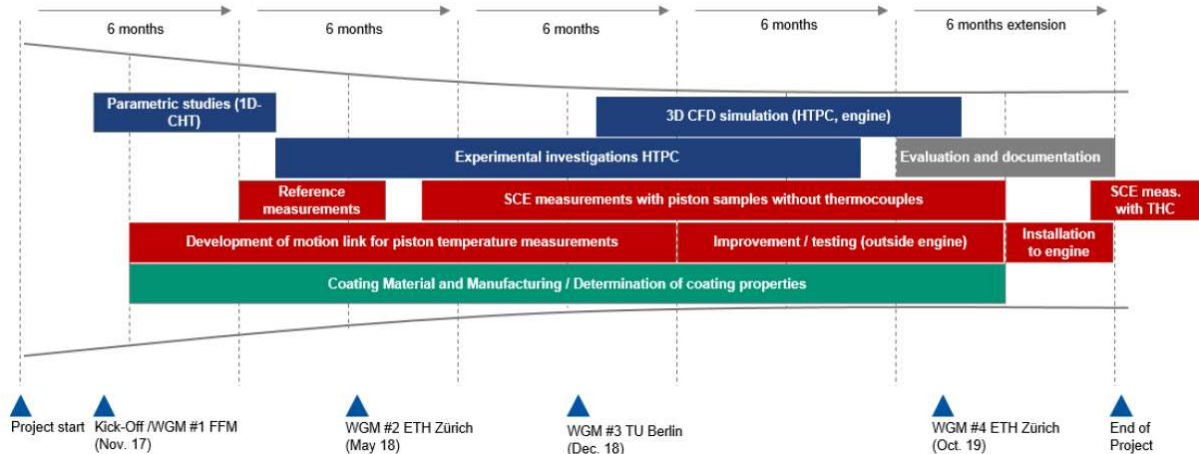


Figure 1. Project timeline and work packages. Courtesy of Oliver Nett / TU Berlin.

1.4 Objectives for work carried out at ETHZ

For the contribution of ETHZ in the project, the most important objectives are as follows:

- 1) For both standard piston surfaces and Thermal Barrier Coatings (TBCs): describe the phenomenology of heat transfer resulting from spray-wall impingement using experiments and 3D CFD simulations
- 2) Attempt to examine and quantify different factors contributing to heat transfer deviating from standard piston surfaces. In particular, discuss whether *non-ideal* properties on solid walls (such as surface roughness or porosity) influence the process in a manner that mitigates advantages from TBCs
- 3) Describe computational methods to aid the industry in the predictive assessment of such non-idealities.

To elaborate on these objectives, let us consider the visualisation in Figure 2. In the uncoated case, i.e. during impingement of a spray on a piston material, the spray combustion-wall impingement process results in some local heat flux, represented by the measured value. The process is influenced both by a (slight) heating up of the wall due to CHT (thermal swing influence), and a possible (slight) increase of heat transfer by surface roughness. If the absence of these factors, the result would correspond to the base wall heat transfer value indicated by the horizontal dashed line.

Considering the coated case in a similar scenario, we can assume for the base wall heat transfer value to be similar to the uncoated case. However, now the material and its surface structure impose far greater effects on the near-wall flow. First, as the surface temperature rises substantially more due to the hot impinging jet, heat flux decreases due to the decrease of gas-wall temperature difference (thermal swing influence). In contrast, a higher roughness of the surface can promote far higher additional heat transfer from the gas to the solid.

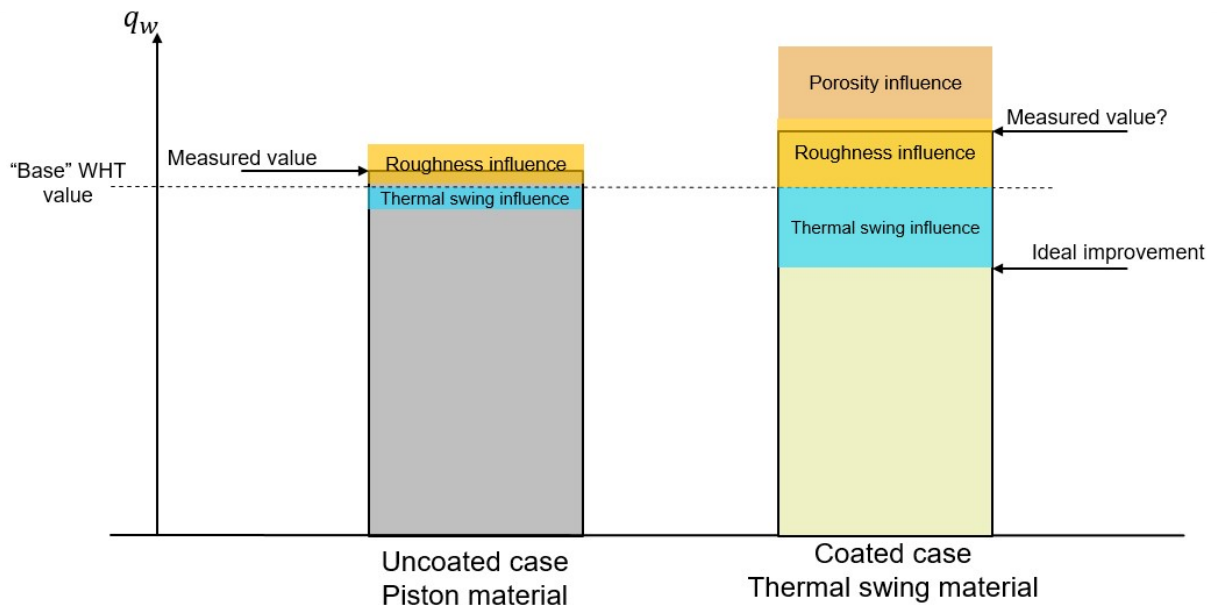


Figure 2. Schematic of heat flux measurements in the uncoated and coated cases, and an illustration of the different factors of heat flux formation.

In addition to the two counteracting impacts of thermal swing and surface roughness, the porosity of coating surfaces has recently been indicated as a contributor to increased heat losses [3]. It is expected that the functionality of coatings in engine conditions presents a more complex scenario than variations in local heat flux. However, the purpose of this report is to focus on the detailed, local phenomena instead of the full engine process.

1.5 Synergy between work carried out by ETHZ and the other institutes

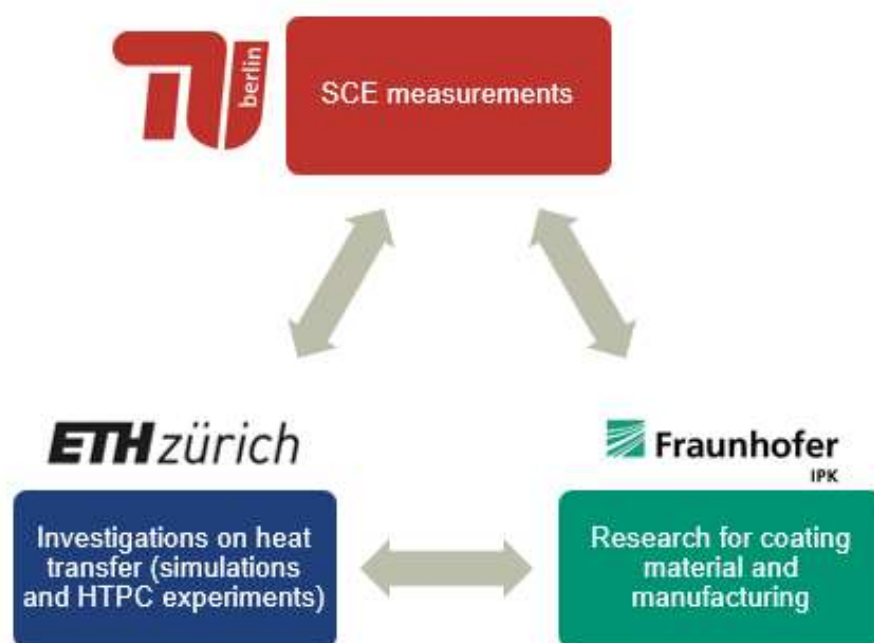


Figure 3. Schematic of the collaborative task areas in the project.



ETHZ and Fraunhofer IPK

ETHZ prepares impingement plates and heat flux sensors to be tested in the HTDZ, and dispatches these to HTDZ for coating. In addition to carrying out coating, Fraunhofer IPK carries out a characterisation of the produced surfaces, including in-depth surface roughness metrics. Moreover, the material property characterisations made by Fraunhofer IPK are employed throughout the computational studies carried out by ETHZ.

ETHZ and TU Berlin

The researchers at TU Berlin are responsible for actual engine measurements within the project. These experiments function in adding efficiency metrics that cannot be ascertained only from cell-like heat flux experiments. To complement the HTDZ simulations, the TU Berlin engine configuration will be explored in simulations at ETHZ, using the methodologies and coating configurations in the HTDZ simulations.

2 Research Methodology

In this chapter, the methodologies used to carry out the research in the work packages are presented. These involve both experimental and computational techniques, and, in some work packages, a combination of the two. First, the fundamentals of near-wall fluid flows and heat transfer are briefly outlined. Experimental and computational methodologies are detailed in the work package specific descriptions.

2.1 Planned coating materials to be studied



Figure 4. Planned coating materials to be studied: porous aluminium (left), zirconia + sealer (second left), zirconia (second right), zirconia + aluminium (right)

In addition to the nominal materials (HTDZ: steel; Engine: aluminium), the initial set of materials to be studied contains four varieties:

- Porous aluminium (sample A): to study the combined effect of roughness and porosity with a non-insulating material
- Zirconia + sealer (sample B): Porous zirconia whereupon a sealing agent has been applied: the objective is to study how sealing of the pores (along with an ostensible decrease in roughness) impacts heat transfer
- **Zirconia** (sample C): this is **the baseline coated case** to be studied, and includes both a porous structure and a rough surface
- Zirconia + aluminium (sample D): The point of this variety is to study potential improvements from reflection, i.e. the decrease of radiative heat transfer, in comparison with the baseline case



Sensor failures

During the coating process of the sensor-plate combinations at Fraunhofer IPK, wherein both the impingement plate and the centrally located sensor are uniformly coated, several sensors failed to produce a coherent output after the process:

- Only sample C survived the process, while the other sensors were deemed non-functional.
- After completing HTDZ measurements with sample C, the sensor-plate installation was sent to be sealed in accordance with sample B
- Measurements in the project were then focused on sample C, and the renewed sample C (corresponding to the original intent of sample B)

2.2 Basics of heat transfer

Fourier's law and the heat equation

Conductive heat transfer is determined by Fourier's law

$$q_i = -\lambda \frac{\partial T}{\partial x_i} \quad (1)$$

where q_i is the heat flux vector, T is the temperature and λ is the thermal conductivity. In fluids, this heat flux enters the full conservation equation for enthalpy. However, in isotropic solid media where convective processes are absent, the evolution of temperature in time t and space x_i is determined by the heat equation:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) \quad (2)$$

where ρ is the density and c_p is the material heat capacity. In the case of constant material properties, the heat equation can also be written as

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x_i^2} \quad (3)$$

where α is the thermal diffusivity. In engineering, the heat transfer coefficient h is an important quantity, relating heat flux and the area available for heat transfer:

$$h = \frac{q_w}{A(T_w - T_f)} \quad (4)$$

where a positive q_w denotes heat flux into the gaseous domain and fluid temperature T_f can e.g. be a representative bulk temperature in the gaseous domain. Similarly, heat flux can be expressed with the heat transfer coefficient by $q_w = hA(T_w - T_f)$. Importantly, h is a convective heat transfer coefficient and includes the effect of turbulent flow motion. The relative impact of convective heat transfer (in relation to purely conductive heat transfer) is expressed by the Nusselt number Nu :

$$Nu = \frac{hL}{\lambda} \quad (5)$$

where L is a characteristic length between the locations of fluid and wall temperatures.



Conjugate heat transfer

Conjugate heat transfer refers to the interaction between fluid and solid heat transfer. The gas-solid heat transfer therefore influences the temperature distribution in both mediums, which in turn affects the future heat transfer processes. While conjugate heat transfer phenomena always exist in gas-solid heat transfer, its significance to the gas-wall heat transfer process can be either close to zero or very high, depending on the material properties of the solid wall.

Material property influence on CHT

The material properties on the piston are very influential towards the CHT characteristics that can be expected. Temperature swing denotes the ability of the wall material to adapt to the surrounding gas temperature, thus reducing heat losses [4].

As stated by Andruzkievicz et al. [5], the amount of temperature swing ΔT can be related to the material properties as follows

$$\Delta T \sim \frac{1}{\sqrt{\rho * c * \lambda}} \quad (6)$$

Effectively, materials with low density, heat capacity and thermal conductivity are proponents to higher variation of surface temperature and hence of thermal swing effects. In Figure 5, this relationship between material properties and thermal swing is shown graphically for both real and hypothetical engine-relevant materials,

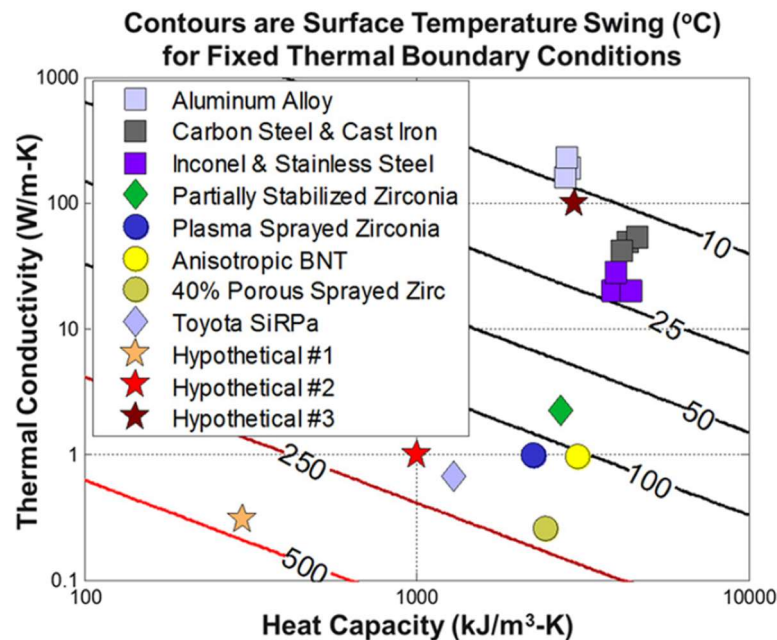


Figure 5. The amount of thermal swing expected with different materials during a cyclic engine process [5]

Heat transfer in numerical simulations

Real fluid flow processes in engines are inherently dependent on the convective processes and small-scale eddies of turbulent flows. In computational fluid dynamics (CFD), a number of levels of fidelity exist to describe fluid flow phenomena and heat transfer:

- Zero/One-dimensional process simulations (e.g. GT-Power): here, gas-wall heat transfer models are typically based on bulk (average) quantities, prominently including the Woschni and Hohenberg formulations. In the absence of any spatial dimensionality (often the case in in-cylinder models) heat transfer within the gas phase occurs only between different flow components.
- Three-dimensional simulations with statistical turbulence models (Reynolds-averaged simulations; RANS): In the gas phase, turbulent heat transfer is governed by modelled turbulent heat flux q_m . In eddy-viscosity turbulence models (employed in this work), this quantity has been formulated in analogy to conductive heat transfer: $q_{i,m} = (\mu_t / Pr_t) (\partial T / \partial x_i)$, where μ_t is the turbulent viscosity (yielded by the turbulence model) and Pr_t is the turbulent Prandtl number. Gas-wall heat transfer is determined from the local flow field variables either by integrating to the wall or by wall modelling.
- Three-dimensional scale-resolving simulations (Large-Eddy Simulation – LES; Direct Numerical Simulation – DNS): These methodologies numerically resolve the governing equations such that the actual turbulent convective transport processes can be either partially (LES) or fully (DNS) described.

Figure 6 displays an example of a wall-modelled large eddy simulation carried out for wall-impinging spray combustion [6], shows key characteristics of scale-resolving simulations, namely local vertical (eddy) structures of varying length scales and instantaneously asymmetrical flow structures.

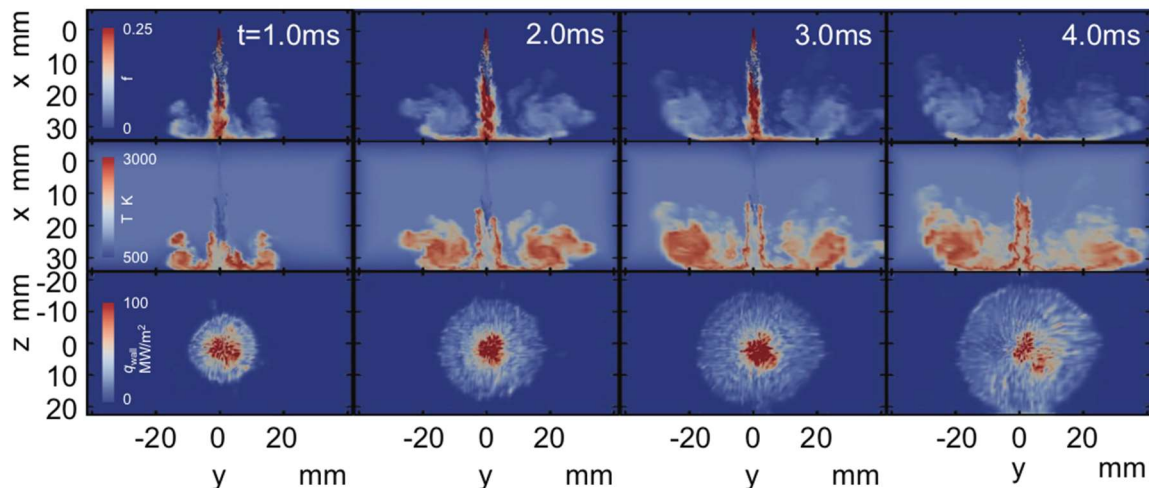


Figure 6. Mixture fraction cutouts (top), temperature cutouts (centre) and wall heat flux surface distributions (bottom) in a wall-modelled large eddy simulation of spray combustion [6]

The example of Figure 6 is then also equivalent to a single experimental injection-impingement process, or a “shot” in an experimental spray combustion bomb. In contrast, a RANS simulation is by nature ensemble-averaged, providing a statistical description of turbulence. Hence, a single simulation attempts to recreate the statistical outcome of a large number of realizations.



2.3 WP1: Parameter study to define optimum material properties

Model formulation and testing for the 1D-CHT simulations has been completed; the governing equations are discussed below. Starting from Fourier's law of heat conduction:

$$q = -\lambda A \left(\frac{dT}{dx} \right) \quad (7)$$

By rearranging this equation and since for a 1D simulation A reduces to unity; following Mruk et al. [7] we relate the steady-state wall inner surface temperature T_w to the ambient air temperature T_c as:

$$T_w = T_c + q \left(\sum_i \frac{g_i}{\lambda_i} + \frac{1}{h_c} \right) \quad (8)$$

Where $\dot{q}$ is the heat flux through the wall, g_i and λ_i are the thickness and thermal conductivity of the i^{th} layer (be it an insulation layer, bonding layer or the metal itself; see Figure 7) and h_c represents the heat transfer coefficient on the coolant side. When applying these results in a 3D-CFD context, care must be taken to account for the varying metal thicknesses at various physical locations due to the complex geometry. However results presented in [3] show that any temperature drop occurs almost entirely in the insulating layer; the metal temperature remains nearly constant regardless of the metal thickness.

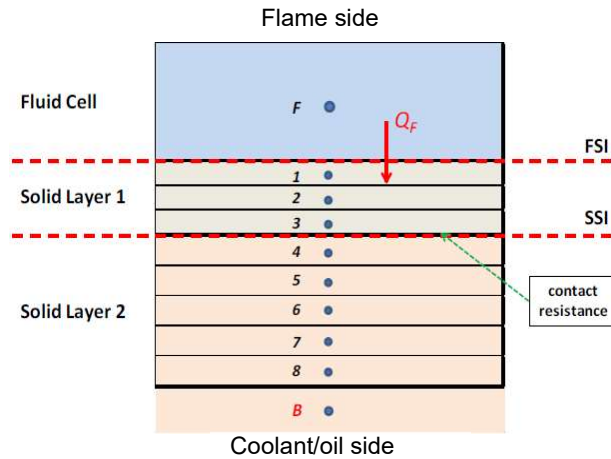


Figure 7. Illustration of multiple solid layers and interface with fluid cell.

The above formulation can be applied to a cycle-averaged calculation where the average heat flux is known. However, in order to incorporate a transient behaviour we solve the 1D elliptic equation:

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c_p} \frac{\partial^2 T}{\partial x^2} = \frac{\lambda}{\rho c_p} \frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) = \frac{\lambda}{\rho c_p} \frac{\partial}{\partial x} \left(\frac{q}{\lambda} \right) \quad (9)$$

Where t is time, x is space comprising all layers of insulation as well as metal, λ , ρ and c_p are the thermal conductivity, density and specific heat respectively, all functions of x (due to the different materials in each layer). Equation (9) will be solved numerically to obtain the temperature T as a function of time and space. The result of this solution procedure is the time-varying surface temperature T_w for a given heat flux.

The higher the surface temperature, the more the isolating effect of the material, however if the surface temperature stays at a high level during the intake stroke (typical for thermal-barrier coatings TBCs such as ceramics), this can lead to heating up of the charge air and have an adverse effect on emissions and component fatigue, as well as increased knocking tendency. On the other hand, if the surface



temperature changes rapidly in time (typical for thermal-swing materials TSMs), the insulating effect can be realized without the associated disadvantages of thermal-barrier coatings.

2.4 WP3: Experimental characterisation of wall heat transfer for coated and uncoated pistons in an optically accessible high pressure and high temperature chamber

2.4.1 The high pressure and temperature cell

The experiments have been performed in the high-pressure high-temperature cell of the LAV, which is a constant volume chamber (CVC) with a combustion chamber of 110 mm of diameter and a depth of 60 mm. The CVC is equipped with a large frontal optical access of 90 mm of diameter and four smaller side optical accesses, each of 42 mm of diameter; which give excellent access for the application of various optical diagnostic techniques of sprays and jets.

The cell body has six electrical heaters on the body and two valves for the inlet of fresh air and the outlet of exhaust gases. The cell can be operated in two modes:

1. Electrical heating: In this mode the body can be heated up to 700 K and is usually filled with air up to 80 bar. This mode is ideal for cases with low temperature or low pressure, also for non-reactive injection events in which an inert environment of nitrogen or gas mixtures is required.
2. H₂ pre-combustion: In this mode the cell body is heated up to 500 K and filled up to 30 bar, then an additional charge of air and hydrogen are injected into the chamber and ignited by a spark plug. This combustion causes the chamber pressure and temperature to rise over 100 bar and 1000 K, respectively.

The measurement conditions (pressure, temperature) are very well controlled and reproducible on both operational modes. The high-pressure chamber is ideal for studies of diffusion flames including beam propagation (liquid and vapour). Figure 8 shows the CVC with the injector mounted on the side in order to take advantage of the main window for visualization.



Figure 8. Constant volume cell with the injector mounted on the side.

2.4.2 Precombustion and injection

To achieve a proper temperature and pressure of the ambient species in the chamber, the constant volume chamber was first filled with air at a certain pressure. A specific mass of hydrogen and additional



air are then injected into the chamber air and ignited via a spark plug. The pre-combustion event of the hydrogen leads to high temperature and pressure conditions at the time of injection, which would not be possible only with the electrical heating. The consumption of oxygen during this pre-combustion event was designed to obtain the oxygen concentration required for the investigations. As the peak pressure is reached and progressively drops to the trigger pressure, the injection is triggered at the right moment. In this investigation, the trigger pressures are 60.7 bar and 52.9 bar that represent gas-averaged temperatures of 900 K and 800 K. As the fuel injector is triggered with an energizing time of 4000 μs , it takes some time for the injector to actually raise the needle and allow the fuel flow in chamber. This time is in addition to the ignition delay time, i.e. from the emergence of fuel until the onset of high temperature ignition. The net sum of these times creates a time delay between fuel injection trigger and actual auto-ignition event of the fuel. The oxygen concentration can be simply estimated by the consumption of hydrogen combustion. In this investigation, the oxygen concentration is 15% in volume.

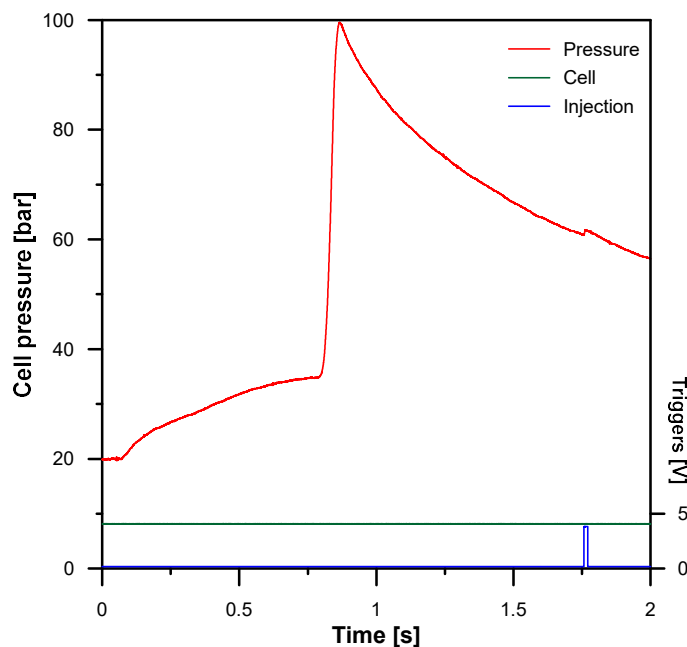


Figure 9. Pressure trace measured inside the CVC during a pre-combustion and an injection event. Trigger signals of the beginning of cycle and injection event are shown at the bottom.

Figure 9 shows the pressure evolution inside the cell during a cycle using hydrogen pre-combustion. It can be seen that the trace begins from 20 bar at 0 s, which corresponds to the filling pressure. Then it gradually increases to 35 bar at 0.8 s due to the added mass of hydrogen and air of the pre-combustion system. After the spark is sent and the hydrogen-air mixture ignites, the pressure rises quickly reaching a peak of 100 bar. Once combustion is complete the pressure starts dropping due to heat losses through the walls and a trigger signal for the main injection is sent once the target pressure is achieved. The trigger signal that starts the whole cycle can be seen as “Cell” and the trigger signal for the main event “Injection” is shown when the pressure reaches 60 bar.

For these experiments the base conditions are 900 K of ambient temperature at a density of 22.8 kg/m³ and 15% (volume) of oxygen, which leads to an ambient pressure of around 60 bar. For some cases, a variation in ambient temperature has been performed at 800 K and the same density.

A single hole axial magnetic injector with a 90 μm nominal orifice diameter was used to inject n-Dodecane into the combustion chamber. The nominal injection pressure was 1,500 bar and the



energizing time was set at 4,000 μs . For some conditions, variations in injection pressure were performed at 500 bar and 1,000 bar; as well as a different energizing time of 1,500 μs .

2.4.3 Impingement plate and wall heat flux sensor

In order to be able to measure and quantify spray impingement induced heat losses through the wall and variations in wall surface temperature a special heat flux sensor was used. This sensor is designed by Dr. Müller Instruments for specific applications and is manufactured on demand. The specifications can be found in Table 2.

In order to mount the heat flux sensor in the combustion chamber, an impingement plate was designed to fit in place of one of the small optical accesses on the opposite side of the injector. This way, the spray would penetrate into the chamber and impinge the plate after combustion had taken place. Figure 10 shows the impingement plate, which has a hollow design which, allowing sensor mounting and removal while the plate is fixed in the CVC. The plate also presents a flat surface so the sensor can be mounted flush on the plate.

Table 2. Technical data of the heat flux sensors used for the experiments.

<u>Technische Daten:</u>	
Thermoelement:	Typ E (als Sonderanfertigung ist auch Typ K möglich)
Material:	Typ E: Chromel – Constantan (Zentrum), koaxial Typ K: Chromel – Alumel (Zentrum), koaxial
Temperaturbereich:	Typ E: - 200 bis 900 °C Typ K: -200 bis 1170°C
Empfindlichkeit:	0,5 K ist die kleinste messbare Temperaturänderung
Wärmestrom:	20 KW/m ² bis 20 MW/m ²
Haltbarkeit ohne Renovierung für Typ E:	Raumtemperatur: Monate 615°C: 35 Minuten 715°C: 8 Minuten
Ansprechzeit:	3 μs
$\sqrt{\rho c k}$	ca. 9500 W $\sqrt{\text{s/m}^2\text{K}}$
Maße:	MCT 19: d = 1.9 x 26 mm MCT 36: d = 3.6 mm x 17 mm MCTB48: d = 4.8 x 25 mm Sensor MCT 19, 36 und 48 kann im Bereich ihres Durchmessers 1,9, 3,6 und 4,8 mm gekürzt werden
Durchmesser:	1,9, 3,6 und 4,8 mm
Empfindlichkeit:	Typ E: ca. 63 $\mu\text{V/K}$, (s. IEC-584 T1), kalibriert Typ K: 39.9 $\mu\text{V/K}$, kalibriert
Empfindliche Spitze:	kann beliebig der Oberfläche angepasst werden

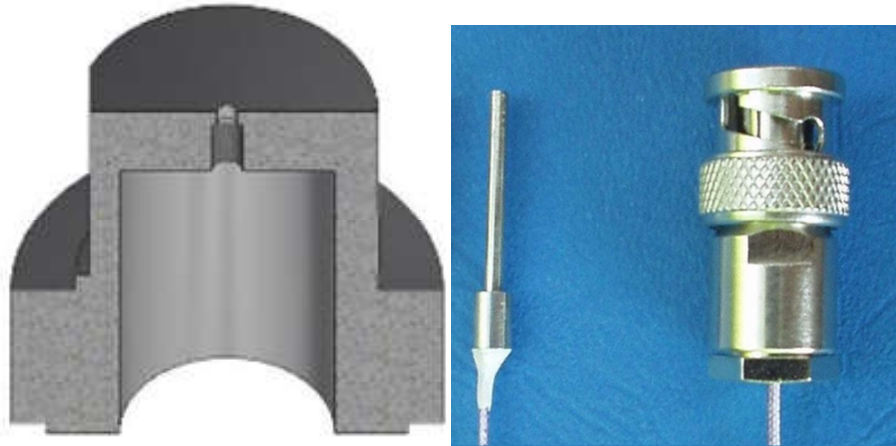


Figure 10. Impingement plate with hollow body and threaded surface to mount sensor (left) and 2mm heat flux sensor with standard BNC connector (right).

2.4.4 Optical diagnostics: broadband chemiluminescence & OH-chemiluminescence

In order to visualise the spray, detect the ignition time and track the spray evolution inside the combustion chamber, two optical techniques have been applied.

Broadband radiation was measured to record the overall luminosity emitted by the flame and visualize the direct impingement of the flame on the plate. This radiation corresponds mainly to the soot thermal luminosity during the diffusion combustion phase. This type of radiation may have two kinds of contributions, chemiluminescence and incandescence. Under most operating conditions, the latter is the fundamental one as it depends on the amount of soot and its temperature, therefore it will be used for a qualitative analysis of such parameters. Figure 11 shows a sample image of broadband radiation, wherein the cross denotes the injector position and the top right corner shows the scale for reference.

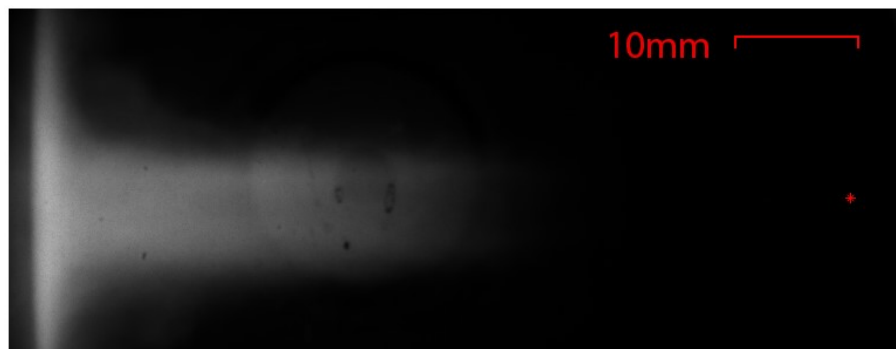


Figure 11. Sample broadband chemiluminescence image; scale shown at the top right. The cross marks the nozzle tip position.

The optical setup is shown in Figure 12 in which a high-speed camera is pointed at the front window with a field of view from the injector tip up to the impingement plate, covering roughly 80 mm. The camera used was a Photron HSS-X recording at 40,000 FPS and to focus on the spray a Nikkor 105 mm f/2.8 micro lens was used.

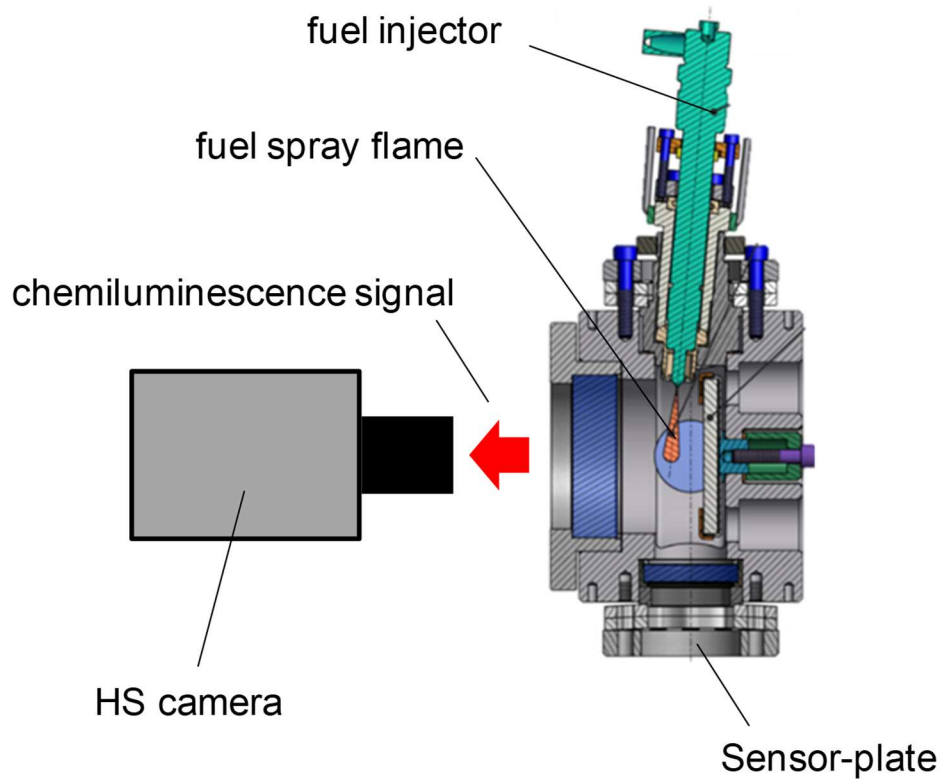


Figure 12. Optical arrangement of the broadband chemiluminescence technique.

OH* chemiluminescence was used to determine the burning area; from this, two parameters were obtained. One is the distance from the nozzle to the base of the flame, which will be referred to as “flame base”; the other is the distance from the nozzle to the tip of the flame, which will be referred to as “flame tip”. This technique records radiation at 310 nm, which is controlled by the OH* radical, being a marker of the diffusion flame limits, and thus of the lift-off length for diesel sprays [8]. The OH* chemiluminescence occurs at stoichiometric conditions and high temperatures, therefore being a good marker of the lift-off length [9]. Additionally, the wavelength band of 310 nm that corresponds to the chemiluminescence of the OH* radical is the strongest one and therefore best for determining the lift-off length [8, 9].

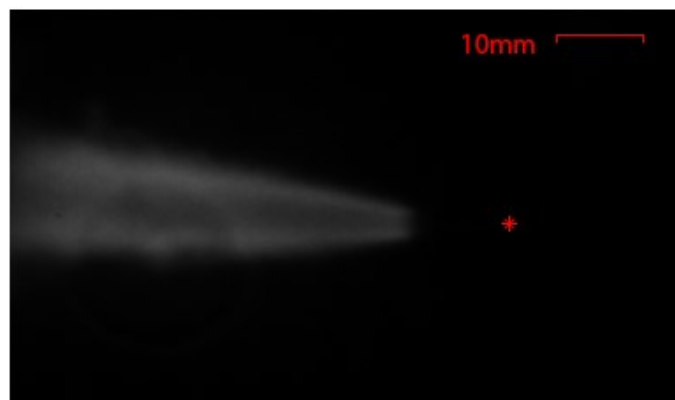


Figure 13. Sample OH* chemiluminescence image; scale shown at the top right and the cross marks the nozzle tip position.



Figure 13 shows an image of OH* radiation, where again the cross denotes the injector position and the top right corner shows the scale for reference. These images are similar in appearance to the broadband ones, but with different spectral information; the lift-off length is calculated as the closest zone to the nozzle where flame can be found [8]. Correspondingly, the flame penetration is calculated as the farthest value from the nozzle tip. The optical setup is shown in Figure 14, which is very similar to the one shown in Figure 8; the main difference is the use of an image intensifier due to the weaker signal of the OH*. The camera used was a Photron HSS-6 coupled to an IRO image intensifier, both synchronized and recording at 40,000 FPS. To focus on the spray a Sodern 100 mm f/2.8 UV lens was used and to filter the other wavelength besides OH* a 310 nm bandpass filter was placed in front of the lens.

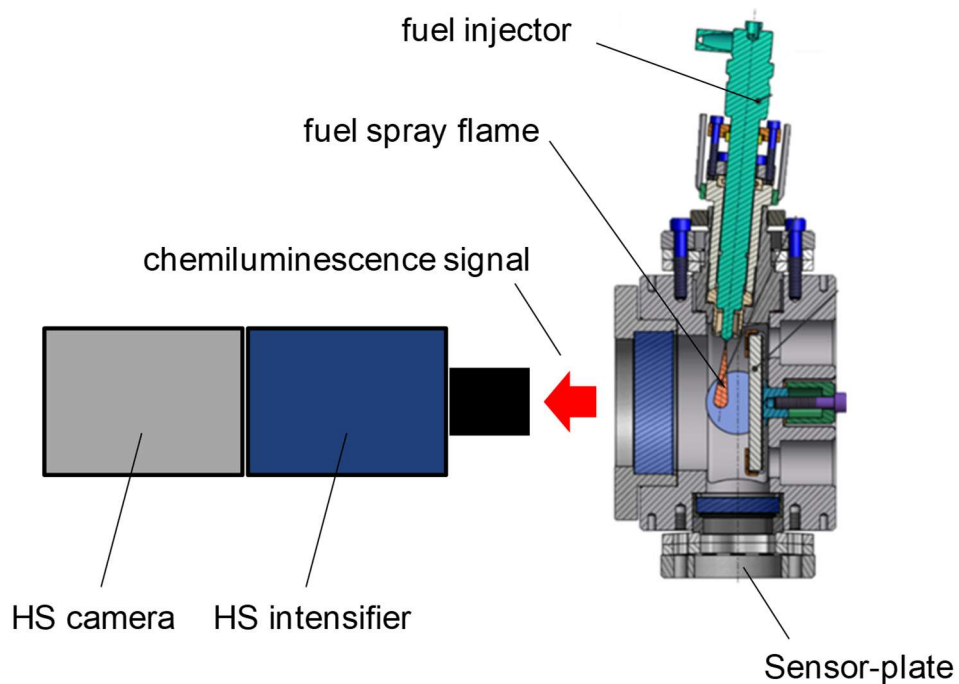


Figure 14. Optical arrangement of the OH*chemiluminescence technique.

In order to quantify the flame-base and -tip penetration from the image a MATLAB processing routine was developed. First, an average background image is calculated for each repetition and based on that image and a threshold; a mask is generated to define the region of interest. Then, the area of the flame is computed, and based on that region the flame-base and -tip are calculated as the closest and furthers points from the injector, respectively. Figure 15 shows the steps of the processing, first the raw image as it is recorded by the camera, then a binary mask that defines the spray region, a masked images in which only the pixels that are considered to be part of the flame are shown and, last, the final image with the calculated contour.

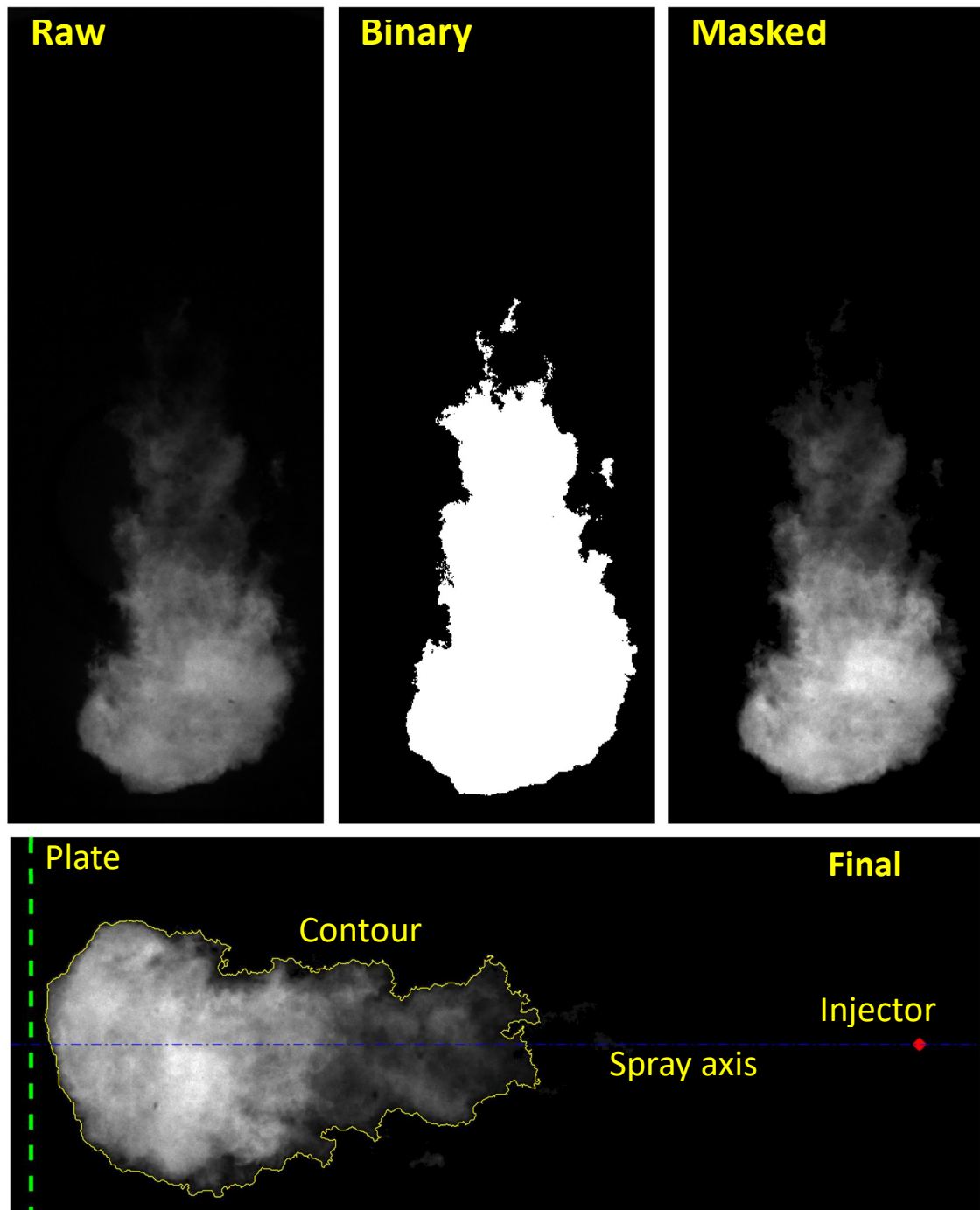


Figure 15. Steps for the processing of chemiluminescence images. Raw image (top left), binary mask (top centre), masked image (top right) and overlay of raw image with flame contour, plate position, injector and spray axis (bottom).

2.4.5 Wall heat flux measurement: processing of coated results

Figure 16 displays the difference between the physical situations of the uncoated and coated cases. While in the uncoated case the sensor is located directly at the gas-solid interface, the coated case has the sensor embedded within the solid surface.

Effectively this means that:

- the uncoated measurement is a direct representation of the wall heat flux and temperature
- the coated measurement indicates wall heat flux and temperature within the wall, at the sensor-coating interface

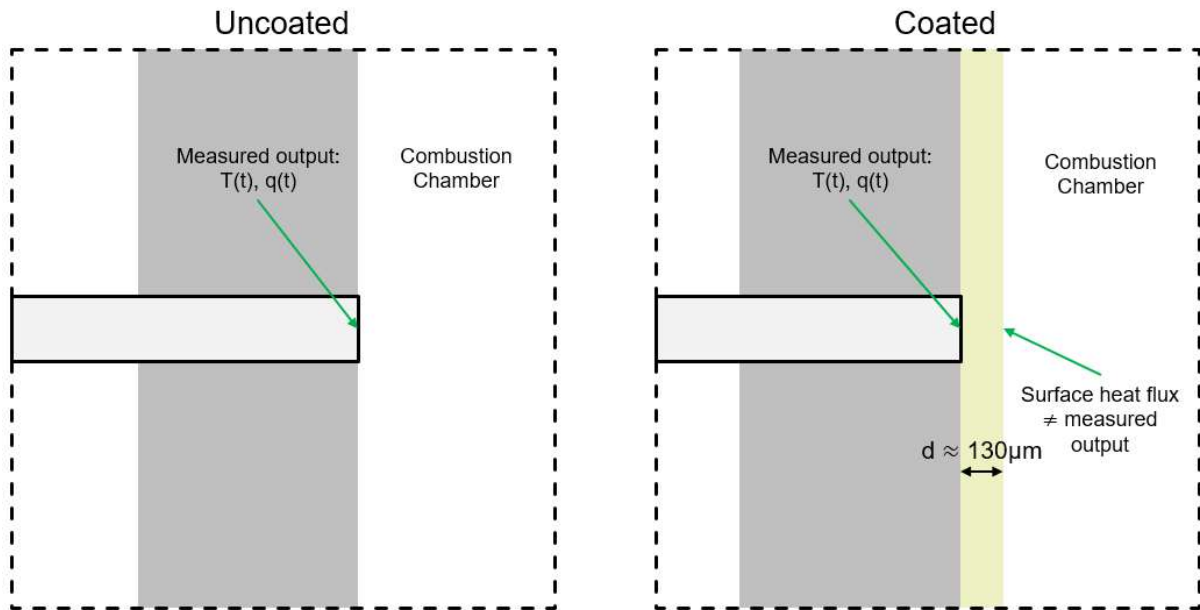


Figure 16. Schematic of the sensor position and outputs in the uncoated and coated cases

To solve for the actual wall heat flux on the gas-coating interface, we have to carry out some reverse-engineering. A schematic of the mathematical problem governing the situation is shown in Figure 17. Here we assume that the problem is described by the heat equation in one dimension (an assumption further assessed in Section 3.1.2).

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} + \frac{1}{\lambda} \frac{\partial \lambda}{\partial T} \left(\frac{\partial T}{\partial x} \right)^2$$

$$T(x, t = 0) = T_0$$

$$q(x = x_L, t) = q_1 \quad \begin{array}{c} \text{coating thickness} \\ \hline x_L \quad \quad \quad x_R \end{array} \quad q(x = x_R, t) = q_2$$

Figure 17. Problem setting for obtaining the wall temperature and heat flux at x_R , from measured data at x_L

Let us start by describing what we know and what we do not know in the situation described by Fig 17.

Known measurement data:

- Heat flux at x_L , i.e. q_1 , which is provided as a function of time
- Temperature at x_L , i.e. T_1 , also provided as a function of time

Unknowns:

- Heat flux at x_R , i.e. $q_2 = q_w$, as a function of time
- Temperature at x_L , i.e. T_1 , also provided as a function of time



- Temperature distribution at $x > x_L$ as a function of time

The problem is hence an ill-posed, inverse problem of the type where the boundary condition q_2 needs to be solved for. The nature of the problem is accentuated by the fact that there is a finite diffusive time scale $t_\alpha = \Delta x^2 / \alpha$ where Δx is the distance between the sensor and the gas-coating interface. This crucially means that responses to heat flux inputs at x_R are not instantaneous, but faced with a characteristic delay. The solution to such inverse problems is not as straightforward as for a corresponding forward problem, where all initial and boundary conditions are known. To solve the problem, one can choose between two alternatives:

- Solve the problem using bespoke techniques for inverse problems [10]. It should be noted that while the solution of forward diffusion problems is usually straightforward, the inverse is difficult and sensitive to measurement noise. This is due to the fact that the physical diffusive process itself loses information when time progresses – effectively, it is very difficult to recover a ‘perfect’ solution to such problems.
- Solve the problem by iteratively searching for a fitting solution in a forward problem. This approach is the one applied in this work, utilising our prior knowledge relating to the phenomenology of the associated hot jet impingement. Specifically, the uncoated measurements inform us of (i) the time scale of heat flux ramp-up, (ii) the time scale of high heat flux (continuous injection) and (iii) the decreasing trend of heat flux after end of injection.

Solution workflow

Solution attempts to the inverse problem are made by iteratively solving for a forward heat equation problem in time, modifying the boundary condition at the right-hand side of the 1-D domain (i.e. the gas-coating interface). In fact, the problem in Figure 17 can be formulated in two ways:

- a) Select the heat flux $q_2(t)$ as the unknown boundary condition to be modified. This is a gradient (Neumann) boundary condition. The surface temperature $T_2(t)$ will then be an output of the computation
- b) Select the surface temperature $T_2(t)$ as the unknown boundary condition to be modified. This is a Dirichlet boundary condition. The surface heat flux $q_2(t)$ will then be an output of the computation

The solution criterion for the forward problem is then to match both of the boundary conditions at $x = x_L$ as a function of time. As this correspondence cannot be directly forced, here again a choice is made

- c) Select the measured heat flux $q_1(t)$ as the (Neumann) boundary condition. This means that the match between the simulation result and temperature trace $T_1(t)$ is the solution criterion
- d) Select the measured temperature $T_1(t)$ as the (Dirichlet) boundary condition. This means that the match between the simulation result and heat flux $q_1(t)$ is the solution criterion

In this work, a) and c) were selected, leading to a problem defined by two Neumann boundary conditions as seen in Figure 17. The finite difference solver for this problem is implemented in the widely used MATLAB software.

A final, important piece of the problem is the material property of the coated material. These were provided by Fraunhofer IPK, who characterised both porous and non-porous properties of zirconia.



Table 3. Thermodynamic properties of non-porous zirconia (courtesy of IPK; * represents extrapolated values).

Temperature	Heat capacity	Thermal diffusivity	Thermal conductivity
°C	J/gK	mm ² /s	W/mK
20	0.45*	0.39	0.92
50	0.46	0.39	0.93
100	0.48	0.38	0.96
150	0.50	0.37	0.95
200	0.51	0.35	0.93
300	0.53	0.33	0.90
350	0.54	0.31	0.87
400	0.54	0.31	0.86
450	0.55	0.30	0.85
500	0.56	0.29	0.84
600	0.58	0.28	0.84

Table 4. Thermodynamic properties of porous zirconia (courtesy of IPK; * represents extrapolated values).

Temperature	Heat capacity	Thermal diffusivity	Thermal conductivity
°C	J/gK	mm ² /s	W/mK
20	0.45*	0.45	0.84
50	0.46	0.44	0.84
100	0.48	0.43	0.86
150	0.50	0.41	0.85
200	0.51	0.40	0.85
300	0.53	0.37	0.81
350	0.54	0.35	0.78
400	0.54	0.34	0.77
450	0.55	0.33	0.76
500	0.56	0.32	0.75
600	0.58	0.31	0.74

2.5 WP4: 3D-CFD with Conjugate Heat Transfer

WP4 consists of two main computational tasks, both of which entail conjugate heat transfer:

- 1) Simulation of the high pressure temperature cell (HTDZ)
- 2) Simulation of the OM651 engine

The main features of the HTDZ simulations are as follows:

- Axisymmetric RANS simulation
- Spray simulation with Lagrangian particle tracking (LPT)
- Experimentally characterised BOSCH diesel injector
- Conditional moment closure (CMC) combustion model for non-premixed combustion, validated extensively for the present (Spray A) conditions
- Implementation of novel rough wall heat transfer model

The main features of the OM651 engine are as follows:

- RANS simulation in a fully representative 3D engine domain



- Spray simulation with LPT
- ECFM-3Z combustion model calibrated for the case
- Implementation of novel rough wall heat transfer model

2.5.1 HTDZ: case setup, computational grids and workflow

Figure 18 attempts to elucidate the workflow for the HTDZ simulations, which are the main platform for model validation and local heat transfer studies. The workflow is divided into four stages:

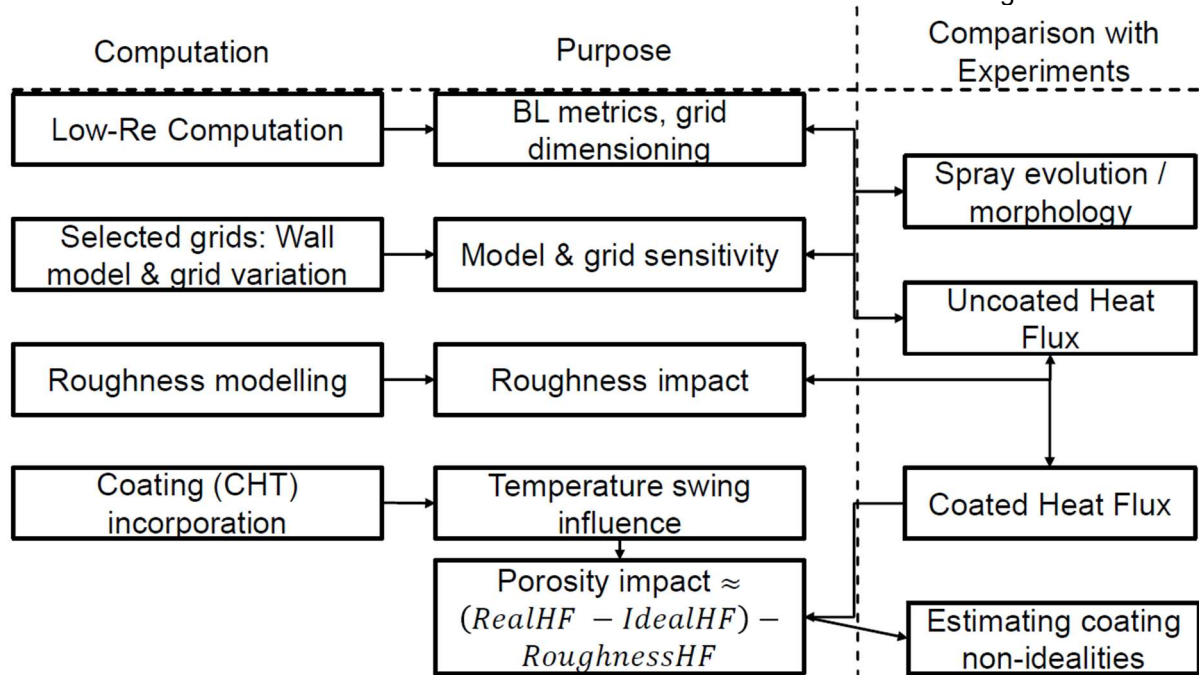


Figure 18. Workflow of the HTDZ simulations

S1: Grid definitions

First, as the computation involves a high-velocity jet impinging on a solid surface, preliminary computations were made to study boundary layer metrics, namely:

- The wall viscous length scale $\delta_{w,v} = \nu_w / u_\tau$, signifying how refined wall normal-resolved grids are required to be
- The boundary layer thickness, determining the maximal cell wall distance in which the assumption of a turbulent boundary layer is valid

The purpose of these preliminary investigations is to determine suitable grid dimensions for (wall-normal-resolved) low-Reynolds number computations, and for different wall modelled computations.

S2: Model and grid sensitivity

The next step was to incorporate different grids and wall models for a sensitivity study. With different models, the primary point of interest was then the level of heat flux on the surface in comparison to (i) the experiment and (ii) the high-resolution low-Re computation. Importantly, this step is used to select the approach to be used for the remainder of cases.

S3: Incorporation of wall roughness model

The roughness modelling involves three different sections:

- 1) Determining an effective roughness metric from measured quantities
- 2) Incorporating a suitable rough-wall momentum transfer model



3) Incorporating a suitable rough-wall heat transfer model

S4: Solid wall properties for 1-D CHT computations

In this step, the investigated material properties and the auxiliary 1-D computational grid are provided in the 3D computations (according to Table 3, Table 3 and Figure 19). The combined observations of S3 and S4 permit a joint evaluation of CHT (including temperature swing) and roughness effects, and whether one appears to be more pronounced in the test case.

Figure 19 shows the grids employed in the HTDZ simulations. The grids are axisymmetric as the solution of the ensemble-averaged problem is not expected to have three-dimensional features. Crucially, this choice facilitates a high grid resolution close to the wall.

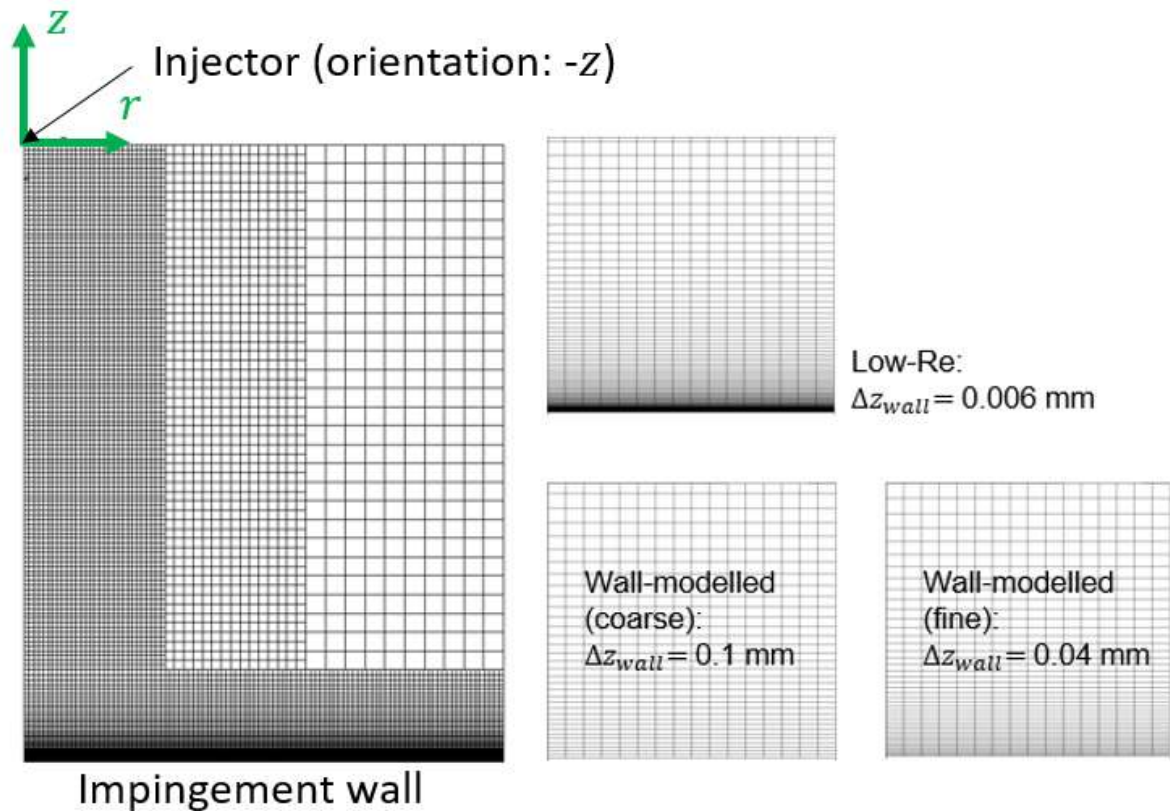


Figure 19. Computational grids for the HTDZ: full grid view (left) and different near-wall treatment variants (right).

While the computational setup is simplified in comparison to the actual cell, two main properties were retained:

- The nozzle-to wall distance is 65.8 mm
- The volume represented by the domain (i.e its revolutionary extrusion) is 0.542 litres

These properties ensure that (1) the jet impingement process is depicted in a realistic intensity, and that (2) the pressure response due to combustion is realistic. The volume is initialised with the following conditions corresponding to the ECN Spray A:

- Temperature: 900 K, absolute pressure: 60 bar, O₂ mass fraction 0.1744, H₂O mass fraction 0.0624, N₂ mass fraction 0.7632, CO₂ mass fraction 0.0936



All simulations are performed with the standard $k - \varepsilon$ turbulence model with a so-called round-jet correction. This means that the model constant $c_{\varepsilon 2}$ is set to 1.52, which has been noted to improve jet flow predictions. The turbulent Prandtl number is set to a constant value of 0.9.

2.5.2 Spray modelling and injector characterisation

Injector characterisation

The Bosch injector in question has been previously characterised, meaning that its outlet diameter and discharge coefficient have been evaluated. This is important as the mass flow rate corresponding to a given injection pressure has a considerable impact on spray penetration and hence also the impingement of the combusting gas jet.

The key parts of the characterisation are shown in Figure 20. The injection rate is approximated to a piecewise linear form. In addition to an electrical delay of $\Delta t_e \approx 300 \mu s$, a hydraulic delay of $\Delta t_h \approx 110 \mu s$ is incorporated to describe the ramp-up to full mass flow rate. In contrast to the nominal (manufacturer-provided) injector outer orifice diameter of $90 \mu m$, a diameter of $104 \mu m$ was measured. Accordingly, a discharge coefficient (the ratio of actual to ideal mass flow rate) of 0.79 has been measured. The injection mass flow rate is given by

$$\frac{dm}{dt} = C_D \rho_f A \sqrt{\frac{2\Delta p}{\rho_f}} \quad (10)$$

Where A is the orifice area, ρ_f is the liquid fuel density (the density of n-dodecane at 373 K) and Δp is the injection pressure differential. With an injection pressure of 1500 bar and a backpressure of 60.7 bar, this results in a mass flow rate of 2.99 mg/ms.

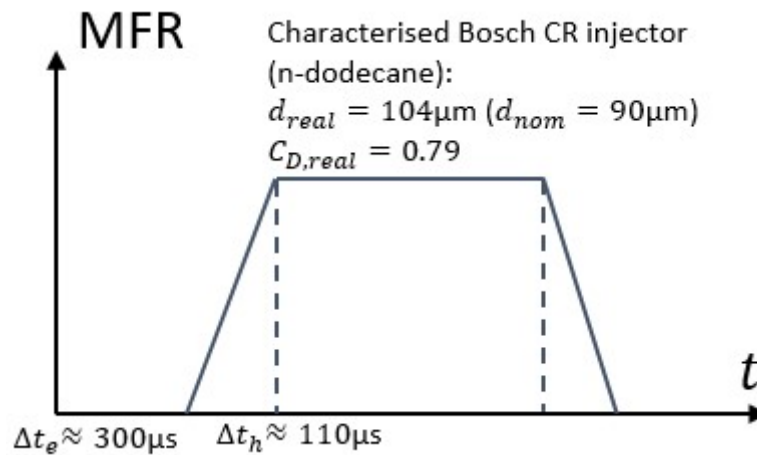


Figure 20. Characterisation of the simulated Bosch injector, in terms of mass flow rate vs. time. Ramp-up and ramp-down are provided with a hydraulic delay of $110 \mu s$ while injector diameter and discharge coefficient are also based on measurements.

Spray modelling

The spray modelling is based on a standard Lagrangian Spray Tracking (LPT) approach in Star-CD. The present approach employs gradient-based interpolation between the gas and solid phases, a turbulent dispersion model and a droplet collision model. As the spray in question is a high-pressure diesel spray, aerodynamic secondary breakup is a dominant part of the process. The Reitz-Diwakar Atomization model [11] is utilised for breakup modelling.



2.5.3 Combustion modelling

Cell simulations: Conditional moment closure (CMC)

The conditional moment closure (CMC) model [12] was employed for the simulation of the HTDZ cases. For the present conditions, close to those of the ECN Spray A, the model has been validated extensively [13] and is expected to provide good predictions.

Explorative engine cases: ECFM-3Z

The 3-zones extended coherent flame model (ECFM-3Z)[14], calibrated by IAV, was employed for the engine case. This model, computationally less costly than the CMC approach, is a good fit for the full cylinder engine cases.

2.5.4 Wall treatment

Wall treatment in Reynolds-averaged simulations is carried out using one of two methods

- A) Solving for the governing equations down to the wall (where the wall-normal grid spacing is specified such that $\Delta y^+ = O(1)$). This solution employs a turbulence model closure that attempts to provide the exact boundary condition for the statistical turbulent quantities. Such models are termed low-Reynolds turbulence models. In this case, the wall boundary conditions follow directly from the physical boundary conditions at the wall with finite-volume gradient approximations.
- B) Solving for the governing equations away from the wall and bridging a small distance between the wall and the inner location with a model. This type of approach can be termed a wall-modelled approach and the turbulence model used in conjunction is a so-called high-Reynolds number variant. The task of the wall model is to determine the interaction between the wall and the surrounding flow, meaning that it provides for:
 - a. Wall shear stress
 - b. Wall heat flux
 - c. Source terms for statistical turbulent quantities

Wall functions and the law of the wall

The ‘law of the wall’ (LotW) refers to the fact that the relationship between near-wall velocities and wall shear stresses can be described in a straightforward manner, using an algebraic relationship between scaled quantities. In the most commonly used form, the LotW reads

$$u^+ = \frac{1}{\kappa} \ln(Ey^+) \quad (11)$$

Where κ is the von Karman constant ($\kappa \approx 0.41$) and $E \approx 9.0$. Importantly, the scaled quantities read $u^+ = u/u_\tau$ and $y^+ = \rho u_\tau y / \mu$ and the scaling variable is the wall shear velocity $u_\tau = \sqrt{\tau_w / \rho_w} = \sqrt{\nu_w (\partial u / \partial y)_w}$ where subscript w denotes values at the wall. In ideal flows, meaning e.g. developed and smooth flat-plate, pipe or channel flows with zero pressure gradient, the LotW holds remarkably well for turbulent flows at various Reynolds numbers.

From the LotW it is possible to infer the solution (i.e. the wall shear stress, via the scaling variable u_τ) by iteratively solving an equation of the type $f(y^+) = 0$ by using the Newton iteration technique. Indeed, this is the way such models are utilised in wall-modelled large eddy simulations. However, for RANS computations there is an additional pathway which is even more convenient: with the assumption of local turbulence equilibrium at the wall (production rate = dissipation rate), the wall shear velocity can be described simply by



$$u_\tau = C_\mu^{1/4} k^{1/2} \quad (12)$$

Where $C_\mu = 0.09$ and k is the turbulent kinetic energy at the wall-adjacent cell centre (while at the wall $k = 0$). This leads to a wall shear stress expression of

$$\tau_w = \rho u_\tau^2 = \rho C_\mu^{1/2} k \quad (13)$$

While the fact that wall shear stresses would be directly related to the near-wall turbulent kinetic energy appears overly simplistic, it is a result of the application of the assumption of (i) a near-wall constant stress layer and (ii) local turbulence equilibrium. Then, while equations (11) and (13) are equivalent in ideal flows, there are some differences to their functionality in complex flows, such as the ones handled here. Indeed, as the turbulent kinetic energy k is governed by a transport equation, its behaviour at locations such as impingement result in a considerable difference to a direct application of the LotW, especially when heat transfer is concerned.

Heat transfer modelling and the thermal law of the wall

In addition to the low-Re approach (where flow and turbulence quantities are computed up to the wall) two wall models have been applied in this work. These include the (i) standard wall function, and (ii) the modified Angelberger wall function.

Standard wall function

$$T^+ = \begin{cases} Pr * y^+ & , y \leq y_T^+ \\ Pr_t(u^+ + P) & , y \leq y_T^+ \end{cases} \quad (14)$$

Where temperature scaling follows $T^+ = c_p \rho (T_w - T) u_\tau / q_w$ and the additional term reads

$$P = 9.24 \left[\left(\frac{Pr}{Pr_t} \right)^{3/4} - 1 \right] \left[1 + 0.28 \exp \left(\frac{-0.007 Pr}{Pr_t} \right) \right] \quad (15)$$

and the scaled transition distance is defined from the equation $Pr * y_T^+ - Pr_t \left[\frac{1}{\ln} \ln(E y_T^+) + P \right] = 0$.

Modified Angelberger wall function

In this wall treatment, the scaled thermal law of the wall appears similar as in the standard wall function

$$T^+ = \begin{cases} Pr * y^+ & , y \leq y_T^+ \\ Pr_t(u^+ + P) & , y \leq y_T^+ \end{cases} \quad (16)$$

However, the scaling for temperature is different, with

$$T^+ = - \frac{\rho_w c_p u_\tau T_w}{q_w} \ln \frac{T}{T_w} \quad (17)$$

The formulation is based on [15] with slight modifications in the Star-CD code [16]. The practical implication of the logarithmic term in this equation signifies that the model takes into account the effects of variable fluid properties of the near-wall cell due to the considerably varying near-wall temperature.



2.5.5 Rough wall modelling

Rough wall impact on near-wall fluid flows

Rough wall flows are encountered a plethora of flow components in engineering. From the purpose of many engineering processes (as indicated by e.g. the Moody diagram), increased roughness increases the resistance imposed by the walls on the surrounding fluid flow.

The similarities and differences between smooth and rough-wall flows have been recently studied. As indicated by Schulz and Flack [17] in their experimental campaign, the impact of roughness on the flow is limited to within a short distance of the near-wall vicinity. What this means in practice is that

- Rough walls induce higher wall shear stresses, i.e. flow resistance
- Turbulent flow characteristics (orientation and trends of Reynolds stresses) outside of the near-wall vicinity are similar to those in smooth-wall flows

What this implies is that it is meaningful to attempt to model rough near-wall processes with an approach bridging the gap between a (coarse) wall-adjacent cell and the wall, effectively with a modification of existing wall functions.

For the purpose of modelling rough wall flows in this work, it would be beneficial to develop a robust, yet simple, model to account for the roughness effects. This involves several steps:

- Having a suitable model to modify existing wall models to account for rough wall frictional resistance
- Connecting measurable surface roughness metrics with the quantities used by the models
- Modelling the relationship between rough wall momentum and heat transfer effects

Surface roughness is clearly a measurable quantity on solid walls. By measuring the distribution of point heights on a surface, one can quantify

- The average roughness on the surface (R_a)
- The root-mean-square roughness (R_{rms})
- A statistical distance between peaks and valleys on the rough surface (R_t)

Where R_t is determined by measuring surface heights over five separate one-dimensional lines and averaging the results. When rough-wall flows were first studied in the mid-1900s, the experimental setup involved coating surfaces with sand grains of different sizes [18]. These studies paved the way towards a standard metric for roughness: the sand-grain equivalent roughness, denoted here by R_s . Evidently real rough surfaces deviate from this form, making it non-trivial to connect real surfaces to the observations in the measurements. Figure 21 shows rough wall mean flow profiles from experiments [19].

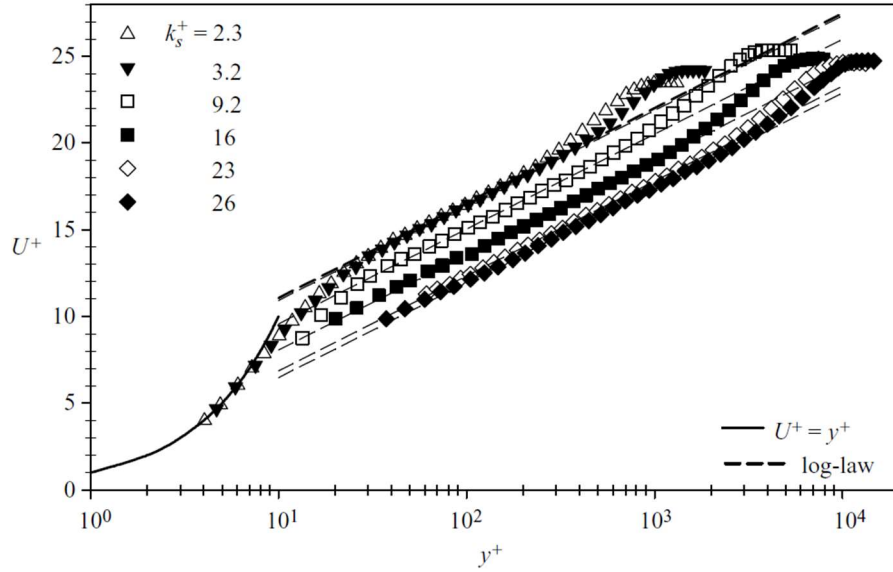


Figure 21. Changes to the position of the logarithmic layer of turbulent flows due to increasing scaled roughness [19].

The varying logarithmic laws in Figure 21 can be described with a slightly modified logarithmic law

$$u^+ = \frac{1}{\kappa} \ln(Ey^+) - G \quad (18)$$

Where G is usually a piecewise function of R_s . Effectively, when G increases, the log-law line will shift downwards, indicating an increased wall shear stress. Star-CD employs the following formulation:

$$u^+ = A + \frac{1}{\kappa} \ln\left(\frac{y^+}{R_s^+}\right) \quad (19)$$

Where $A = 8.5$ and R_s^+ is a scaled roughness, with the scaling functioning similarly to general distance scaling, $R_s^+ = \rho R_s u_\tau / \mu$. This formulation has been fitted with the data of Nikuradse [18].

Model for R_s

From the perspective of incorporating real surface properties in models, it is useful to try to evaluate the relationship between R_s and the measurable metrics R_a , R_{rms} , R_t . Flack & Schultz [20] investigated many roughness correlations and attempted to create a new one by examining detailed material surface properties (such as the roughness PDFs), the measurable metrics and effective frictional increases. They found that the RMS roughness R_{rms} and the skewness of the roughness PDF s_R were the most promising candidates to function as a baseline for a model that predicts the sand grain-equivalent roughness from the directly measurable quantities. The model they formulated reads

$$R_s = 4.43 R_{rms} (1 + s_R)^{1.37} \quad (20)$$

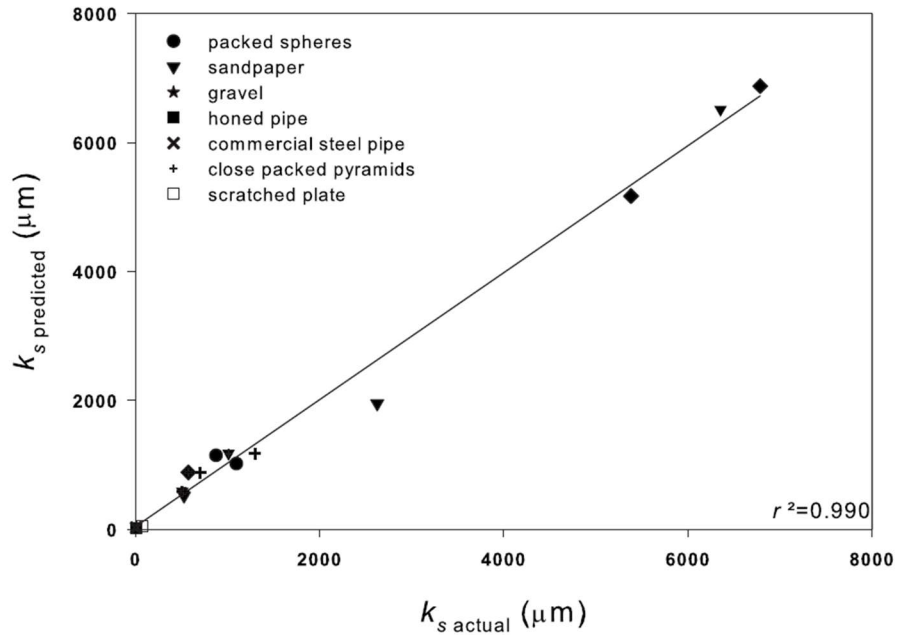


Figure 22. Comparison between actual and model-evaluated sand grain-equivalent surface roughness. Adapted from [20].

The skewness of the PDF effectively signifies whether there are more prominent peaks (positive s_R) or valleys (negative s_R) on the surface. Figure 22 shows how this model performs in a number of test cases with large differences in the surface structure; the correspondence is evidently excellent.

Heat transfer models: Strong Reynolds analogy

A straightforward intuitive argument presents that, as the surface area of rough walls is increased in comparison to smooth equivalents, there is more area available for heat transfer between the wall and the surrounding fluid. One can also state that the turbulent flow motion at the nominal wall position does not necessarily follow the conventional boundary conditions: in particular, turbulent fluctuations cannot be statistically assumed to approach zero as wall distance approaches zero.

Between rough wall induced momentum and heat transfer the conventional wall models in CFD follow the Reynolds analogy, i.e. that wall momentum and heat transfer increase and decrease similarly:

$$q_w \approx \tau_w \frac{c_p(T_w - T)}{u} \quad (21)$$

The Reynolds analogy RA can be defined as

$$RA = \frac{2St}{C_f} \quad (22)$$

Where $St = h/\rho u c_p$ is the Stanton number and $C_f = \tau_w/0.5\rho u^2$. A normalised Reynolds analogy factor RA/RA_0 is of special interest (RA_0 being the factor for a smooth wall) as it describes the relative increase of heat transfer in comparison to that of the momentum transfer:

- $RA/RA_0 > 1$: heat transfer is proportionally greater than momentum transfer
- $RA/RA_0 = 1$: the Reynolds analogy is fulfilled
- $RA/RA_0 < 1$: heat transfer is proportionally smaller than momentum transfer



In general, the Reynolds analogy is not fulfilled in rough-wall flows. The following represents an attempt to model this deviation using recently emerged literature.

Model for RA/RA_0

Recent work on understanding how the Reynolds analogy factor behaves in real flows includes papers by Bons et al. [21] and Forooghi et al. [22, 23]. The latter performed high-resolution DNS computations in channels with both artificial and real roughness elements. In the artificial cases, the types and scales of roughness elements were altered, while in the real roughness cases, measured surfaces of turbine blades and IC engines were utilised.

It is worth keeping in mind that despite the qualitative similarities between factors such as Reynolds stresses (turbulent momentum transfer) and turbulent heat fluxes, different phenomena are in play in the momentum and energy equations. One specific phenomenon is that of (pressure-induced) form drag, which is a term in the momentum equation but does not appear in the energy equation. Interestingly, rough-wall surfaces do impose a degree of form drag on the flow, and this is cited as one dominant reason why heat and momentum transfer do not match in rough-wall flows [23].

Forooghi et al. [23] found that, across their simulated cases (and the experiments of Bons et al. [21]) the relative impact of roughness on heat transfer could be modelled in a very simple manner by using the scaled roughness R_s^+ :

$$\frac{RA}{RA_0} = 0.55 + 0.45 * \exp(-R_s^+/130) \quad (23)$$

This formulation satisfies two constraints:

- 1) In the case of smooth walls, RA/RA_0 tends to 1
- 2) In the case of highly rough walls, RA/RA_0 tends to a constant value (0.55)

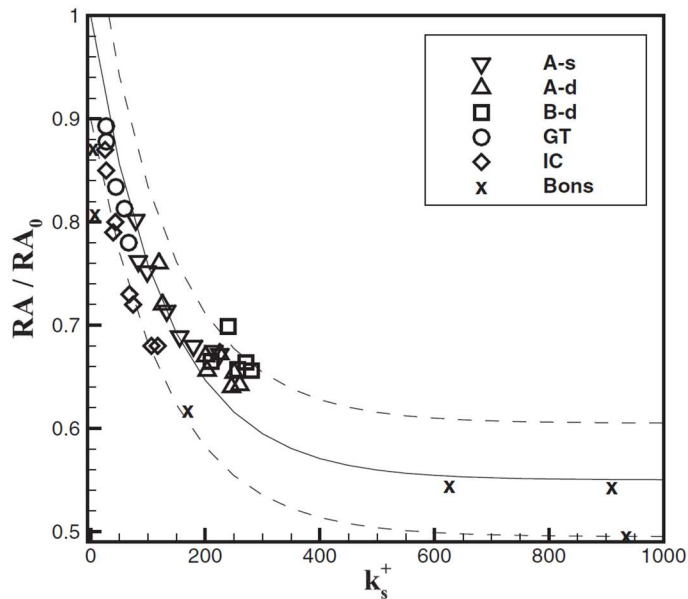


Figure 23. Performance of the model for scaled Reynolds analogy factor (solid line) and its correspondence with both computational and experimental references (markers). Adapted from [23].

The functionality of this model in terms of the reference data can be seen in Fig. 23. Clearly, some deviations exist to the model graph depending on the condition and R_s^+ region, but the fit is reasonable

overall. It should be noted that the authors state that finding a parametrisation based on R_s^+ is far better than can be achieved for any directly measurable, physical roughness parameter.

The primary practical implication of Figure 23 is that the increases of heat transfer on rough walls can be quite substantially smaller than for the momentum transfer. Effectively, if one does not apply this correction, but uses a methodology to model rough wall flow momentum transfer, one risks a considerable overestimation of the heat flux estimate.

2.5.6 OM651 computational grid, workflow and case setup

The simulation of the TUB Mercedes-Benz OM651 engine is carried out in collaboration with IAV. The operating condition in question is as follows:

- Engine speed 2,000 1/min, BMEP 20 bar, compression ratio 16.2, rail pressure 1800 bar, injected fuel mass 59 mg
The following wall temperatures were prescribed based on estimates: Piston crown: 546 K; Cylinder head: 508 K; Liner: 439 K; Intake valve face: 621 K; Exhaust valve face: 722 K

The fuel-air charge is influenced by swirl motion and the configuration involves a swirl number of ca. 2.1 throughout compression.

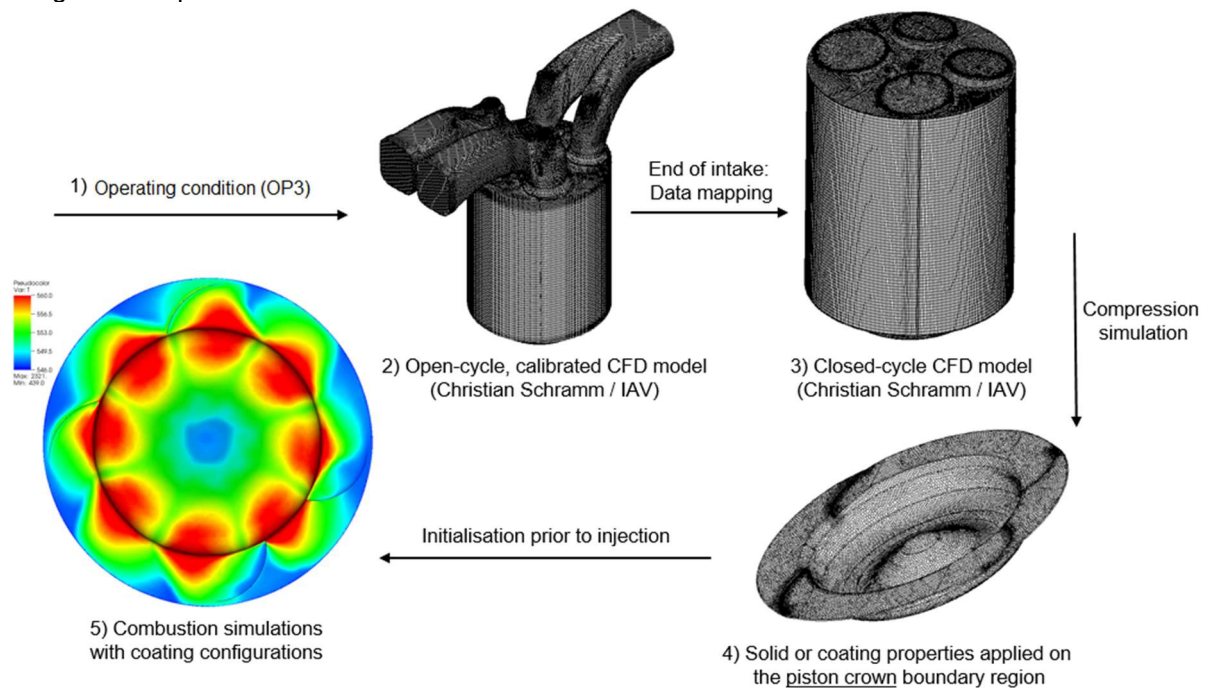


Figure 24. Schematic of the workflow in the engine simulation cases. The workflow includes both open-cycle simulations (carried out at IAV) and closed-cycle simulations

The focus of this work is to simulate the power stroke in a closed cycle configuration and examine coating effects therein. However, there are several preceding steps that have been carried out in order to get to the power stroke simulation. The workflow includes two separate types of CFD models, the open-cycle model (simulating all four engine strokes) and the closed-cycle model (simulating only compression and power strokes).

For the open-cycle model (which includes the gas exchange), initial and boundary conditions have been provided via a GT-Power process simulation model. The open-cycle model has been calibrated in detail at IAV. At the end of the intake stroke in the open-cycle model, variables are mapped to the closed-



cycle geometry, and the compression stroke is simulated with this configuration. Prior to injection timing, coating properties are applied to the piston crown boundary region where the sprays impinge. Finally, the combined 3D/1D-CHT simulation is carried out with the specified piston crown.

The closed-cycle grid includes 1.7 million cells at BDC and 0.6 million cells at TDC. The grid is composed of both hexahedral and polyhedral cells. The combustion chamber walls are covered with a 0.2 mm prismatic layer. The es-ice plugin is employed for mesh movement with cell layer removal. Computations presented here include

- smooth and rough aluminium pistons
- smooth and rough porous zirconia coatings
- smooth and rough high-velocity low-pressure (HVLP) thermal barrier coatings recently presented by the University of Madison-Wisconsin [24]

The two first variants are then directly related to the engine experiments, while the final material is a state-of-the-art material with highly compatible material properties for thermal swing. For these cases, the standard wall model in Star-CD is adopted as a basis. Rough walls in all cases have sand grain-equivalent roughness of 115 μm .

3 Results

3.1 Computational characterisation of applicable materials

3.1.1 1-D CHT simulations to assess insulation materials and configurations

For the standalone approach (Figure 25), the input heat flux to Equation (3) is obtained, for the purpose of sensitivity studies, from literature or from previous experience in similar engine-relevant operating conditions. It is expressed using a time-varying heat transfer coefficient and gas temperature. A wide variety of materials can be tested with this procedure, which only requires the density, specific heat and thermal conductivity of the individual layers.

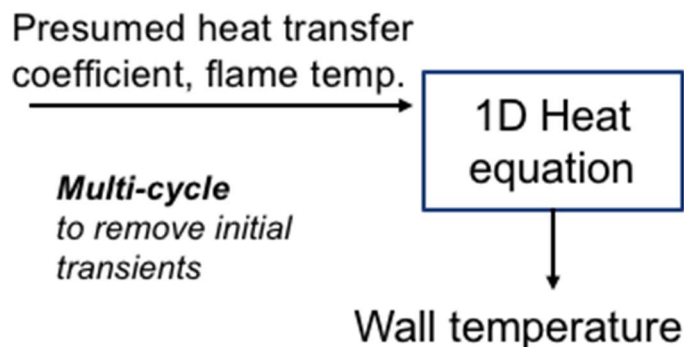


Figure 25. Schematic of standalone 1D-CHT computation.

The parametric variation of thermal conductivity, density and specific heat capacity considered for the study is shown in Figure 26. Parameter values are taken for materials typically representing either TSM-like or TBC-like behaviour based on data for widely available materials (e.g. Zirconia).

It must be noted that the standalone 1D-CHT method does not consider spatial variations. These can be significant especially in diesel combustion, which is classically characterised by thermal stratification, depending on operating load, turbulent flow field or duration of injection. A high stratification of solid



component temperatures may also have negative effects on durability. Spatial variations are considered in the integrated CHT-CFD approach in WP4.

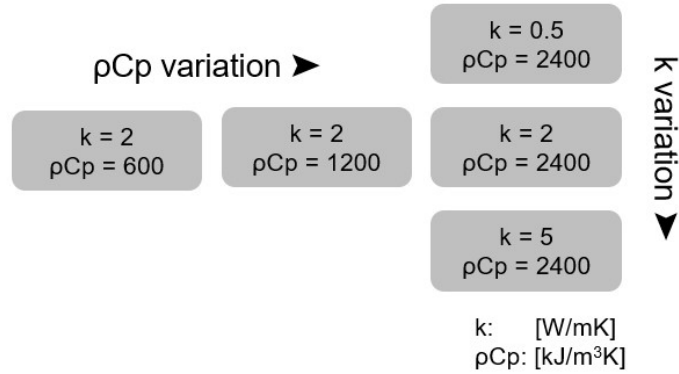


Figure 26. Operating conditions.

A thicker coating reduces temperature swing amplitude and increases cycle-mean temperature. This leads to reduced net heat loss, increased fresh air heating, as can be seen in Figure 27:

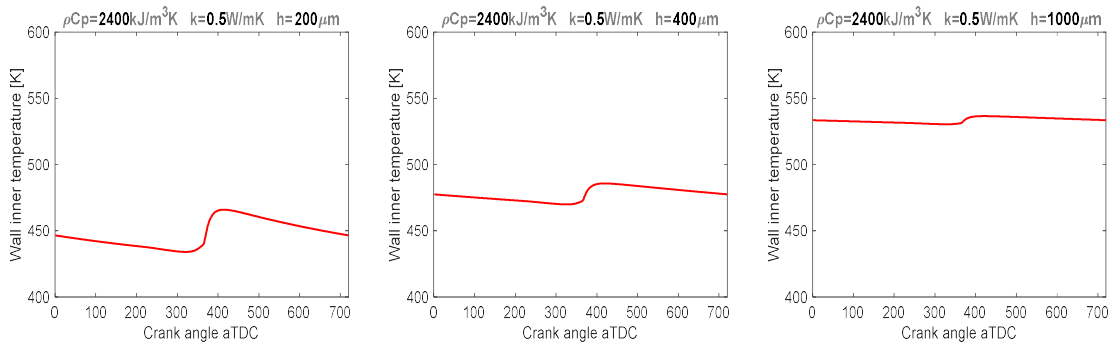


Figure 27. Influence of coating thickness (200, 400, 1000 μm).

Thermal conductivity λ affects cycle-mean temperature but not temperature swing amplitude. Lower λ results in reduced net heat loss, increased fresh air heating; as shown in Figure 28. On the other hand, heat capacity ρC_p affects only temperature swing amplitude and not the cycle-mean temperature, as seen in Figure 29. The net heat loss is not appreciably influenced by ρC_p .

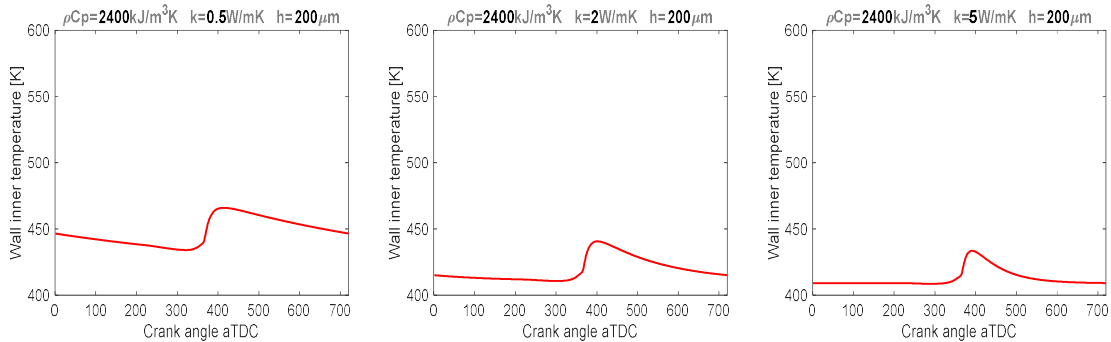


Figure 28. Influence of thermal conductivity (0.5, 2.0, 5.0 W/mK) for coating thickness 200 μm.

In summary, the temperature swing amplitude increases with a reduction in either density, specific heat capacity, or thickness of the coating, and is not greatly affected by the thermal conductivity. Further,

only changing the density or specific heat capacity does not cause an appreciable change in the net heat loss. The cycle-mean temperature is increased by a reduction in thermal conductivity (or a thicker coating), but is unaffected by density or specific heat capacity. Between TBCs and TSMs, there are differences in both specific heat as well as thermal conductivity, the combined effect of which leads to improved insulation in TSMs without the disadvantage of intake air heating.

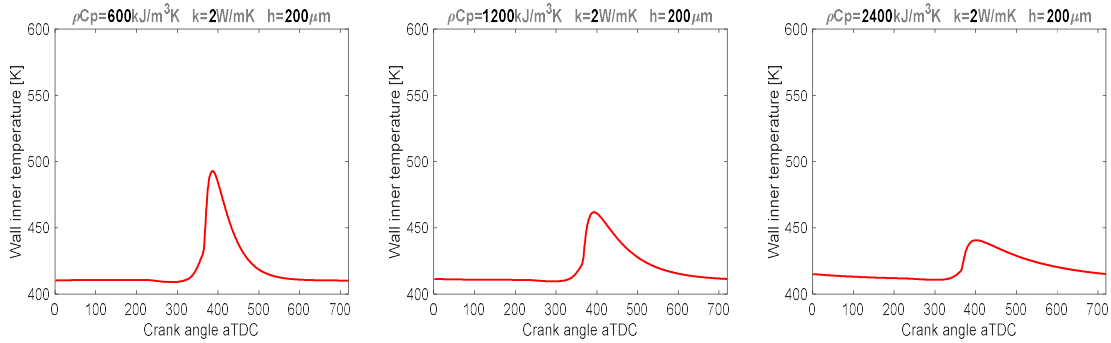


Figure 29. Influence of specific heat capacity ($\rho C_p = 600, 1200, 2400 \text{ kJ/m}^3\text{K}$) for coating thickness $200 \mu\text{m}$.

3.1.2 Examining the validity of the 1-D CHT assumption in engine conditions

The previous type of 1-D investigation was extended to two dimensions to determine the impact of wall-tangential heat transfer within the wall. A spatial heat flux distribution was provided to a surface in a cyclical manner following the principle presented in the previous, more simplified approach. The spatial distribution of an impinging diesel spray was emulated with a Gaussian function, resulting in a high peak at the time of maximum heat transfer rate, and a near-constant value otherwise.

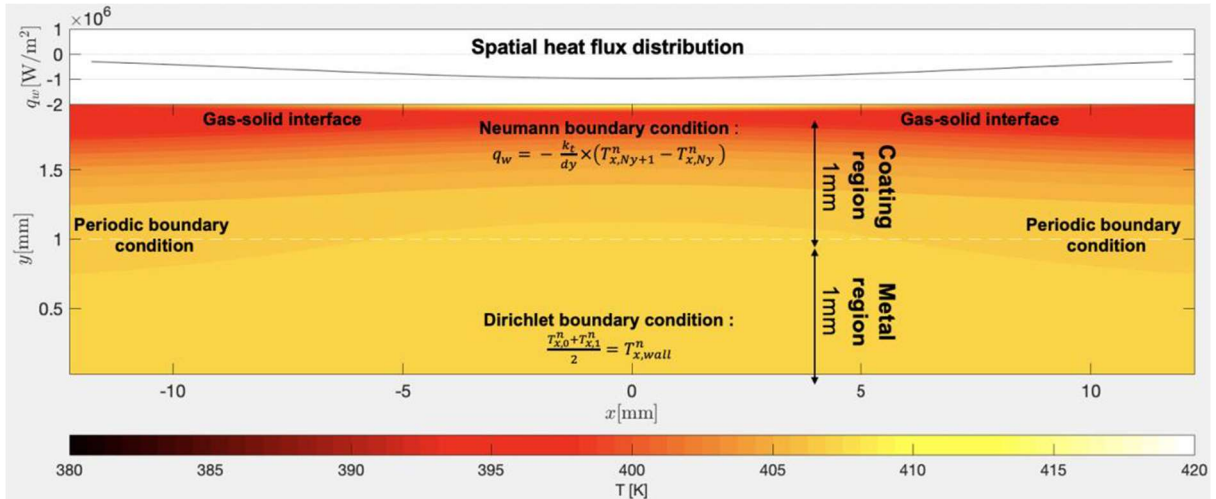


Figure 30. Schematic of the simulation setup for 1D/2D comparisons.

To carry out a comparison between 1D and 2D assumptions, the 2D solid configuration was run in two modes, with different numerical operators: (i) with the full 2D stencil governing multidimensional heat transfer, (ii) with a simplified stencil where only wall-normal heat transfer is effective. Note that in both cases, the heat flux boundary condition does have spatial variability. The following conclusions are made based on the campaign:

- A thermal swing material exhibits the highest differences between 1D and 2D heat transfer assumptions



- These differences are however small (fractions of K) and are not assumed to pose a marked impact in 3D computations.

3.2 Heat transfer experiments in the high pressure and temperature cell

3.2.1 Spray morphology: broadband chemiluminescence

Figure 31 shows the flame-base and tip penetration from broadband radiation and it can be seen that all base and tip curves overlay with each other, respectively, proving that the conditions inside the chamber have remained the same for all four sensors. Moreover, the trends show that the flame base stabilizes after ignition has started and only increases after fuel stops being injected. On the other hand, the flame tip continuously grows as the spray penetrates further into the chamber and stops only once it hits the impingement plate.

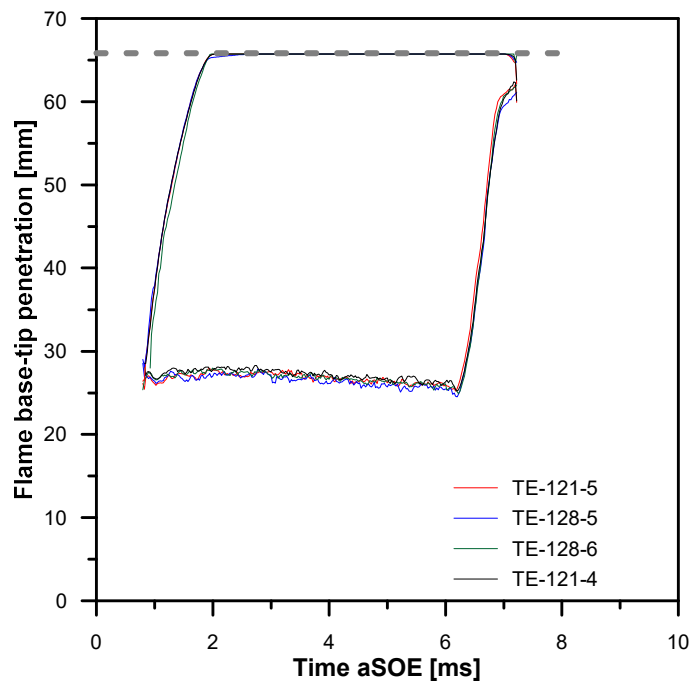


Figure 31. Flame-base and -tip penetration for all four sensors under the same conditions using broadband radiation.

Figure 32 shows a comparison of the parameters obtained using both optical techniques, and although the trends are similar, there are important differences to point out. OH* is a precursor of combustion and appears before soot is formed, therefore the flame base measured with OH* chemiluminescence is closer to the nozzle than the one measured with broadband chemiluminescence. Once OH* and soot appear within the spray, the tip detected via either method grows as the spray enters further into the chamber. As mentioned in the previous paragraph, the tip of the spray stops as it impinges the plate, however, the flame tip detected with OH* seems to stop before only because that is the end of the field of view of the camera.

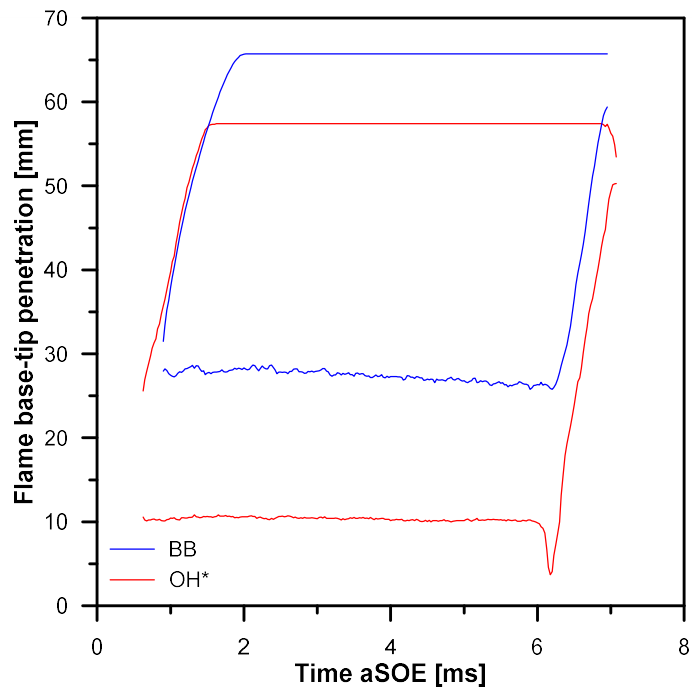


Figure 32. Comparison of flame-base and -tip penetration using OH* and broadband chemiluminescence.

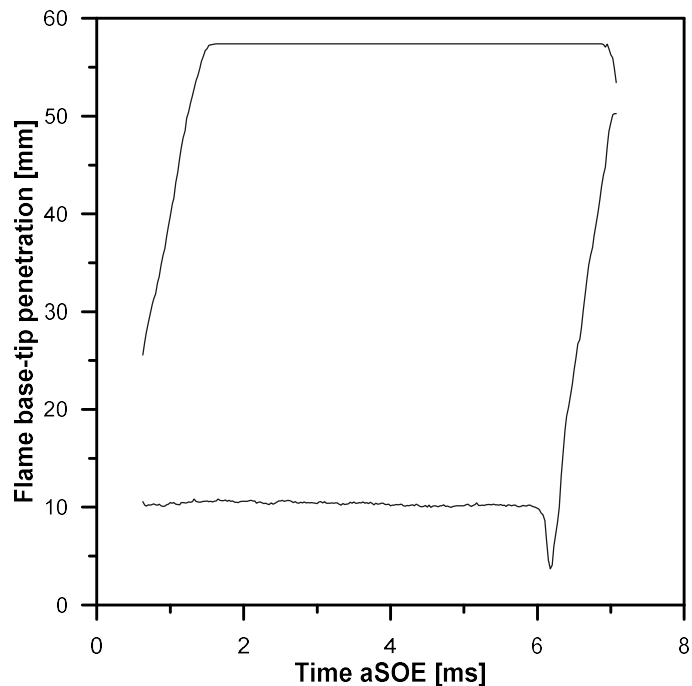


Figure 33. Flame-base and -tip penetration using OH* chemiluminescence.

Figure 33 shows the isolated curves for flame-base and tip using OH* chemiluminescence. As opposed to the trend described in Figure 31, the flame base briefly goes back in the direction of the injector before lifting off completely. This is called combustion recession and happens after injection has finished and there is no longer an equilibrium between the flame speed and injection velocity, so the flame travels back toward the injector.

Figure 34 shows a comparison of the flame-base and -tip penetration at 800 K and 900 K of ambient temperature using OH* chemiluminescence. It can be seen that although the flame tip seems to appear at a similar position in both cases, the one corresponding to the higher temperature has a higher slope. This is due to the larger momentum from the premixed combustion causes the tip of the spray to accelerate faster. The flame-base is further from the injector for the lower temperature case due to the lower reactivity of the environment.

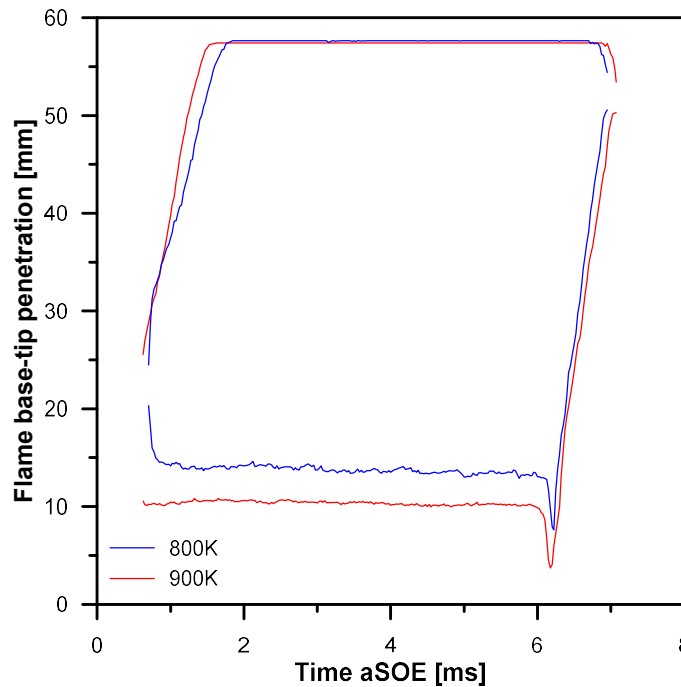


Figure 34. Comparison of flame-base and -tip penetration at 800K and 900K of ambient temperature using OH* chemiluminescence.

3.2.2 Wall heat flux measurements: uncoated case

Two experimental campaigns have been performed. First one with uncoated plates to understand the wall heat transfer and study its behaviour under different conditions. Second, another campaign using a Zirconia-coated plate to understand the effects of coating.

Figure 35 shows the heat flux measured using one plate and four different sensors, this was done to identify possible sensitivity differences among all sensors. Figure 36 shows the heat flux using the four sensors mounted on a separate plate each. From both figures it can be seen that there is little variation among sensors and plates, indicating that the conditions inside the cell are repeatable and that the sensors yield sufficiently similar results. Looking at the trend of the heat flux, it remains close to zero up to 2.5 ms due to the injection delay and the time needed for the spray tip to reach the plate. Once the spray impinges on the plate, the heat flux rapidly increases with a peak around 10 MW/m² and then stabilizes at a lower value of around 8 MW/m² for the diffusion-flame. Finally, injection stops at around 7.5 ms and the heat flux decreases back to the base value.

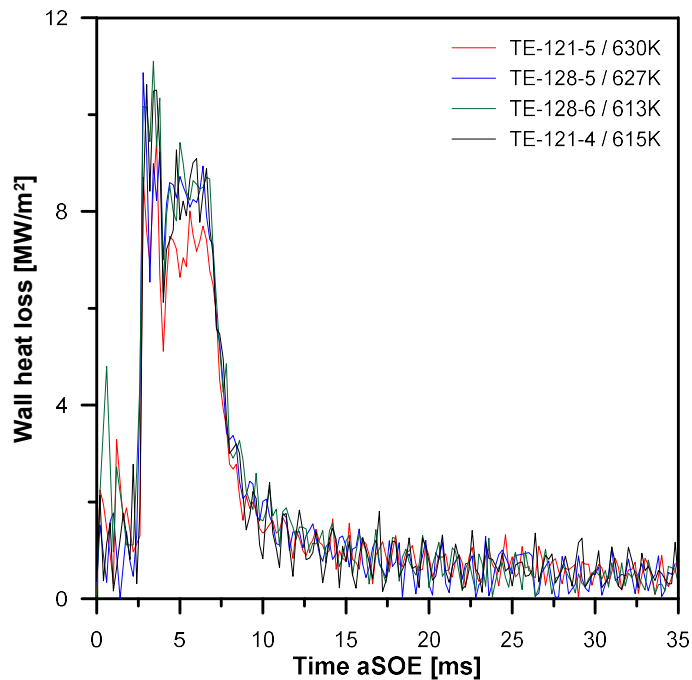


Figure 35. Comparison of heat flux measurements under the same conditions using the same impingement plate and four different sensors.

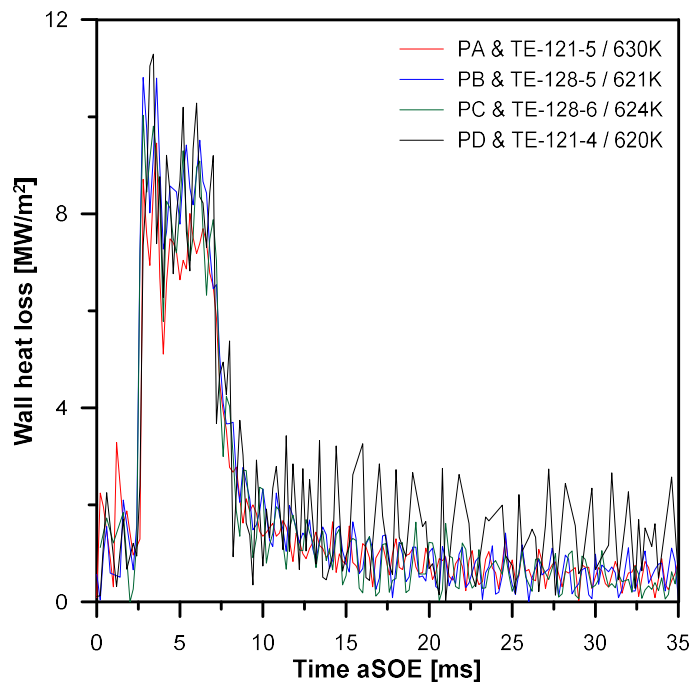


Figure 36. Comparison of heat flux measurements under the same conditions using four different plate-sensor combinations.

A similar comparison can be made from Figure 37, where the surface temperature variation is shown for all sensors mounted on separate plates. The cell body is heated up to 500 K and the temperature variation is caused by the flame impinging the plate surface. Similarly to Figure 35 and Figure 36, there is no significant temperature increase up to 2.5 ms due to the injection delay and the time need for the spray tip to reach the plate. However, once the spray impinges on the plate, the temperature increases rapidly with a peak around 50 C° at around 7.5 ms and decreases slowly to the base value.



As opposed to the trend of the heat flux in which a peak can be seen at the time of impingement, followed by a stabilized phase cause by the diffusion flame, the temperature increases continuously as long as the flame is heating up the surface. Once the flame burns out, both curves start to decrease.

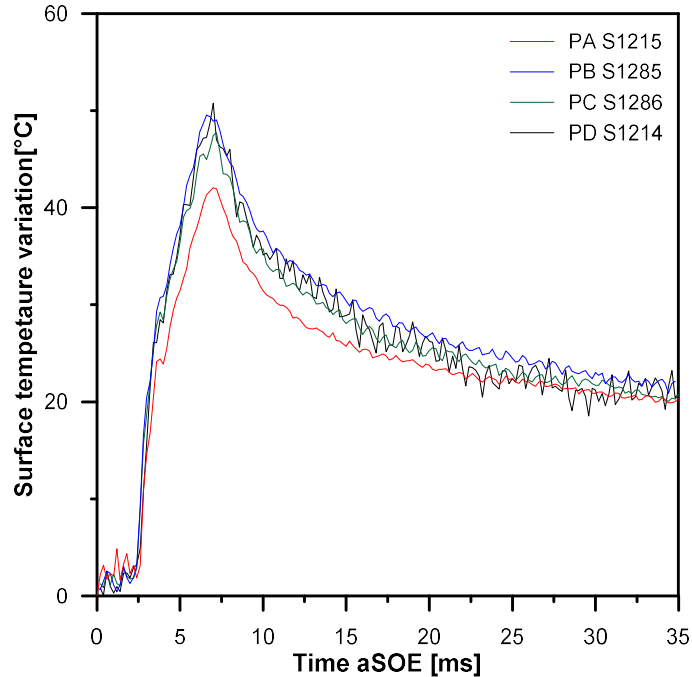


Figure 37. Comparison of surface temperature measurements under the same conditions using the same impingement plate and four different sensors.

The effect of the ambient temperature variation of 800 K and 900 K is shown in Figure 38 for the heat flux and in Figure 39 for the surface temperature. It can be seen that the heat flux traces are very similar for both cases, the main difference is that the heat flux begins earlier for the case of 900 K. This is caused by the acceleration of the flame tip due to the earlier combustion, which causes the flame to reach the plate earlier than in the case at 800 K. For the temperature variation there is a constant offset between both cases, in which the case at 800 K presents a lower temperature increase than the 900 K case. This is expected as the lower ambient temperature will cause the flame to have a lower temperature. Although the peak of surface temperature seems to happen at a very similar time for both cases, around 7.5 ms, the rising slope also differs for the aforementioned reasons.

Figure 40 and Figure 41 present the heat flux and temperature variation at different energizing times. Looking at the longest energizing times, 1 ms, 1.5 ms and 4 ms, it can be seen that they present the same initial phase, in which the heat flux starts at the same time and the peak also reaches very similar values around 10 MW/m². The main difference can be noted in the stabilized phase caused by the diffusion flame which is proportional to the injection duration. The case for 500 μ s has different behaviour due to the fact that a much smaller amount of fuel is injected into the chamber, causing it to overmix and ignite later than the other cases. Since a smaller amount of fuel is burned the flame reached the place for a shorter amount of time causing the peak and duration of the heat flux to be smaller.

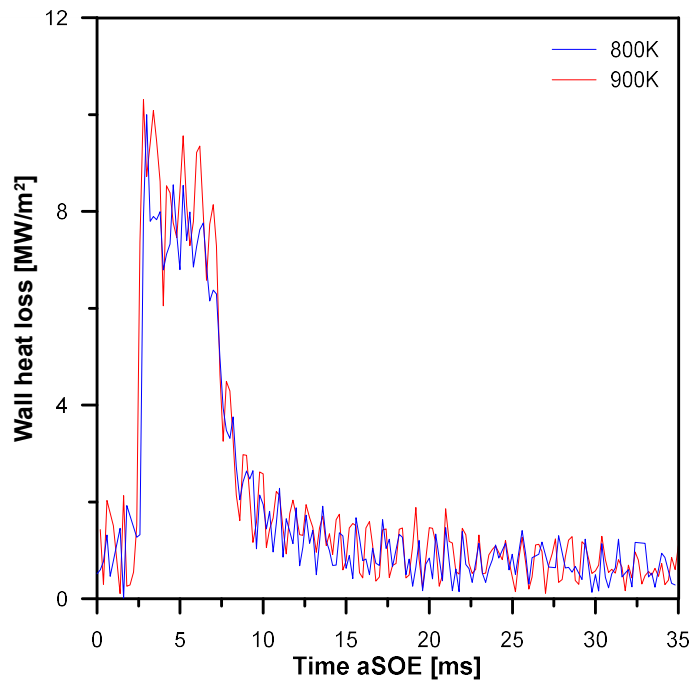


Figure 38. Comparison of heat flux measurements under the 800K and 900K of ambient temperature.

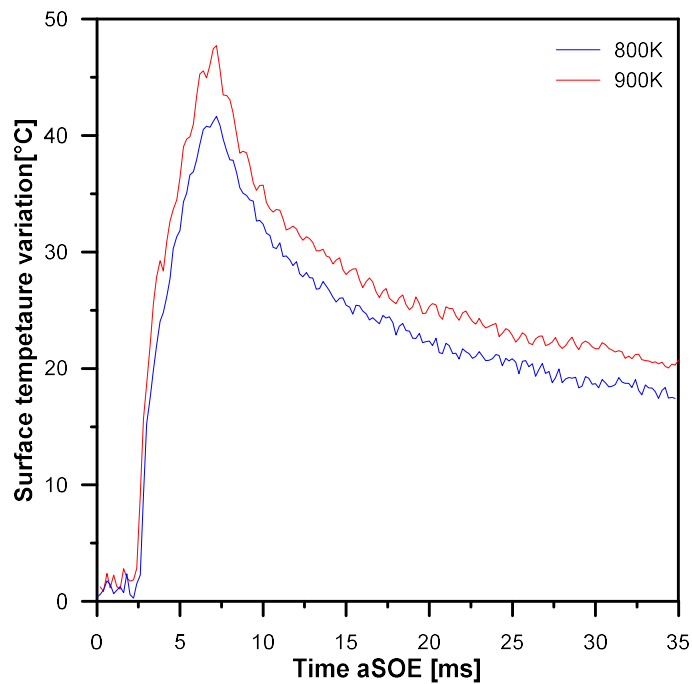


Figure 39. Comparison of surface temperature under the 800K and 900K of ambient temperature.

A similar pattern can be seen for the temperature variation, where the cases with longer injections have similar temperature increase phases which are different only by the time in which the peak is reached. These times are consistent with those seen in Figure 38 and are proportional to the injection duration. The difference in peak temperature variation is also linked the smaller amount of fuel injected and the short diffusion flame phase.

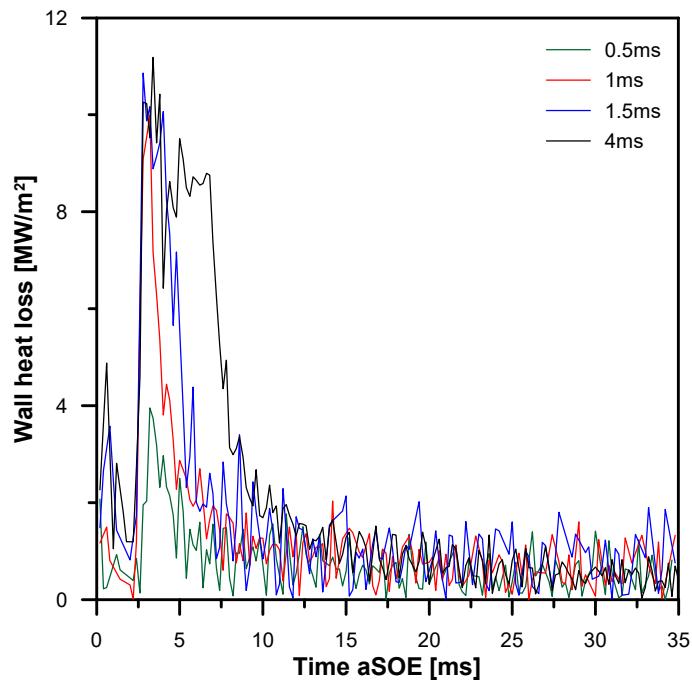


Figure 40. Comparison of heat flux measurements under the same ambient conditions with four different energizing times.

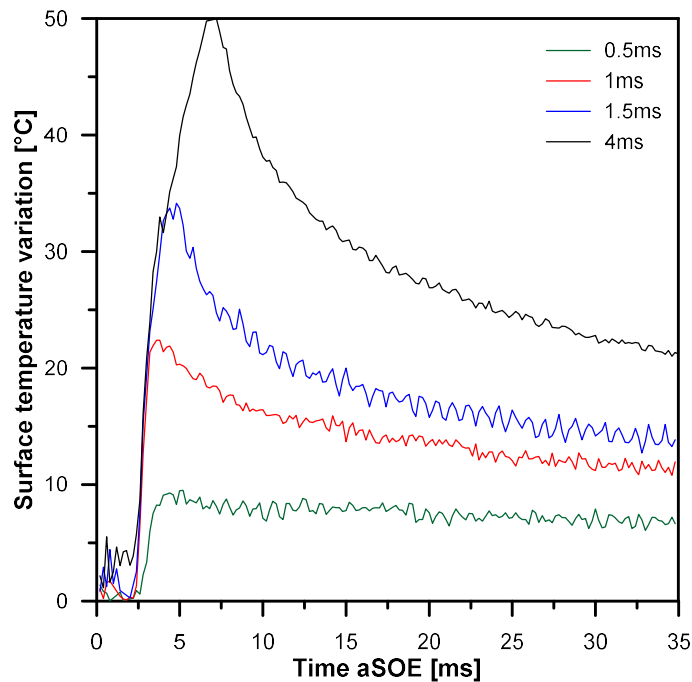


Figure 41. Comparison of surface temperature under the same ambient conditions with four different energizing times.

Figure 42 presents the heat flux for a combination of injection pressures and energizing times, 500 bar for 1.5 ms, 1,500bar for 1.5 ms and 1,500 bar for 4 ms. The cases at 1,500 bar, show the same trends seen in Figure 40, in which the longer injection dominates the stabilized phase cause by the diffusion flame. On the other hand, the case at 500 bar presents a peak at a much later time due to the lower tip velocity caused by the injection pressure. This effect combined with the shorter injection duration, causes the peak to be smaller and to have virtually no stabilized phase, as the injection stops at a similar time in which the flame reaches the plate.

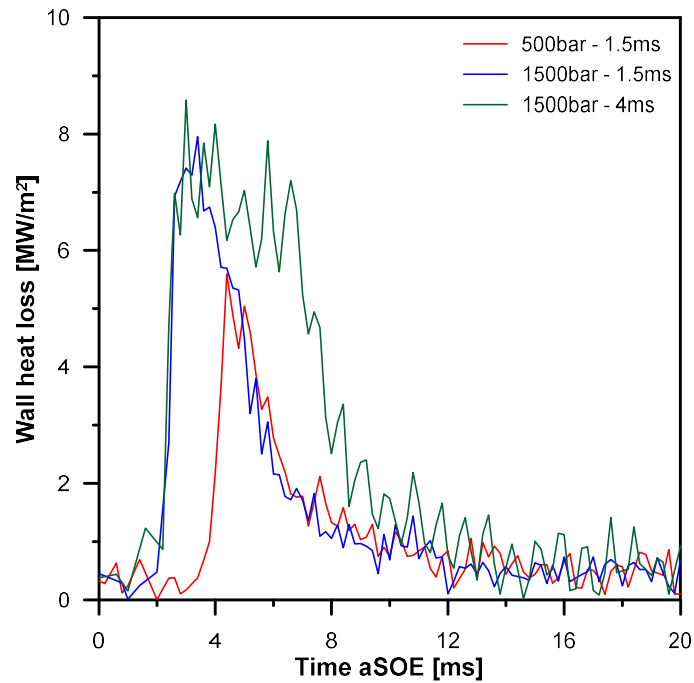


Figure 42. Comparison of heat flux measurements under the same ambient conditions with three combinations of injection pressures and energizing times.

3.2.3 Wall heat flux measurements: coated case

Figure 43 and Figure 44 present the heat flux and temperature variation between an uncoated and a zirconia coated plate (C).

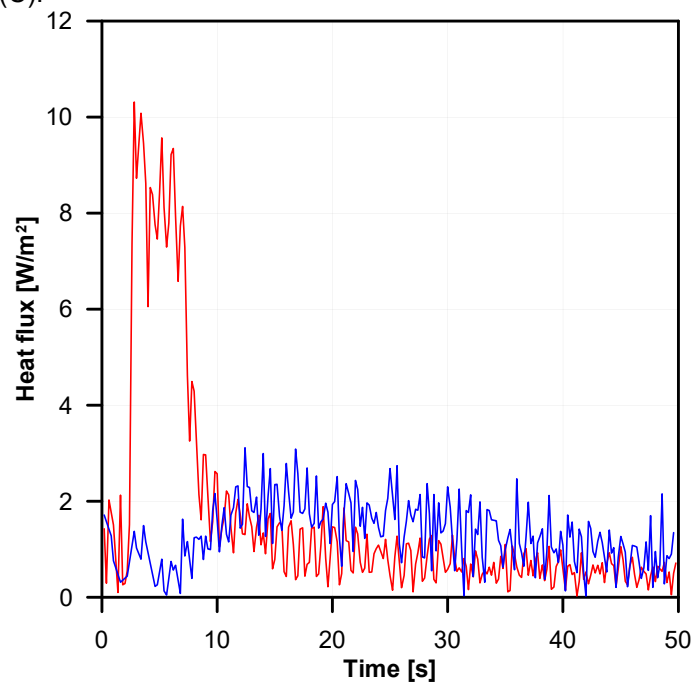


Figure 43. Comparison of heat flux measurements under the same ambient for an uncoated and a zirconia coated plate.

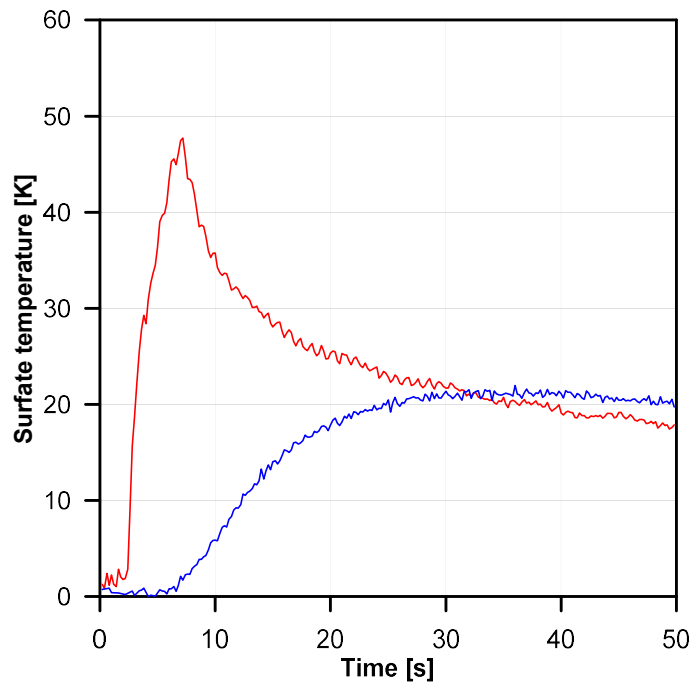


Figure 44. Comparison of surface temperature measurements under the same ambient for an uncoated and a zirconia coated plate.

It can be seen that the coated plate presents a much higher latency, in which the maximum heat flux is only a fraction of the uncoated reference, 2 MW/m^2 compared to 10 MW/m^2 . A similar trend is noted with the sensor temperature. However, observing these coated results is misleading as the measurement location within the coating considerably distorts the impression of the surface heat flux. Hence, the techniques described in Section 2.4.5 are employed in recovering the true surface heat flux.

3.2.3.1 Inferring surface heat flux from embedded sensor output

Porous zirconia coating, $130 \mu\text{m}$

Figure 44 shows the difference between the raw (ensemble-averaged) measured output in the uncoated (red) and coated (blue) cases. Applying the techniques in Section 2.4.5 2, Figure 45 shows the result of the iterative solution procedure. In the top frame, the blue curve represents the (filtered) measured heat flux which serves as the boundary condition at $x = x_L$, whereas the solution attempt is shown by the black curve.

It is seen that the heat flux increase to its maximum value happens in a time scale of ca. 1 ms – in contrast, the decreasing portion is much longer-lasting, as is expected from the uncoated experiments. The comparison between measured and simulated temperatures, i.e. the solution criterion, shows a good match over the simulated time. From the results, it is worth pointing out the following:

- Both the heat flux and the temperature measured at the sensor beneath the coating show distinctly different temporal trends and wholly different magnitudes than the surface quantities. This contrast concisely shows why it is imperative to carry out the present type of analysis.
- The solution criterion, i.e. the temperature trace at the bottom of Fig. 45, is very sensitive to the setting of the RHS Neumann boundary condition (the heat flux profile). Indeed, even a q_2 change of a few per cent will change the sensor temperature correspondence dramatically. This is a strong indicator that the attempt in the top frame is indeed a good solution approximation for the present situation.

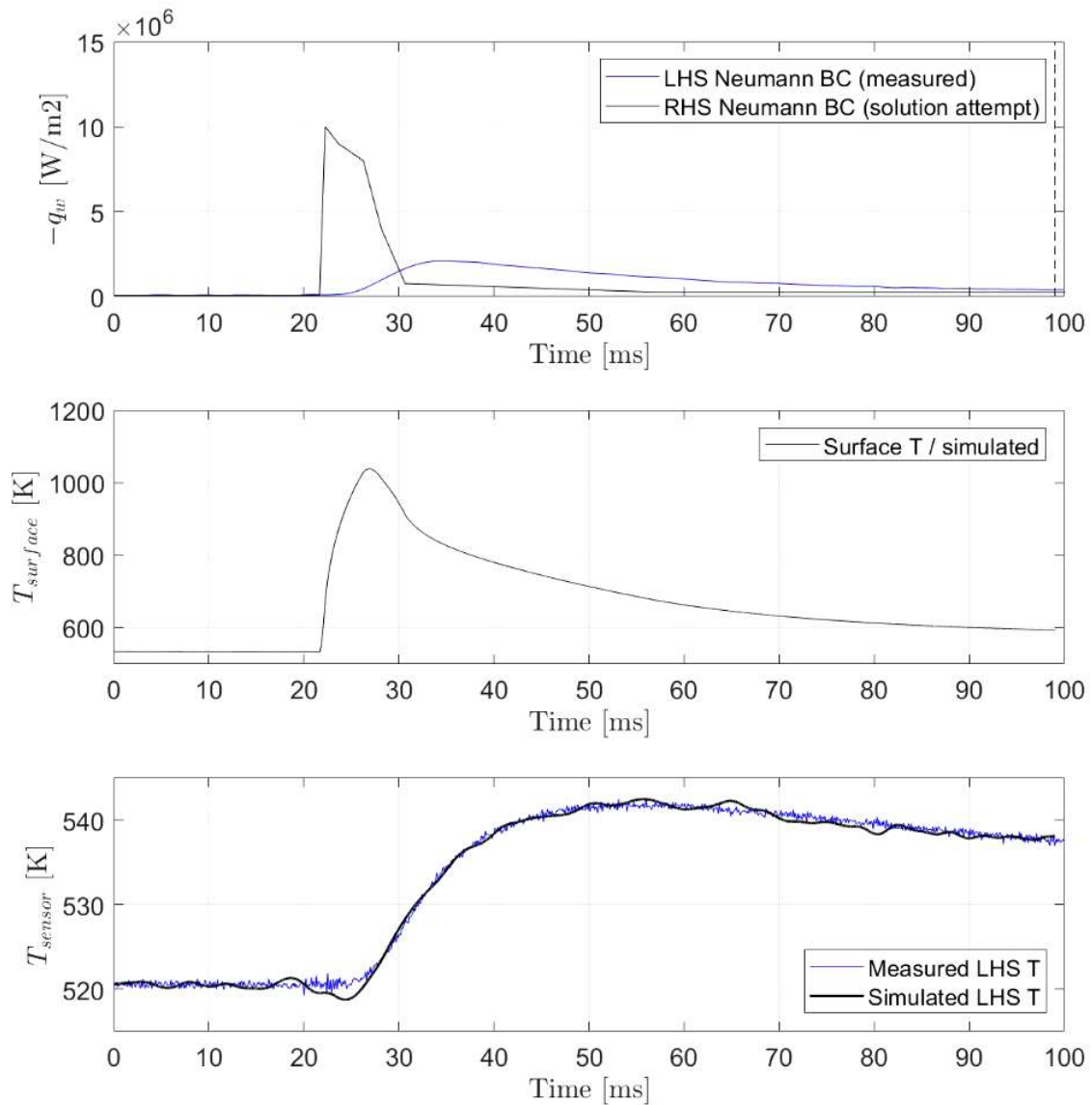


Figure 45. Visualisation of the solution heat flux (top), associated surface temperature evolution (centre) and the solution criterion sensor temperature (bottom).

The obtained result then begets additional questions:

- 1) How does this solution attempt compare with the uncoated heat flux?
- 2) How sensitive is the solution to uncertainties such as the coating layer thickness?

Fig. 46 shows the result from the above procedure compared with the uncoated result. In the figure, it is noted that the (black and magenta) profiles are remarkably similar in terms of their magnitude and shape. The indication hereof is then that the coated heat flux likely does not differ much from the uncoated one.

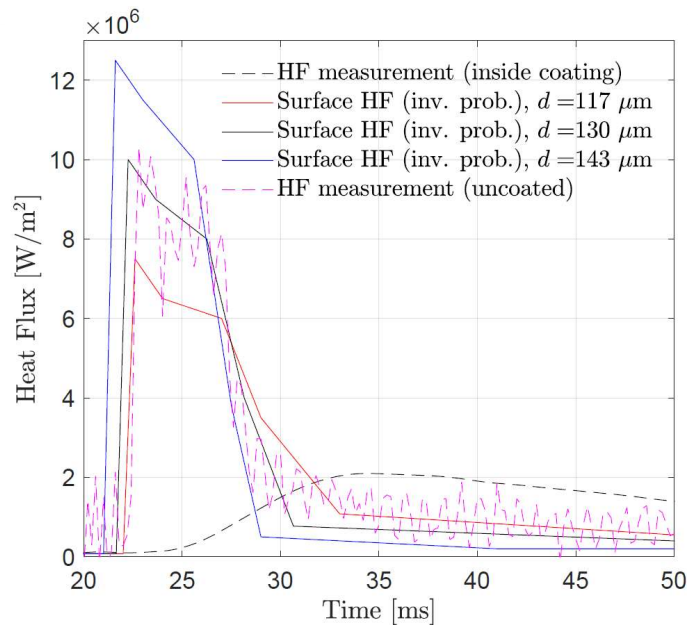


Figure 46. Measured surface heat flux (uncoated), heat flux within the coated surface, as well as three inverse solutions to the coated heat transfer problem with different thickness assumptions

However, it is prudent to carry out an uncertainty analysis as to the impact of the actual coating thickness. Figure 46 shows the impact of either decreasing or increasing the coating thickness by 10 % in comparison to the nominal thickness of 130 μm .

Each solution in Figure 46 is representative of a situation where the sensor temperature signal in Figure 45, i.e. the solution criterion, is fulfilled. As can be observed, the thickness influences primarily the magnitude of the indicated heat flux. As a secondary impact, the “tail” of the heat flux profile changes.

3.3 Heat transfer simulations using 3D CFD

The simulations carried out, and their purpose for furthering the objectives of the project, are present in Table 5 and Table 6.

The following sections describe the results of these simulations, starting from phenomenological correspondence analysis and continuing towards quantitative metrics.



Table 5. List of HTDZ simulations, carried out with a sector mesh and the CMC combustion model.

Cell Simulations					
ID	Near-Wall Approach	Grid	Roughness	Coating / CHT	Purpose
A-001	Low-Re	Wall-normal-resolved	None	None	Determine Characteristic Thermal BL scales for grid generation
B-001	Wall-modelled / Standard	Wall-modelled / Fine	None	None	Determine approach performance and grid sensitivity
B-002	Wall-modelled / Angelberger	Wall-modelled / Fine	None	None	Determine approach performance and grid sensitivity
B-003	Wall-modelled / Standard	Wall-modelled / Coarse	None	None	Determine approach performance and grid sensitivity
B-004	Wall-modelled / Angelberger	Wall-modelled / Coarse	None	None	Determine approach performance and grid sensitivity
C-001	Wall-modelled / Angelberger	Wall-modelled / Fine	None	1DCHT / steel properties	Determine CHT influence on uncoated results (if any)
D-001	Wall-modelled / Angelberger	Wall-modelled / Fine	None	1DCHT / 130µm coating / zirconia	Determine indicated influence with "ideal" (smooth, sealed) coating
D-002	Wall-modelled / Angelberger	Wall-modelled / Fine	Zirconia roughness (~115µm R_s)	1DCHT / 130µm coating / zirconia	Determine Roughness influence on coated results

Table 6. List of engine simulations, carried out with a full combustion chamber mesh and the ECFM-3Z combustion model.

ID	Near-Wall Approach	Roughness	Coating / CHT	Purpose
E-001	Wall-modelled / Standard	None	1DCHT / Aluminium properties	Baseline case
E-002	Wall-modelled / Standard	Zirconia roughness (~115µm R_s)	1DCHT / Aluminium properties	Determine roughness impact on baseline case
E-003	Wall-modelled / Standard	None	1DCHT / 130µm coating / Zirconia	Determine indicated influence with "ideal" (smooth, sealed) coating
E-004	Wall-modelled / Standard	Zirconia roughness (~115µm R_s)	1DCHT / 130µm coating / Zirconia	Determine impact with a realistic roughness value with the present project components
E-005	Wall-modelled / Standard	None	1DCHT / 130µm coating / UWM-HVLP	Determine indicated influence with "ideal" (smooth, sealed) version of HVLP spray coating
E-006	Wall-modelled / Standard	Zirconia roughness (~115µm R_s)	1DCHT / 130µm coating / UWM-HVLP	Determine impact with a hypothetical roughness value equivalent with the present project components

3.3.1 HTDZ simulations: Spray morphology

The spray evolution is observed here using both temperature contours and virtual luminosity. The latter allows us to compare with the experimentally observed soot luminosity. A line of sight luminosity is computed as

$$L_v(r, z) = \int_s f(r, z) ds \quad (24)$$

$$f(r, z) = A * F_{V,soot} * T^4 \quad (25)$$

Where $F_{V,soot}$ is the soot volume fraction and A is an empirically defined constant. The integral L_v is computed for each point in the perpendicular projection plane to the camera, using the ensemble of corresponding points in the r, z plane (i.e. along the dashed lines).

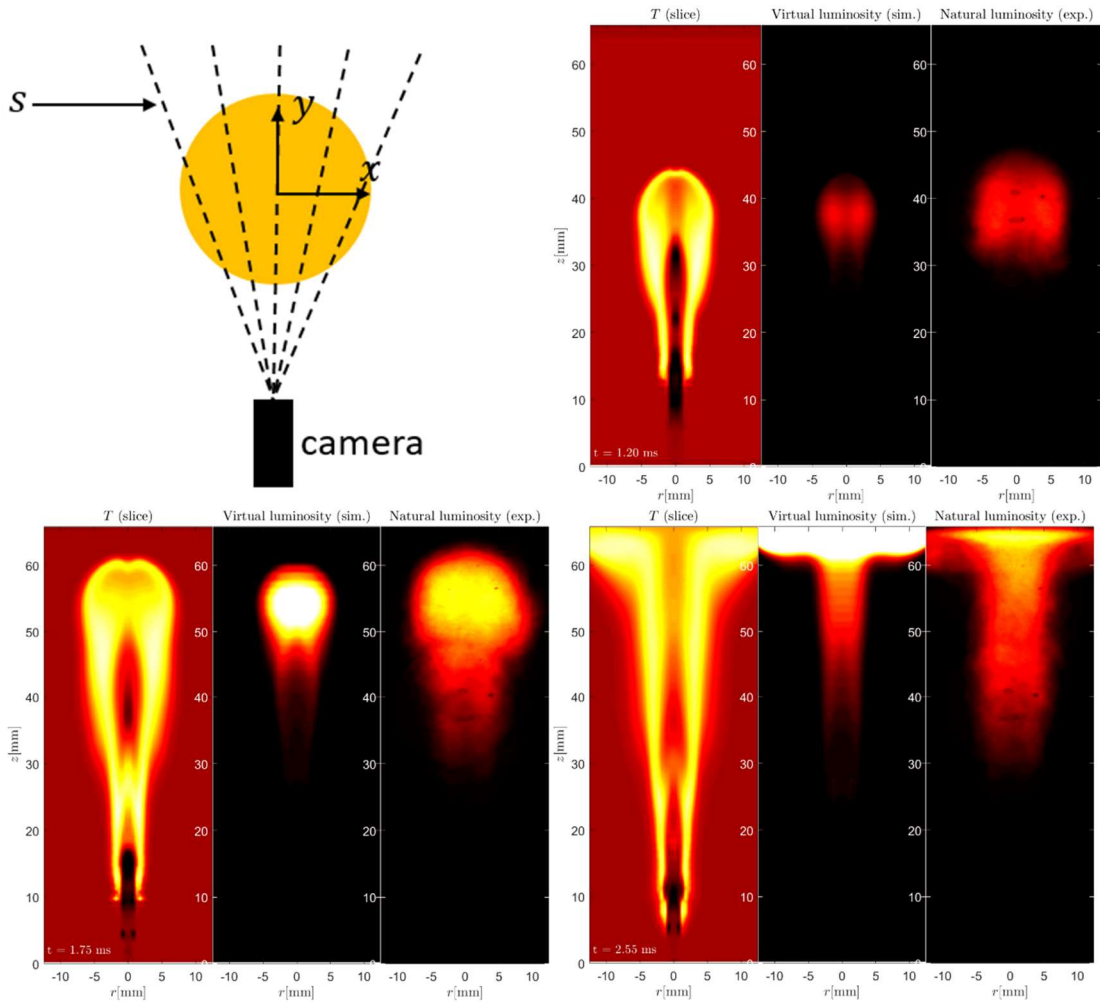


Figure 47. Virtual luminosity images from 1.20ms, 1.75ms and 2.55ms after the electrical start of injection.

Overall, in terms of the luminosity metric, the qualitative nature of the spray plume, as well as its penetration rate, are replicated well. This should not however be surprising given the prior experiences with the present modelling platform. The differences between the temperature field and virtual luminosity metrics however highlight the usefulness of the latter in assessing the correspondence to experiments.

3.3.2 Wall heat flux trends between models and grids

Figure 48 shows the evolution of wall heat flux at the sensor location for both the uncoated experiment and the uncoated simulations. Within the imaged time span, all results are consistent in the shape of the traces: the initial low heat flux (due to the high chamber temperature from pre-combustion) is followed by a rapid rise, up to the range of 10 MW/m², when the combustive plume impinges the wall.

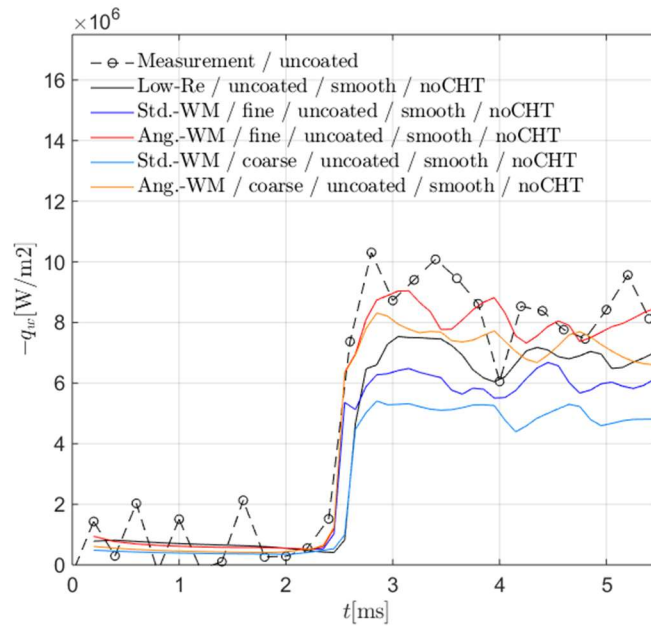


Figure 48. Wall heat flux evolution between the uncoated experiment, low-Re simulation, and wall-modelled simulations.

From Figure 48, the differences between model and grid-specific predictions can be ascertained. The (high near-wall resolution) low-Re computation displays heat flux levels slightly lower than those in the experimental reference. This discrepancy increases considerably with the standard wall model, which appears to considerably underpredict wall heat flux. Such a result can be expected based on prior literature [25]. In contrast, the modified Angelberger model provides slightly increased heat fluxes in comparison to the low-Re computation. These computations provide the closest correspondence to the experimental reference. The most positive aspect of the modified Angelberger model is its low dependence on mesh sizing: the coarse wall-modelled grid (which is the most relevant for engine simulations) provides a result very close to that of the finer variant, and to that of the reference experiment and low-Re computation.

It is worth reminding that the present investigation does not aim to provide a definitive indication regarding the fundamental ability of heat transfer models. In order to investigate these abilities thoroughly in the present configuration, heat fluxes should be measured at several different locations. Indeed, the past literature regarding heat transfer models in impinging jets [26, 27] show that models result in strikingly variable correspondence depending on the case at hand and the examination location. Moreover, there are differing perspectives on which model performs best. Fundamentally, the contribution of this work is to employ an approach correspondent to experimental observations, and to show sensitivities of different wall-dependent variations.

Figure 49 shows the expected result when it comes to CHT effects in the uncoated (steel) material. While measurable CHT effects exist also in the steel surface case, their effect is too small to have a significant impact on the comparisons at hand. Hence, the uncoated cases without CHT were maintained as a baseline for the coated simulations.

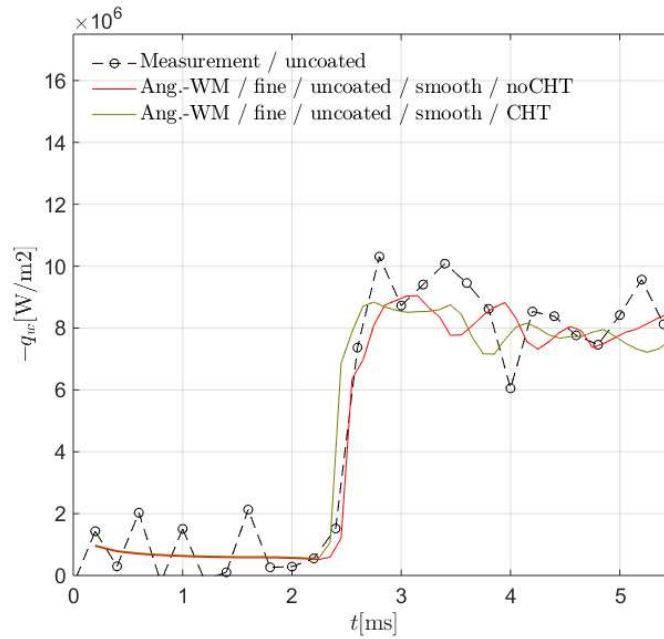


Figure 49. Wall heat flux evolution in the uncoated case between non-CHT and CHT simulations.

3.3.3 Wall heat transfer in the Zirconia-coated HTDZ simulation

Prior to simulating the coated zirconia case, its surface properties are assessed with the aid of measurement data from Fraunhofer IPK. Thermodynamic properties are provided from the basis of Table 3, and surface properties are processed according to detailed measurements.

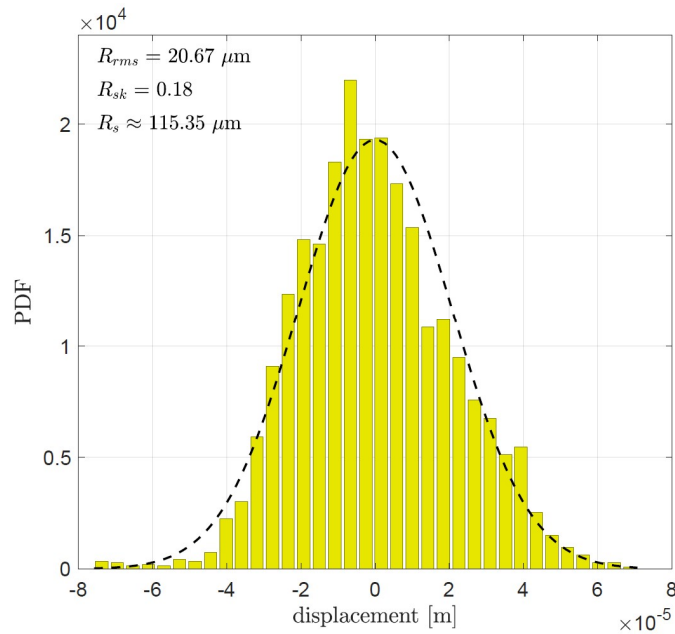


Figure 50. Roughness PDF of the zirconia-coated surface. (data origin: Fraunhofer IPK)

Figure 50 shows the roughness PDF of the zirconia-coated surface, as well as a corresponding Gaussian distribution. The PDF has a slight positive skewness. An estimate of the sand-grain roughness is computed based on Eq. (14) and provided as an input to the simulation.



Ideal coating – smooth zirconia

From Figure 51, the comparison between smooth zirconia and the baseline simulation, some important phenomenological aspects can be distinguished:

- The initial heat flux upon impingement is not significantly affected. In this stage, the wall temperature is close to that of the uncoated reference.
- This initial peak heat flux instance is followed by a rapid wall temperature increase. This ensues in a rapidly decreasing heat flux, hence fulfilling the purpose of thermal swing materials
- When the injection is sustained and the combusting plume continually hits the wall, the increase in temperature slows down, and the heat flux begins to approach a steady-state level. In the present case, this steady-state level is ca. 25 % lower than in the uncoated case.

In accordance with the core principles of thermal swing materials, the zirconia coating in the ideal (rough, sealed-surface) case is expected to provide tangible heat flux mitigation benefits.

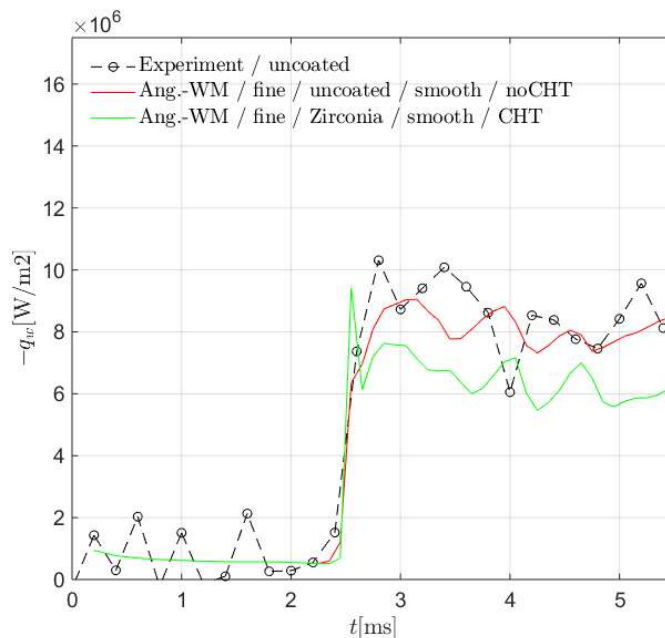


Figure 51. Heat flux evolution in the baseline case and with an ideal (smooth) Zirconia coating.

Realistic (rough) Zirconia coating

In the examination of the realistic zirconia coating, the roughness model components presented in Section 2.4.5 were incorporated as part of the analysis. Figure 52 displays the heat flux trace for the rough zirconia coating, with the smooth case as reference. Primary observations are that

- The initial heat flux following impingement is noticeably higher here than in the ideal zirconia case. The difference is in the order of 20-25 %
- This initial heat flux is also higher than in the uncoated reference case, indicating that the rough zirconia coating would in fact increase heat losses at the early stage
- When time progresses, the heat flux reduces close to the level of the uncoated reference. This is, again, due to the thermal swing: the surface of the rough zirconia heats up significantly – in fact, even more than the ideal zirconia coating

In contrast to the ideal zirconia case, this result appears to suggest that the incorporated coating does not bring heat flux benefits, and possibly even introduces a slight detriment. However, such an inferiority/superiority depends also on the time scale of the process: the lengthier the heat flux sensitive



process is, the more potential the thermal swing material has to eventually overcome the initial heat loss detriment.

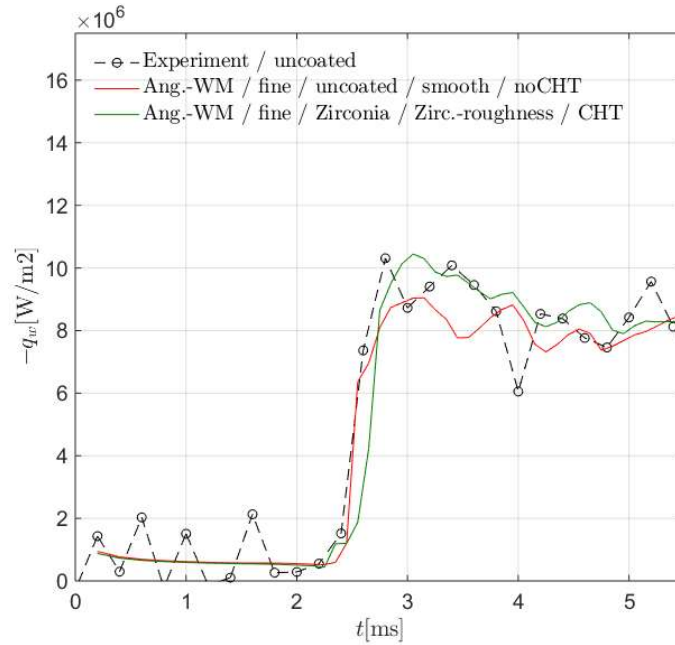


Figure 52. Heat flux evolution in the baseline case and with a realistic (rough) Zirconia coating.

To complement the observations using the coated measurements, Figure 53 shows the inverse problem solution previously discussed in Section 2.4.5 as a reference. The exact case here employs the nominal coating thickness of 130 μm .

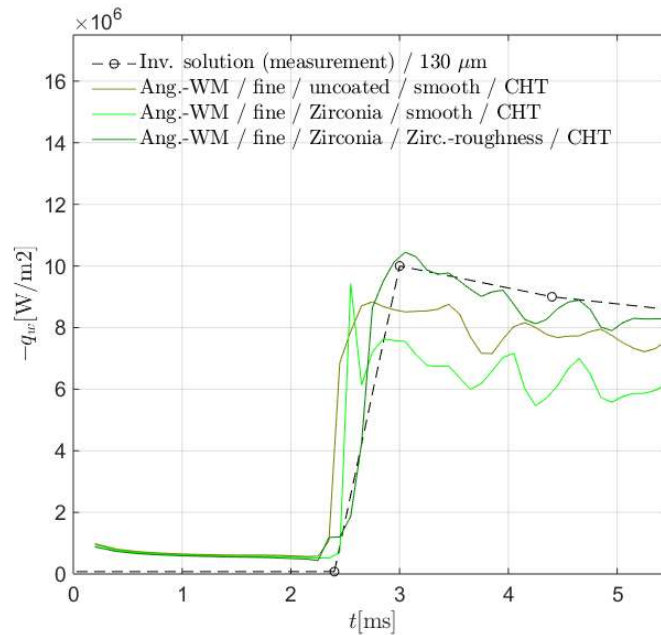


Figure 53. Wall heat flux evolution for cases with CHT. Here, the reference result shows the iteratively determined solution for the inverse problem (WP3; coated experiment).

The heat flux trace obtained through analysis of the wall-embedded heat flux sensor outputs coincides very well with the result of the 3D CFD computation which includes the model for rough walls. This is



quite a remarkable result as the two cases are start from completely independent points. Furthermore, Figure 54 shows the evolution of surface temperature in the same case. To provide a meaningful comparison with the uncoated case, the CHT variant of the baseline case is provided as another point of comparison.

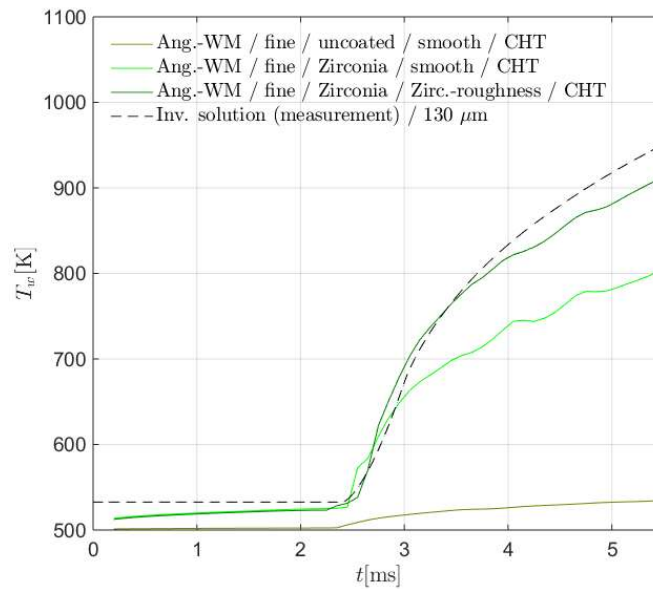


Figure 54. Surface temperature evolution in CHT computational cases, with the iteratively solved inverse problem solution (coated experiment) as the reference.

The increase of surface temperature is expectedly lowest in the uncoated (steel) case, where a temperature increase of ca. 30 K is achieved. From the simulated cases, the highest surface temperature increase is noted in the rough zirconia case. This is a logical result as the gas-wall heat flux is higher than in the ideal case. Corresponding to the wall heat flux comparison in Figure 53, the surface temperature trend matches very well between the backward-engineered experimental analysis and the rough zirconia computation.

In order to more comprehensively understand the impact of rough wall heat transfer, it is instructive to observe situation as a function of roughness. Figure 55 shows how much (i) wall shear stress and (ii) wall heat flux are increased due to changes of (a) roughness or (b) near-wall flow intensity. The figure employs iterative solutions for rough wall functions in addition to the Reynolds analogy factor.

The dashed line in the figure indicates the region of interest for the present zirconia-coated cases. The vertical axis range has been chosen so that it fits the relevant spray-wall impingement intensity encountered in the engine cases. It is noted that the present range of roughness provides a considerable change in the wall shear stress, and a moderate increase of the wall heat flux. The increase in wall heat flux can be expected to be in the range of 20-50 %. It is however also seen that decreasing the roughness, even by a small fraction, could considerably alleviate heat losses. The analysis suggests that, in the present scenario, one could limit heat transfer losses to ca. 35 % by limiting the surface roughness to ca. 50 μm (sand-grain-equivalent).

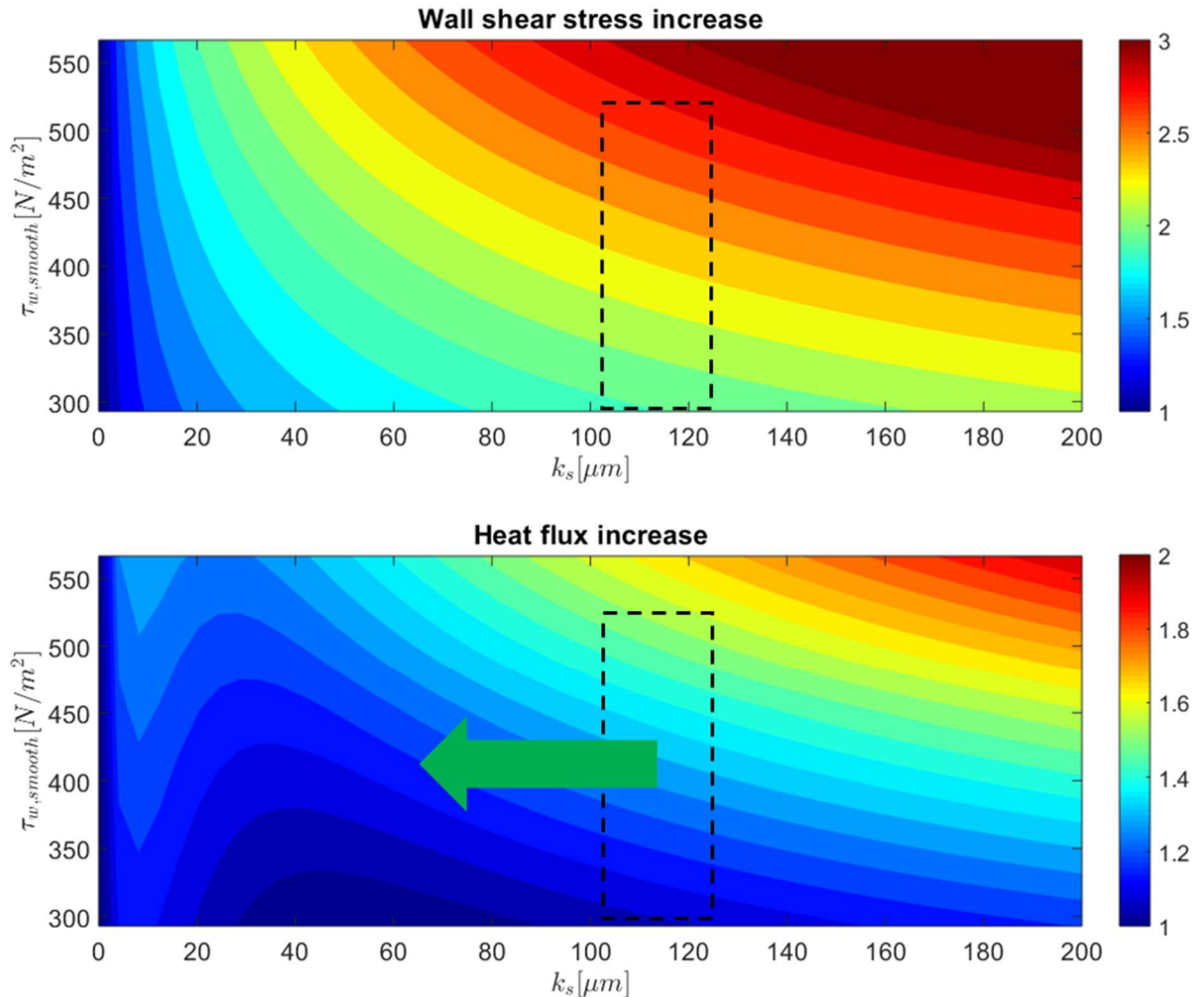


Figure 55. The impact of increasing dimensional wall roughness and near-wall flow intensity on increases of wall shear stress and wall heat flux. Dashed line indicates presently applicable region in the zirconia-coated case.

3.3.4 Explorative simulations in the OM651 metal engine configuration

Figure 56 displays the temporal evolution of the total combustion chamber heat flux during the expansion stroke. It is firstly noted that there are some heat transfer differences between cases already before spray impingement, due to roughness. As the initialisation for each case was similar, these differences would be somewhat mitigated if the compression stroke was also computed with each coating. After impingement, the rough aluminium case experiences the highest wall heat transfer, a trend that continues until EVO, as seen in the cumulative graph. In contrast, lowest heat transfer levels are experienced by the smooth UWM-HVLP coating, as should be expected. The material in the focus of the present project, zirconia, places on both sides of the uncoated aluminium reference, depending on whether the surface is smooth or rough. In the rough case, while peak averaged heat fluxes are slightly lower than with aluminium, the cumulative indication is of a small disadvantage. This result is in good agreement with the cell experiments and the engine experiments. In the case of smooth zirconia, heat transfer advantages exist but are indicated to be much smaller than for the UWM-HVLP coating. Again, it is worthwhile to iterate that this coating has been not experimented with in the project, and we do not indicate whether the chosen surface properties can be realistically attained with such a material.

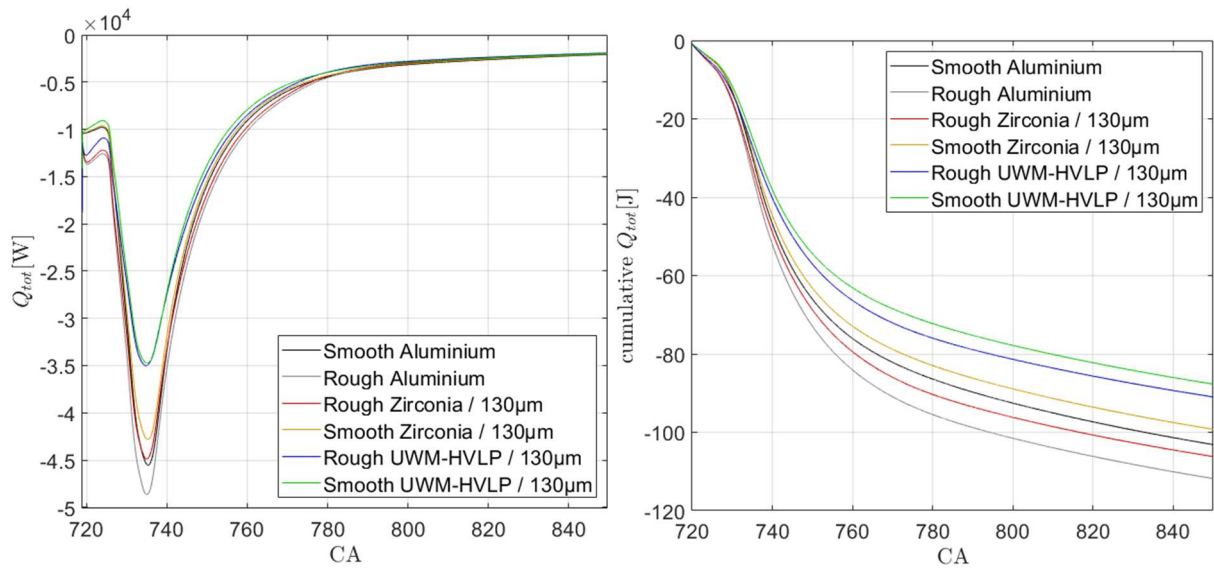


Figure 56. Instantaneous (left) and cumulative (right) evolution of heat transfer during the expansion stroke in the engine simulation cases.

To investigate heat transfer in a spatial manner, Figure 57 displays heat fluxes on the piston bowl after injection, as well as concurrent surface temperatures. The time frame imaged focuses on the region of highest heat flux. Impingement occurs at ca. 725.5 CA, after which the combusting jet begins to advance on the surface of the piston bowl. This process continues and gradually envelops the bowl area in hot gases. The heat flux generally continues to increase up until the injection ceases. It should be recalled that by this time the spray-wall impingement has continued for a significant time scale, about 10 degrees CA. Observing the local nature of heat transfer in the aluminium case, the heat flux pattern looks classical, with high heat transfer at stagnation locations. Correspondingly, local surface temperature increases are small, in the order of 20 degrees. The coated cases display various different trends: in the zirconia-coated simulations, surface temperatures of about 800 K are noted, and peak heat fluxes close to the stagnation region are slightly decreased. The rough zirconia case displays similar trends but with some increase in both heat flux and temperature. It is also apparent that in the case of rough-wall surfaces, heat transfer increases are not limited to the flame impingement region. As the momentum introduced by the sprays drives the entire in-cylinder flow field, roughness effects emerge universally, not just in the immediate flame-wall region.

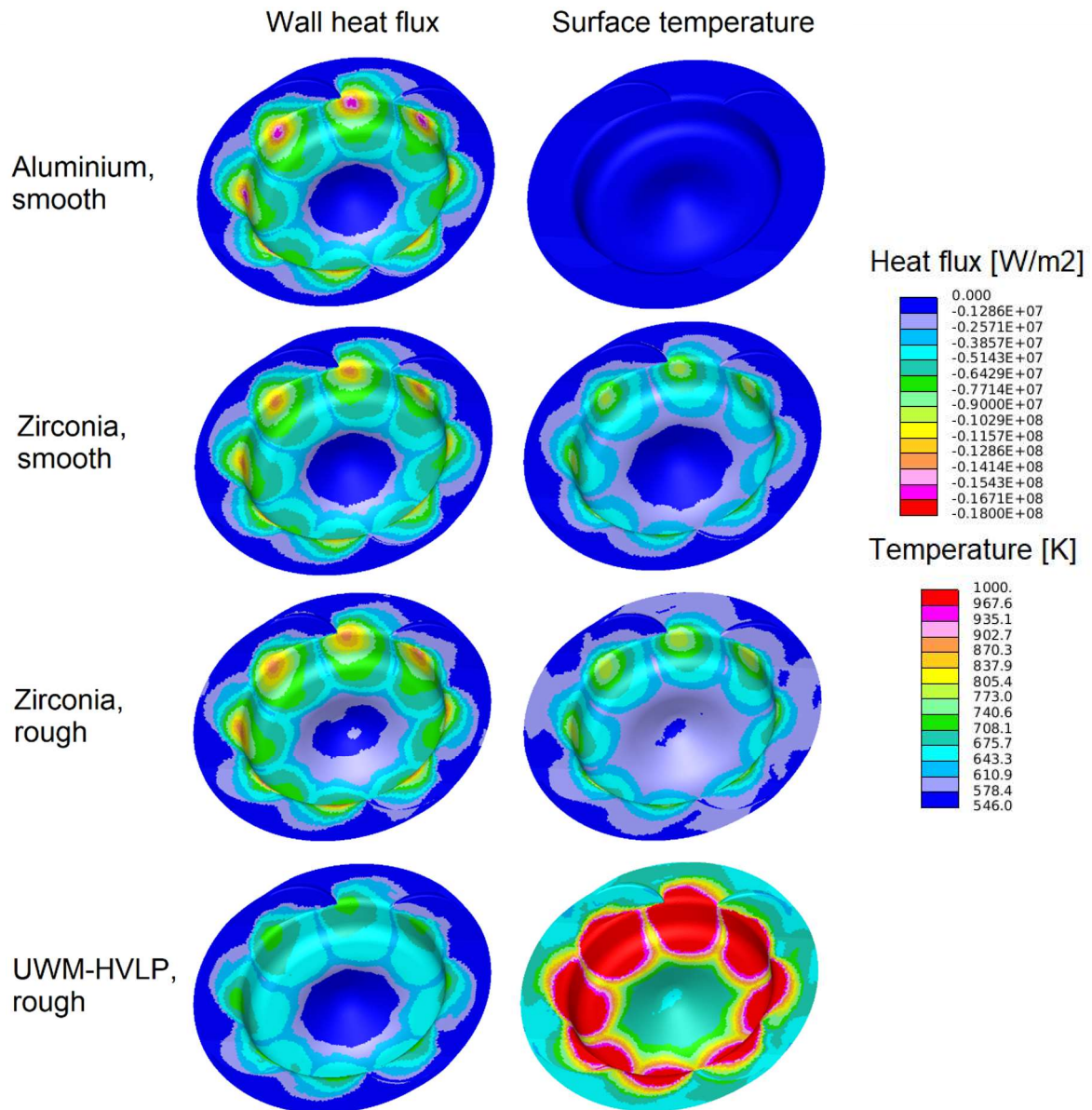


Figure 57. OM651 engine simulation at 15 degrees after TDC, i.e. close to peak heat flux timing. Wall heat flux (left) and wall surface temperature (right) distributions on the piston.

Evidently roughness appears to influence heat transfer characteristics in a significant manner. Several main effects can be discerned from roughness:

- Substantial increase in early, local heat transfer
- A deviation in the spatial distribution of piston heat flux over time in comparison to the uncoated case
- A difference in peak heat flux timing and the temporal heat flux trend

It is noted that both surface roughness and material selection impact the total heat transferred during expansion. These influences are of the same order of magnitude: a small advantage is noted with smooth zirconia, while a similar disadvantage is seen with rough zirconia, compared to the smooth aluminium reference. These factors are reflected in the cylinder pressure trace and hence in the indicated efficiency effects of heat transfer. Figure 60 shows the cylinder pressure traces for the above cases in the early part of the expansion process.



For further insights, let us observe cylinder pressure and mean temperature trends (Figure 58). In accordance with the differences in heat transfer, higher pressures and temperatures are noted in the cylinder especially in smooth-wall cases, and with increasingly capable thermal swing materials. The differences in gas temperature at EVO (here, up to ca. 15 C) are significant as higher temperatures provide more energy to the exhaust stream and to the turbocharger. However, in contrast to the cumulative heat transfer trends, the pressure and temperature appear to be bundled primarily according to roughness. This indicates that there are other discrepancies between the cases besides heat transfer.

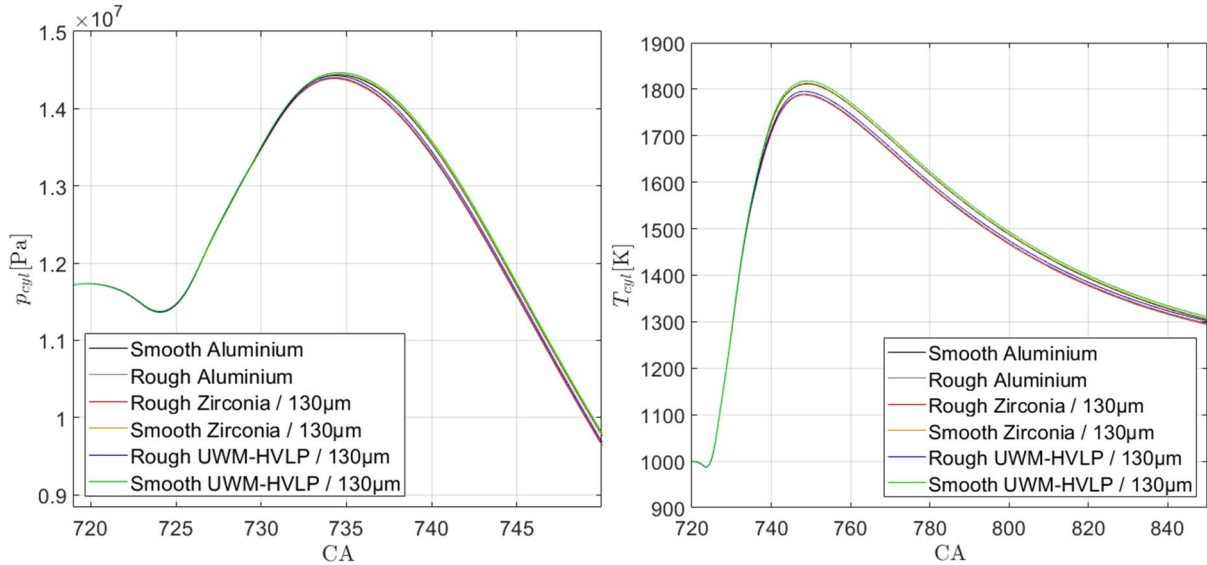


Figure 58. Peak-phase cylinder pressure (left) and temperature (right) traces for the different engine simulation cases in the expansion stroke.

To make further interpretations, let us probe at the gross heat release rate curves (Figure 59). It is noted that in the rough wall cases, a slightly higher heat release is noted in the early part of combustion (A). However, a much larger decrease of HRR is noted later, especially after injection has stopped (B), and the result is clearly reflected in the cumulative trend. This appears to indicate that the charge is impacted by the rough wall and cannot combust as rapidly in the mid-stages of the combustion process. This phenomenon is not a new observation, as combustion retardations with rough surfaces have already been noted in the literature [28].

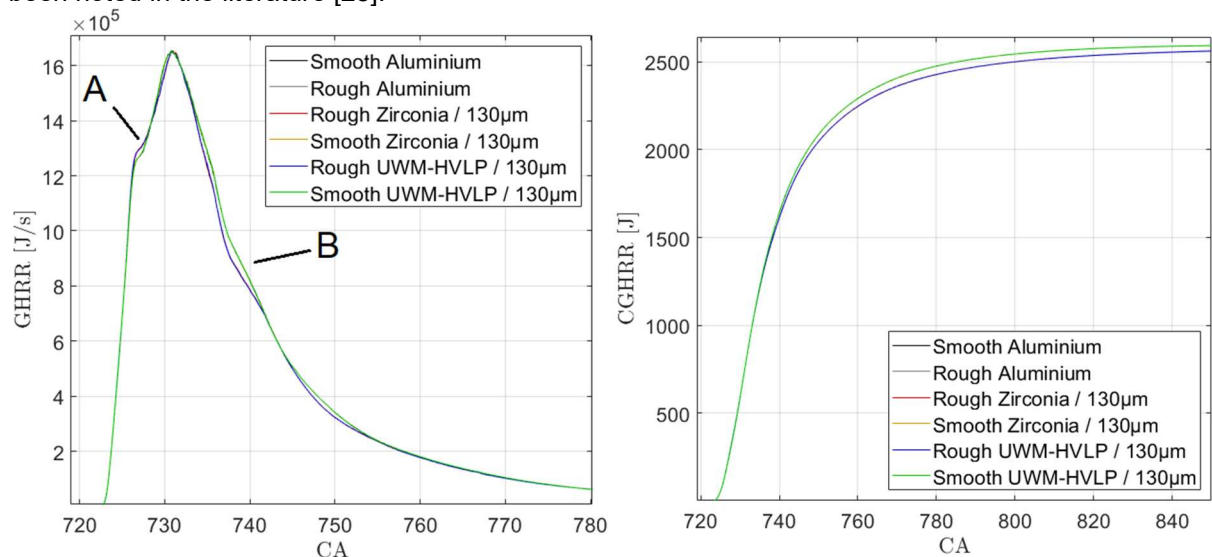


Figure 59. Instantaneous (left) and cumulative (right) gross heat release rates from the engine simulation cases.



It appears, then, that at least two effects of wall roughness have a negative impact on work produced during the expansion stroke:

- Increased initial wall heat transfer. The higher wall heat flux during the early jet-wall impingement lowers the cylinder pressure in the case of rough-wall coatings.
- Retarded heat release. Wall roughness appears to be detrimental to the mid-stages of combustion. The delayed phasing again contributes to decrease cylinder pressure at the early part of the power stroke, leading to an efficiency detriment

To elaborate on these factors, let us observe Figure 60 which shows the differential between work produced during the power stroke, using the different approaches. With this comparison, results from the smooth TSMs are likely the easiest to interpret. The initial heat transfer upon the spray impingement is similar to the aluminium case (S1). After impingement, heat losses decrease due to thermal swing, and cylinder pressure remains at a higher level in comparison to the reference (S2). As the wall is smooth, there is relatively little impact on the charge motion, and the behaviour continues in a smooth fashion. Towards the end of expansion, a small gain in expansion work is noted.

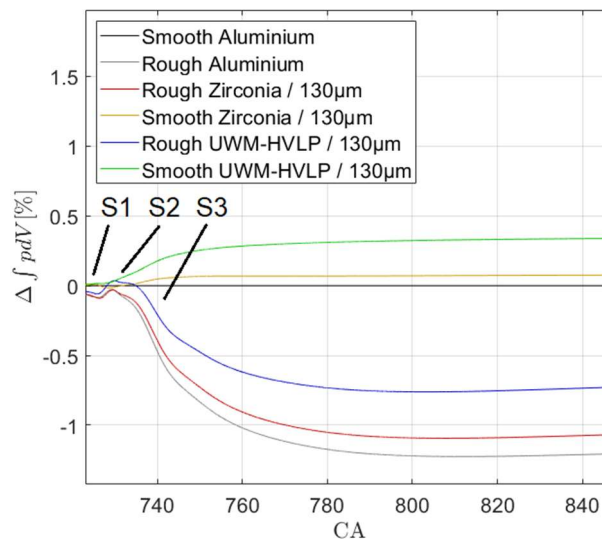


Figure 60. Difference in work done by the piston during the power stroke until exhaust valve opening, with the base aluminium case as the reference level.

With the rough cases, these trends change considerably. The initial stage (S1) sees all rough simulations experiencing higher heat losses, contributing to a work loss. However, as the impact of thermal swing increases (S2), the simulations recover somewhat from this loss. Cases with higher thermal swing improve the most. However, after this time (S3), both rough-wall cases indicate a considerable loss of efficiency. This can be connected with point B in Figure 59 as the rate of chemical heat release is retarded. Evidently, this phenomenon is only indicated to occur in the rough wall cases. It should be noted that in case the Reynolds analogy correction is not applied (not shown here), rough-wall heat fluxes would exceed the present values considerably, and the indication from such cases would be even worse. It is also important to consider the impact of the base heat transfer model selection: the greater the heat base heat transfer, the larger potential benefits arise from thermal swing. Hence, the quantitative indications of the present results are sensitive to such differences.

The observations presented here can be compared with the experimental engine results from TU Berlin. Figure 61 shows results from a GT-Power-based three-pressure analysis from different experimentally tested coatings. The cases compared here are (1) rough aluminium ($R_z = 112.4\mu m$), (2) porous (and rough) aluminium ($R_z = 179.3\mu m$), and zirconia with a very thin aluminium top ($R_z = 115.2\mu m$).



In these engine results it is indeed noted that efficiency is indicated to be influenced by several factors. The components most pertinent to the present simulation results are (1) heat transfer and (2) combustion duration. Comparing the results with the computational results in Figure 56 and Figure 60, it can be noted that the indicated loss components are of similar relationship and magnitude. The positive impact of thermal swing materials can be deemed important, a feature not inherently visible in the experiments. However, the detriments of rough wall increased heat transfer and that of combustion phasing appear to both be of similar importance. The observations as a whole however agree well with the previous engine experiments, and reaffirm that there is most likely a dual negative impact of the roughness of TSM coating roughness that is sufficient to offset the advantages brought purely by thermal swing.

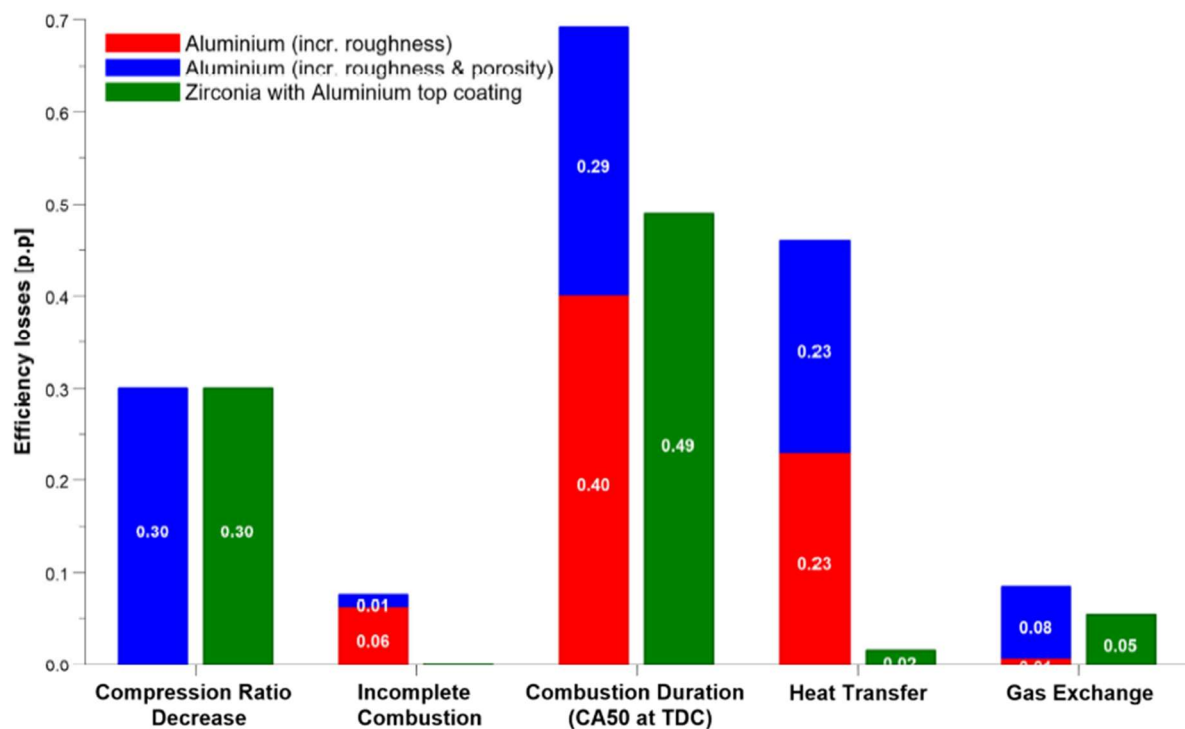


Figure 61. Efficiency detriment contributors (in percentage points) according to GT-Power-enabled cylinder pressure analyses. (courtesy of Oliver Nett, TU Berlin)

4 Main accomplishments and conclusions

The following main conclusions, divided according to work packages, are derived from the results of the study:

WP1

- A simplified heat transfer test platform was constructed to examine material influences on multi-cycle heat transfer processes. Over a number of combustion cycles, the thickness of a coating is highly influential to its temperature, with higher thicknesses decreasing overall heat losses. The combination of lower heat capacity and lower thermal conductivity result in both an increase in temperature and a decrease in heat losses. The nominal material properties can conveniently be improved via a change in porosity – however, this does not account for porosity-induced adverse effects such as embedded fuel, surface roughness or coating degradation.



- A two-dimensional finite difference test platform was constructed to test the applicability of the one-dimensional heat flux assumption. For engine-scale cyclic periods, local heat flux variations and realistic coating material properties, the assumption of one-dimensional conjugate heat transfer in the solid coating material holds well. While TSMs are most sensitive to multidimensional effects, such effects should be assumed to be small in the engine context.

WP3

- Optical broadband and OH*-chemiluminescence imaging has been carried out in a high pressure-high temperature cell (HTDZ), describing the high-level phenomenology of a wall-impinging combustor diesel spray
- Concurrent heat flux measurements have been carried out for both uncoated and coated sensor-impingement plate combinations.

WP4

- The 3D CFD model, employing the CMC combustion modelling approach, was successfully validated against the (i) optical and (ii) heat flux measurements in the high-pressure-temperature cell.
- To account for rough-wall effects in spray-wall impingement, a methodology was implemented based on recent fundamental rough-wall measurements and Direct Numerical Simulations: The methodology accounts for (i) defining a suitable sand-grain-equivalent roughness from measurable surface characteristics, (ii) modelling rough-wall momentum transfer, and (iii) modelling rough-wall heat transfer.
- For heat transfer investigations with significant roughness (as is the case in the present coating materials), roughness effects are important and need to be modelled. Furthermore, it appears imperative that deviations from the Reynolds analogy are modelled: effectively, rough-wall heat transfer does not increase similarly to rough-wall momentum transfer, and the effects of this phenomenon are important to account for when evaluating the suitability of coating materials for heat flux mitigation.
- Combined with the results of WP3, it appears likely that the currently tested zirconia coating does not contribute to lower local heat fluxes in the impingement region. Since the rationale of this observation can be explained only by wall roughness effects, it remains unclear what the effects of coating porosity are on the instantaneous heat fluxes.
- In explorative engine simulations, wall roughness appears to be detrimental to engine efficiency through different mechanisms: first, initial wall heat losses are indicated to be increased even with the thermal swing material coating. The ensuing cylinder pressure decrease is compounded by retarded heat release. This appears to be an effect solely due to the momentum flux effects of the wall roughness.

A primary practical implication of the results in WP3 and WP4 is that rough combustion chamber surfaces should be avoided and/or mitigated as effectively as possible. The present results indicate that roughness encountered in a realistically manufactured coating surface can alone dispel advantages from thermal swing material coatings. The HTDZ simulations and experiments jointly indicate that this is the case in a static configuration. Furthermore, the engine simulations brought other, secondary effects into consideration. Indeed, the case of the ideal (smooth) zirconia coating did indicate tangible advantages in both the HTDZ and the engine simulations.

Returning to Figure 56, Figure 60 and Figure 61 in Section 3.3.4, there is a strong indication from both our present simulations and the experiments of TU Berlin that Diesel engine efficiency losses in thermal swing coatings can result from a combination of factors: while in this study it was possible to model and indirectly determine roughness-induced effects, the impact of porous coatings (beyond their thermodynamic effects contributing to temperature swing) cannot be quantified with the results of the present study.



5 National and international collaboration

This project was carried out in close collaboration with the Fraunhofer Institut für Produktionsanlagen und Konstruktionstechnik (IPK) and the Technical University Berlin (Fachgruppe Antriebssysteme); co-financed and managed on the German side by the FVV Research Association Combustion Engines (Forschungsvereinigung Verbrennungskraft-maschinen e.V.).

The project is closely related to the Swiss Federal Office of Energy project “Investigation of heat transfer (resolved in space and time) by modern combustion processes” (grant no. SI/501546-01) carried out at the University of Applied Sciences FHNW, where the focus is on the development of heat flux sensing technology. A fruitful exchange with the group of Prof. Herrmann and co-workers at FHNW has been established resulting in significant know-how transfer between the two institutes.

This project is further related to two other FVV/CORNET projects “Wall heat transfer in Otto engines” and “Experimentally validated LES models for wall heat transfer in Otto engines”, both co-funded by the Swiss Federal Office of Energy (grants nos. SI/501615-01 and SI/501930-01), where near-wall flow and heat transfer are studied in non-coated Otto engines with pent roof geometry and tumble flow motion. Both are in collaboration with the Technical University Darmstadt (Reactive Flows and Diagnostics group, Prof. Andreas Dreizler and Dr. Benjamin Böhm), performing the experimental investigations in the optically accessible passenger car engine.

Finally, this project is also associated with the CTI financed Swiss Competence Center of Energy Research (SCCER) Mobility, Capacity Area A2 “chemical energy converters”, Topic A2.2 “IC engine powertrain efficiency increase” involving FHNW (Prof. K. Herrmann), EMPA (Automotive Powertrain Technologies, Christian Bach) and ETH Zurich (Aerothermochemistry and Combustion Systems Lab., Prof. K. Boulouchos).

6 Dissemination

The results obtained will be presented at the autumn conference 2020 of the Research Association Combustion Engines (FVV), ensuring wide dissemination in the field. Furthermore, the findings are in preparation for publication in peer reviewed journals.

7 References

1. Dietrich, M., *Hochleistungsschichten im Werkstoffprogramm des BMBF Trends und Potenziale*. 2006, Forschungszentrum Jülich GmbH.
2. Moos, M., R. Janssen-Timmen, and N.a.K. Leonenko, J., *Gesamtwirtschaftliche und sektorale Wertschöpfung aus der Produktion und Anwendung von Fügetechnik in Deutschland*. 2013.
3. Andruskiewicz, P., et al., *Assessing the capability of conventional in-cylinder insulation materials in achieving temperature swing engine performance benefits*. International Journal of Engine Research, 2018: p. 599-612.
4. Kosaka, H., et al., *Concept of “temperature swing heat insulation” in combustion chamber walls, and appropriate thermo-physical properties for heat insulation coat*. 2013. **6**(1).
5. Andruskiewicz, P., et al., *Analysis of the effects of wall temperature swing on reciprocating internal combustion engine processes*. 2018. **19**(4).



6. Kawanabe, H., J. Komae, and T. Ishiyama, *Analysis of flow and heat transfer during the impingement of a diesel spray on a wall using large eddy simulation*. International Journal of Engine Research, 2018.
7. Mruk, A., et al. *Heat Transfer Through Ceramic Barrier Coatings Used in Internal Combustion Engines*. 1994. SAE Technical Paper.
8. Higgins, B. and D. Siebers. *Measurement of the flame lift-off location on DI diesel sprays using OH chemiluminescence*. 2001. SAE Transactions.
9. Gaydon, A., *Flame Structure and Reaction Processes*, in *The Spectroscopy of Flames*. 1974, Springer.
10. Alifanov, O.M., *Inverse heat transfer problems*. 2012: Springer Science & Business Media.
11. Reitz, R.D. and R. Diwakar. *Effect of drop breakup on fuel sprays*. 1986. SAE transactions.
12. Wright, Y., et al., *Simulations of spray autoignition and flame establishment with two-dimensional CMC*. 2005. **143**(4).
13. Blomberg, C.K., et al., *Modeling split injections of ECN "Spray A" using a conditional moment closure combustion model with RANS and LES*. 2016. **9**(4).
14. Colin, O. and A. Benkenida, *The 3-zones extended coherent flame model (ECFM3Z) for computing premixed/diffusion combustion*. 2004. **59**(6).
15. Angelberger, C., T. Poinsot, and B. Delhay. *Improving near-wall combustion and wall heat transfer modeling in SI engine computations*. 1997. SAE Technical Paper.
16. Siemens, *Methodology, STAR-CD version 4.30*. 2017.
17. Flack, K., M. Schultz, and J. Connelly, *Examination of a critical roughness height for outer layer similarity*. 2007. **19**(9).
18. Nikuradse, J., *Laws of flow in rough pipes*. 1950: National Advisory Committee for Aeronautics Washington.
19. Schultz, M. and K. Flack, *The rough-wall turbulent boundary layer from the hydraulically smooth to the fully rough regime*. 2007. **580**.
20. Flack, K.A. and M.P. Schultz, *Review of hydraulic roughness scales in the fully rough regime*. 2010. **132**(4).
21. Bons, J., *A critical assessment of Reynolds analogy for turbine flows*. 2005. **127**(5).
22. Forooghi, P., et al., *Toward a universal roughness correlation*. 2017. **139**(12).
23. Forooghi, P., M. Stripf, and B. Frohnepfel, *A systematic study of turbulent heat transfer over rough walls*. International Journal of Heat and Mass Transfer, 2018. **127**: p. 1157-1168.
24. Andrie, M., et al., *Low heat capacitance thermal barrier coatings for internal combustion engines*. 2019, SAE Technical Paper no. 2019-01-0228.
25. Nuutinen, M., O. Kaario, and M. Larmi, *Conjugate heat transfer in CI engine CFD simulations*. 2008: SAE Technical Paper.
26. Craft, T., L. Graham, and B.E. Launder, *Impinging jet studies for turbulence model assessment—II. An examination of the performance of four turbulence models*. 1993. **36**(10).
27. Zuckerman, N. and N. Lior, *Impingement heat transfer: correlations and numerical modeling*. 2005. **127**(5).
28. Tree, D.R., P.D. Wiczynski, and T.M. Yonushonis, *Experimental results on the effect of piston surface roughness and porosity on diesel engine combustion*. SAE transactions, 1996: p. 112-121.