Netherlands Organisation for Scientific Research

Argon Power Cycle

Scientific summary

The focus of this project is on a revolutionary power cycle that converts energy from renewable fuels into power, with substantially enhanced efficiency by using argon as working fluid. The efficiency of a thermal power cycle is limited by the specific heat ratio of its working fluid. By using argon instead of air the cycle efficiency can be increased by about 25% reaching values above 80%!

A new internal combustion cycle that circulates argon will be explored in this project. Such a closed-loop argon power cycle (APC) would most conveniently burn hydrogen and oxygen, leading to an exhaust stream that is emissions-free and effectively contains only water and argon, which allows for easy separation by condensation. Furthermore, the closed-loop nature of APC makes carbon capture affordable, which enables the use of carbonaceous fuels without greenhouse gas emission. Although combustion in air is more convenient, APC will be preferred when efficiency is critically important. Current concerns about climate change and increasing amounts of intermittent renewable energy sources, make hydrogen energy storage and power generation applications of keen interest.

A major hurdle to take in the development of APC technology is the control of the combustion process. Since both fuel and oxidizer are to be injected, new injection and combustion strategies of fuel and oxidizer in argon will be investigated. The aim to develop and validate an advanced numerical model that will be used to find the optimal combustion strategy. The project encompasses a multi-scale approach that includes an exploration of the fundamental processes in unsteady igniting gas jets by using high-fidelity numerical models and detailed optical diagnostics. This fundamental knowledge is then translated via experimental and numerical studies of lab-scale setups into design tools for APC technologies. Finally, the injection strategies will be investigated on full-scale research engines.

Project description

Overall aim and key objectives

The aim of this project is to enforce a breakthrough in the development of Argon Power Cycle (APC), a revolutionary power generation cycle with ultra-high conversion efficiency. The scientific foundation for this increase is that thermal efficiency is a strong function of the specific heat ratio γ of the working fluid. Since engines typically use air as oxidizer, the specific heat ratio of the working fluid is dominated by that of nitrogen. Ideal working fluids with the highest possible specific heat ratio, however, are monoatomic (noble) gases such as helium, neon and argon. Due to the absence of rotational and vibrational modes, monoatomic gases have a specific heat ratio that is about 25% higher than that of air. For an internal combustion engine, this means that higher temperature and pressure conditions in the cylinder are reached, which increases the boundary work on the piston and reduces the unused heat that leaves the cycle with the exhaust gas.

Figure 1 compares the theoretical thermal efficiencies of Otto cycles using argon and air as working fluid for a range of practical compression ratios *r*. While any monoatomic gas could be used as ideal working fluid, argon is chosen because it is non-toxic, abundant, very affordable, and it facilitates the creation of gas-tight seals. Due to various energy losses such as gas cooling, gas pumping and mechanical friction of the moving parts, the actual efficiency of the engine will be lower than the values shown in figure 1. By reducing these parasitic losses, optimized air-breathing diesel engines for stationary power generation have now reached efficiencies slightly above 50% as demonstrated by commercial products. Thermodynamic model calculations show that if such engines are converted to use argon as working fluid, overall efficiencies may rise to values close to 80% as depicted in figure 1. This tremendous leap in conversion efficiency makes APC a possible breakthrough technology.

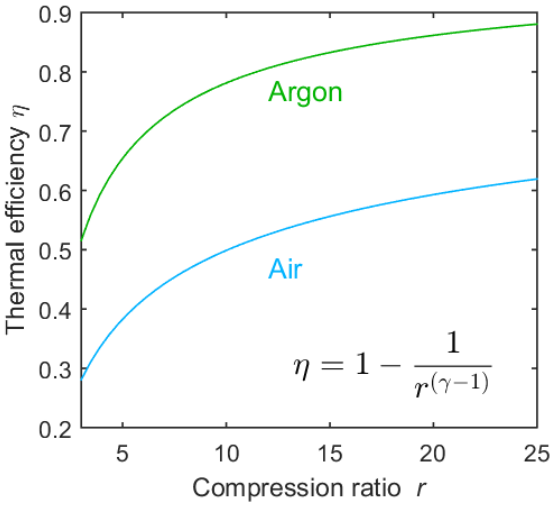

Figure 1: Thermal efficiency of an Otto cycle for different working fluids

Though the superior thermal efficiency of argon cycles is known since the 19th century, current engines almost exclusively use air as working fluid because it is much more convenient. The main reasons are that a) air is free and abundantly available everywhere on earth, and b) it provides the oxygen that is required to burn the fuel and convert the chemical energy into heat. The APC addresses these topics by recirculating the working fluid in a closed loop configuration, also understood as 100% exhaust gas recirculation (EGR). This enables the APC system to freely increase its nominal pressure at no cost, while conserving its valuable working fluid. The oxygen, as the fuel, is added to the system gradually as power output is increased. This, in turn, allows the APC to maintain its high efficiency along the full load range, unlike current power systems, whose efficiency decreases as operational load decreases.

Because the system does not contain any nitrogen, combustion of hydrogen (H_2) is not limited by the generation of nitrogen oxides emissions, effectively rendering a pollution free power system. Although hydrogen is the perfect fuel for the APC, carbonaceous fuels such as natural gas or biogas are also appealing. Combustion of natural gas will allow the system to operate during periods when there is no hydrogen available, increasing its

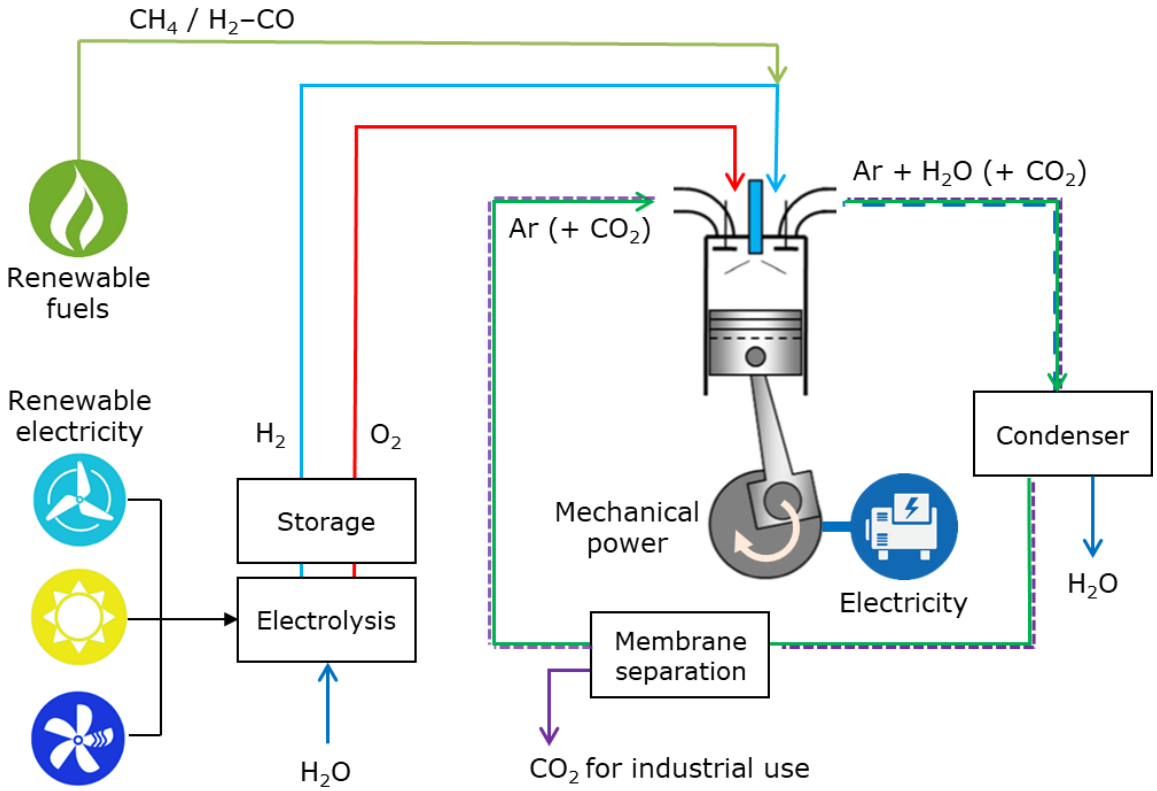

Figure 2: Basic process diagram of APC utilizing renewable energy sources with hydrogen energy storage.

capacity factor and helping it compete with conventional power generation. This flexibility is achieved thanks to the combination of ultra-high thermal efficiency during the fuel conversion process and the features of the high pressure closed loop configuration.

After the fuel conversion has taken place, the exhaust gases leave the cylinder at the nominal boost pressure. The exhaust is dried by means of a condenser operating at the boost pressure and thus higher condensing temperatures. As a result, a more efficient heat transfer system and higher quality heat for ancillary services is made available. When H_2 is being used, the process ends after the condenser (see process diagram in figure 2). In the case of carbonaceous fuels, a membrane gas separation unit follows the condenser. This unit separates the resulting carbon dioxide (CO_2) from the exhaust and delivers the argon back to the engine intake. The high pressure of the exhaust stream and the closed-loop nature of the cycle make this separation possible at a small efficiency penalty of less than 5% by providing a high-pressure gradient across the membrane unit and enabling an increased carbon dioxide concentration on the exhaust stream through its combined recirculation with argon [1]. The CO_2 that is captured in this way can be used for long term carbon storage, enhanced oil recovery, or as industrial feedstock for fuels, chemicals and materials (CO_2 reuse). The extremely high conversion efficiency, fuel flexibility and cost-effective emissions mitigation make the APC a perfect companion to renewable energy.

The APC is ideal for use in a hydrogen energy storage scheme (figure 2). By electrolysis of water, surplus renewable energy is stored as hydrogen and oxygen (O_2), which the APC converts back to electricity at higher efficiencies than existing technologies such as fuel cells (60%) and air-breathing combined-cycle gas turbines (50-60%) while emitting no nitrogen oxides. Furthermore, APC engines, which can be regarded as modified large diesel engines, have a much lower investment cost than fuel cells (~500 EUR/kW vs ~3000 EUR/kW). The operational flexibility and agility of a power plant based on APC engines is

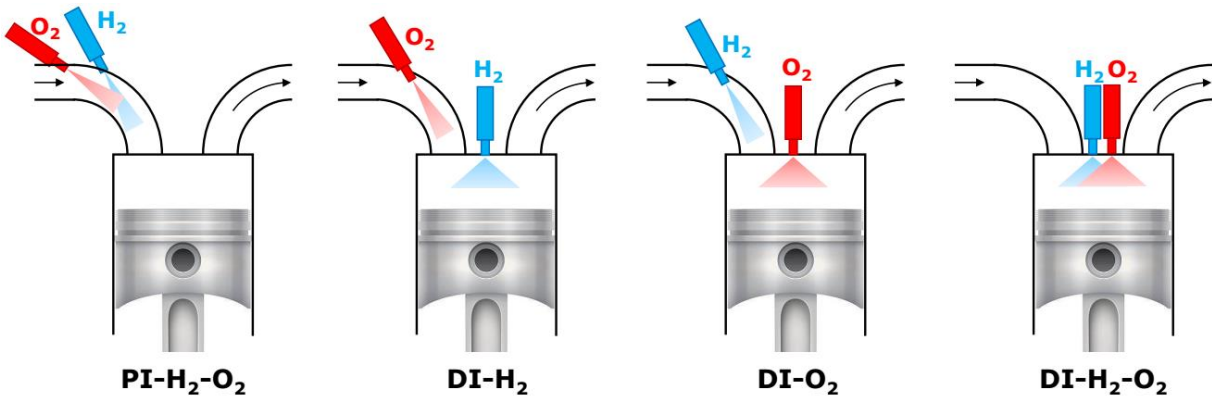

Figure 3: Basic injection configurations for the APC.

another big advantage for the use in conjunction with renewable energy sources. Power plants based on internal combustion engines dispatch power quickly when needed, counteracting the intermittent nature of renewable energy sources (RES).

Challenges and innovative character

As explained in the previous section, the APC is a very promising energy conversion technology that has the potential to play a big role in future renewable energy systems. However, the lack of knowledge and design tools hampers the development of APC technologies that fully exploit the enhanced efficiency and other advantages. Since the first ideas of a hydrogen fuelled argon engine were introduced and patented by Laumann and Reynolds in 1978 [2], only a handful of papers have been published in literature on this topic. Noteworthy are the experimental studies by de Boer and Hulet [3], Kuroki et al. [4] and Killingsworth et al. [5]. They demonstrated the feasibility of the APC in spark-ignition (SI) type engines and confirmed the significant increase in efficiency compared to operation with air. However, the compression ratio r in these SI engines is limited by knock, leading to suboptimal efficiencies (<50%). Due to the high heat capacity ratio of argon, the temperature that results in auto-ignition of the premixed charge is obtained at a relatively low compression ratio (r<8) and thus lower efficiency. **Therefore, we will focus on compression-ignition (CI) engines in this project, which can operate at high compression ratio and consequently have the potential to reach much higher efficiencies.**

APC in a CI engine is a rather unexplored area of research. Very little is known about combustion under these conditions. The major challenge is the injection of the gaseous reactants to control the combustion process. Both fuel and oxidizer need to be injected and subsequently mix, ignite and burn in a controlled way. Too much premixing before ignition results in too high heat release rate and consequent pressure rise, which may damage the engine. On the other hand, the reactants should mix well enough to burn completely. Note that this might be extra challenging when H_2 and O_2 are injected at stoichiometric ratio as provided by the electrolysis of water, and there is no excess air as in conventional engines.

The fact that O_2 needs to be injected into the cycle can be considered a challenge but also an opportunity to further improve the performance of the APC, because it provides an additional degree of freedom to the system. Since both fuel and O_2 can be either injected in the inlet port (Port Injection, PI) or directly into the cylinder (Direct Injection, DI), there are four basic injection schemes, which are schematically shown in figure 3. In this project we will consider hydrogen and methane as fuels. However, we will first focus on hydrogen since it is the perfect fuel for the APC (no gas separation required) and much more affordable to use in numerical simulations.

Port injection of both hydrogen and oxygen (PI-H_2-O_2 in fig. 3) will not be considered in this project, because it leads to a premixed charge, which ignites in an uncontrolled way at relatively low compression ratio as explained before. Therefore, we will focus on the other three, more promising, mixing-controlled DI schemes displayed in figure 3:

1. **DI-H_2**: This injection scheme is closest to that of a conventional CI engine, in which fuel is injected in a compressed oxidizer. Furthermore, port injection of O_2 is convenient since pressure and temperature are relatively low at that point of the cycle. However, not much is known about direct injection of H_2 at high pressures. Since H_2 is very light and diffusive, it may result in weak jet penetration, which is a reasonable concern given the large bore of stationary engines cylinders. For maximum efficiency, low oxygen concentration (to retain high γ) and large bore diameters (to reduce heat loss) are preferred. Will the H_2 jet scavenge all the O_2 from the cylinder? Will it improve, if H_2 is premixed with argon or preheated before injection? Furthermore, strong differential diffusion effects significantly affect the ignition behaviour of H_2 in non-premixed jets [6-8]. How will this influence the combustion process under these conditions?

2. **DI-O_2:** As an alternative, the heavier O_2 could be directly injected, which may improve jet penetration. In this case, O_2 will be injected in a hot compressed mixture of diluted fuel. Combustion under these inverse conditions has never been investigated. How will it affect mixing, ignition, heat release rate and combustion efficiency? This injection scheme could turn out to be a dark horse in the race for best injection strategy.

3. **DI-H_2-O_2:** Direct injection of both reactants promises the highest efficiency, since the penalty of a lower γ due to the presences of other gases than argon in the compression stroke is avoided. Furthermore, it maximizes the benefit of the high pressure at which H_2 and O_2 are stored in tanks by recovering (at least partially) the energy needed for pressurizing them. However, direct injection of both reactants has never been tried and ignition and combustion at these conditions is unexplored. The arrangement of the jets in space and time will have to be investigated. Fundamental knowledge of the interaction of the jets, their mixing, ignition and combustion behaviour, is required to come to an optimal injection strategy preventing too much premixing and its resulting practical problems (engine knock or super-knock). What will be the optimal strategy to control heat release rate and to reach the highest efficiency?

To answer these questions we will employ a multi-scale modelling approach in combination with advanced experiments on dedicated injection and engine setups. High-fidelity numerical simulation tools will be used to investigate the combustion process at the unexplored APC conditions and a predictive full-scale engine modelling tool will be developed in a bottom-up manner. First the fundamental processes at the micro scale will be unravelled by using first principles, direct numerical simulations (DNS). The richness and high level of detail of the resulting DNS data sets, will make it possible to develop reduced-order models for chemistry and turbulence, which enable the simulation of lab-scale experiments at affordable computational cost. In this project, the large-eddy simulation (LES) approach will be combined with an innovative reduced-order tabulated chemistry model for APC combustion. This new turbulent combustion model will be validated with high-quality lab-scale validation experiments and used to explore various injection strategies for APC combustion. Finally, a reliable and efficient modelling framework will be developed to simulate combustion in a full-scale engine cylinder, which will be validated with measurements in a research engine. This newly developed modelling framework can be used to further guide the design of APC technologies.

The proposed research encompasses the first comprehensive multi-scale modelling study of combustion in APC engines. The few studies on APC that have been reported, were all engine experiments. These pioneering works demonstrated the feasibility of APC with H_2, but they did not give insight in the combustion process occurring in the cylinder. However, understanding of the mixing and combustion process is essential to develop a direct injection compression ignition engine. Therefore, in this project, we will acquire this knowledge by performing high-fidelity simulations and detailed experiments in optically-accessible setups. The acquired insight and the newly developed tools will enable us to make the next step and to boost the efficiency of APC engines to unprecedented values.

The proposed modelling work is quite challenging from a computational point of view. At present, engine design and optimization studies in industry are almost exclusively performed by using unsteady RANS (Reynolds-Averaged Navier-Stokes) modelling, which is computationally much cheaper than LES. However, RANS requires a lot of model tuning and, hence, its predictive capability is rather limited. The establishment of LES as a turbulence modelling technique caused a step change in modelling accuracy and it has become the preferred method of choice in most academic studies. By pushing the limits of high-performance computing, we will develop an efficient and accurate LES model for APC combustion and demonstrate its superior performance against established methods. Together with the continuously increasing availability of cheap computing power, possibly in the cloud, this will pave the way to use high-fidelity models in engine development.

Methods and techniques

In this project we will use a series of high-fidelity numerical methods and experimental techniques to investigate the injection of H_2 and O_2 in the APC. These methods and techniques are described in the following sections.

Direct numerical simulation

Direct numerical simulation is the perfect numerical method to unravel the fundamental processes that occur in turbulent reacting flows. It can be considered as the microscope for turbulent flow studies since it resolves all length scales of the flow down to the smallest phenomena. As such, DNS has been successfully used to study the interaction of turbulence and chemistry in a wide variety of combustion problems [9,10]. In DNS, the governing equations which are solved, describe conservation of mass, momentum and energy, and are derived from first principles. In combination with highly detailed and reliable models for molecular transport and reaction kinetics, DNS gives the most accurate prediction of the flow at an extreme level of detail. Basically, all flow variables are available at all locations. Therefore, DNS provides spatially and temporally resolved data for quantities that are hard or impossible to measure experimentally, yet are of utmost importance for the development of multi-scale combustion models. The lack of DNS data for APC conditions impedes the development of such models. Therefore, we will perform DNS of turbulent flows in this project at conditions that are representative for the APC. Local chemical mode analysis of the resulting data sets in the framework of a flame-adaptive coordinate system will give detailed insight in the modes of combustion occurring in APC combustion. The resulting data will provide all the essential information to develop APC combustion models employing reduced-order models for turbulence and chemistry.

In this project, DNS will be performed of APC combustion in a series of configurations with increasing complexity. The following cases will be simulated:

1. *Periodic planar jet:* In this configuration, a high velocity jet surrounded by a low-velocity (or counterflowing) fluid in a periodic domain is simulated. The difference

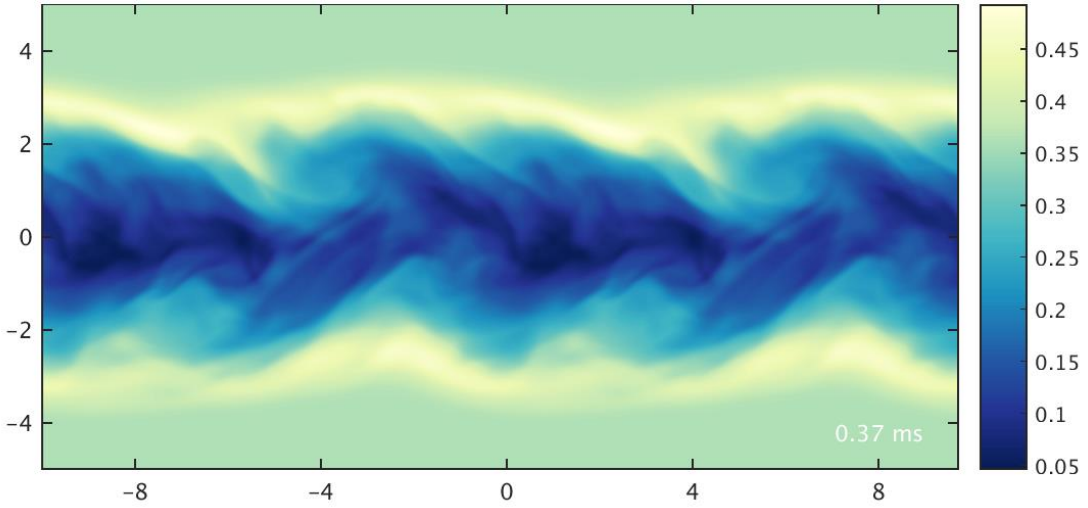

Figure 4: DNS result of a planar periodic jet of a CH_4/H_2 mixture in hot diluted air [15], showing the mass fraction of water averaged along the line of sight. Units are mm.

in velocity creates two temporal mixing layers at each side of the jet. This is a common configuration to study turbulent mixing of two fluids (see, e.g., figure 4) and will be used to study injection of H_2 in premixed Ar-O_2 and injection of O_2 in premixed Ar-H_2, corresponding to DI-H_2 and DI-O_2 in figure 3, respectively.

2. *Periodic planar parallel jets:* This configuration is similar to the previous case but it considers two (or more) parallel jets. With this configuration we will study the interaction of H_2 and O_2 jets in a background of hot argon, which mimics the DI-H_2-O_2 injection scheme of figure 3. DNS of such a three-stream problem has never been performed and will provide new important information on how these streams mix, ignite and burn.

3. *Unsteady round jet:* In this setup, a gaseous jet emerging from an injector will be modelled. This setup features an inlet boundary condition, which makes it possible to prescribe a time-dependent flux of gases into the domain. In this way we can simulate injection events and study the temporal and spatial development of the resulting unsteady round jet. Since this setup requires a much larger domain than the former cases, its DNS is computationally very challenging and unprecedented. Preliminary 2D runs at 40 bar and 1300 K have indicated that such simulations are within reach on large high-performance computing (HPC) clusters.

4. *Multiple unsteady jets:* This configuration is an extension of the previous one in the sense that in this case two jets will be considered. While the previous setup allows to simulate two-stream combustion problems corresponding to DI-H_2 and DI-O_2 injections schemes, this setup involves three streams and resembles the DI-H_2-O_2 injection scheme. The exact configuration (parallel, concentric, …) to be simulated, is to be decided based on results obtained from the other configurations.

The simulations will be performed by using our in-house developed DNS code, which we have used successfully in various studies of turbulent flames [6,7,11-16]. This DNS code solves the governing equations in fully compressible form including detailed models for molecular transport and chemistry. It employs advanced higher-order space and time discretization methods. The code has been parallelized by using MPI and OpenMP and scales very well on high-performance supercomputing facilities. To further enhance the computational performance of the code, we will pursue GPU-acceleration for the calculation of reaction rates and transport coefficients.

Adaptive Flamelet Tabulation for Multi-stream Mixed-mode Combustion

Numerical tools for the modelling of reactive flows in APC should accurately predict complex chemical phenomena such as auto-ignition and extinction. This implies the use of accurate chemical kinetics with a sufficient level of detail that only multi-step, multi-species reaction mechanisms can provide. The combustion chemistry of hydrogen and methane has been thoroughly investigated over the years and detailed highly reliable mechanisms are available. The use of detailed reaction mechanisms in combustion simulations, however, comes at a very high computational cost. Though the reaction mechanisms of hydrogen and methane are among the simplest of all fuels, they still comprise dozens of species and hundreds of reactions and cannot be used directly in simulations of reactive flows in practical applications. To tackle this problem, many methods have been developed, of which flamelet-based tabulated chemistry approaches such as the Flamelet Generated Manifold (FGM) method, have been very successful. The FGM method makes the use of detailed reaction mechanisms in DNS of canonical flows affordable and enables LES of reactive flows in practical engineering applications [17]. In 2000, van Oijen introduced the FGM formalism that combines the advantages of mathematical chemical reduction techniques and laminar flamelet models [18]. Since its first application to premixed laminar flames, the FGM approach has been systematically analysed and extended to include more physical phenomena in different flame types. Heat loss and flame stretch effects combined with preferential diffusion were studied [18-21] and the method was successfully extended to partially-premixed and non-premixed flames [22-28] and flameless (or mild) combustion [8,9]. It was further developed to be used in RANS and LES [9,30-38] of turbulent flames. In all these steps, the FGM method has been carefully validated against simulations using the full reaction mechanism. It was found that FGM simulations reproduce the results of detailed simulations very accurately (see, e.g., figure 5), but that they are typically 100 times faster. Because of these outstanding results, FGM has attracted a lot of interest in the field of turbulent combustion modelling. Today, many experts are using FGM or similar approaches, such as FPI [39] and FPV [40], in their simulations of turbulent flames.

Unfortunately, present flamelet tabulation methods are not suitable to model the complex combustion process under APC conditions, which features auto-ignition, preferential diffusion and mixing of multiple streams. This complex interaction of

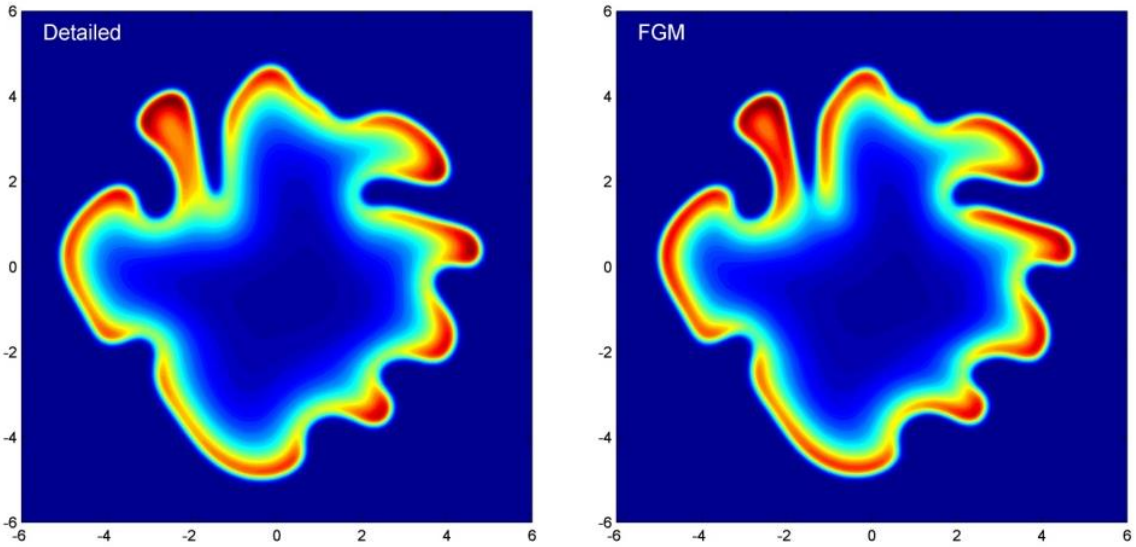

Figure 5: DNS results of the mass fraction of atomic hydrogen in a turbulent premixed CH_4/H_2-air flame kernel computed with detailed chemistry (left) and FGM (right). Same colour scale is used in both plots. The strong preferential diffusion effects are well predicted by using FGM [17].

phenomena may lead to the simultaneous presence of both premixed and non-premixed reaction-diffusion structures as well as mixed forms of these two, which is known as mixed-mode combustion. **Therefore, we propose to develop an innovative adaptive flamelet tabulation (AFT) method which can dynamically adjust itself to the mixing conditions in the flow and the local mode of combustion**. This new AFT method will bring flamelet combustion modelling to the next level and extend its modelling capabilities to include to following phenomena:

1. **Multi-stream mixing:** Flamelet models for non-premixed autoigniting combustion systems usually consider only two-stream problems, fuel and oxidizer, with a single mixing parameter, the mixture fraction. While this approach might be sufficient to model combustion in the DI-H_2 and DI-O_2 injection schemes, it will not work for the DI-H_2-O_2 case, which is essentially a three-stream problem and requires at least a second mixing parameter. However, since both fuel and oxidizer stream might be diluted at different levels due to argon entrainment, a single variable to account for the mixing with a third stream is not enough. Therefore, in the new AFT method, flamelets will be computed for all mixing combinations of the streams that occur in the flow. If this would be done in a preprocessing stage for all theoretically possible combinations, then the resulting look-up table would be huge and impractical to use. The actual mixing combinations occurring in the flow are usually only a small fraction of all possible combinations. Therefore, we propose to develop an innovative method that computes the required flamelets online, i.e. during the flow simulation, for the mixing combinations that are locally present. Following the ideas of in-situ adaptive tabulation [41], these flamelets are stored and reused, when similar mixing conditions occur. When mixing conditions are encountered in the simulation that are not yet stored, the representative flamelet is computed and added to the table. In this way a dynamic flamelet table is formed, which adapts itself to accommodate the actual mixing conditions in the flow.

2. **Mixed-mode combustion:** In existing flamelet tabulation methods, a chemical look-up table is constructed using flamelets that are representative for the reaction-diffusion structures that are expected to occur in the application. However, in general it is not known in advance what kind of reaction-diffusion structures may arise in a combustion problem. Results of DNS with the detailed chemistry will reveal which reaction-diffusion structures are present in APC combustion. It is not unthinkable that both premixed and non-premixed reaction-diffusion structures will occur. Though the reactants are injected separately in the DI-H_2-O_2 case, they may premix to a large degree before they ignite, which will result in a premixed propagating flame front. Unlike existing flamelet methods, the proposed AFT method is very suitable to deal with this mixed-mode combustion regime. By not only considering the gradients of mixing variables but also of the reaction progress variable, the AFT method will be able to identify the local reaction-diffusion structure and define appropriate boundary conditions for the flamelet calculation. A large gradient in progress variable and negligible gradients in mixture fraction (and other mixing variables), for instance, will translate into a flamelet calculation with unburned and burned mixtures as boundaries at equal mixture fraction, effectively representing a premixed flame. When the mixture fraction gradient is not negligible, this may become a front- or back-supported stratified flame depending on the alignment of the gradients.

3. **Autoignition:** Since we are focussing on CI engines in this project, autoignition phenomena should be accurately predicted, which is quite challenging with tabulated chemistry methods. In tabulated chemistry methods, the progress of reaction is usually parameterized by a single variable, which is chosen such that it is monotonously increasing. Often a linear combination of reaction products is

chosen as reaction progress variable. Defining a suitable progress variable, which is monotonous for all conditions in the manifold, is not an easy task. As a result, the progress variable is often a compromise and cannot accurately describe all the different stages of the combustion process. Hydroperoxyl (HO_2), for instance, is a perfect progress variable for hydrogen ignition chemistry, but cannot be used for the final stages of the combustion process, which are much better parameterized by water (H_2O). To solve this problem, we propose to develop a tabulation approach, in which the combustion processes is divided in multiple stages with an optimal progress variable for each stage. Recently, we introduced this idea and demonstrated the advantages of this approach [16]. However, there are still many important questions to be answered. How should the boundaries of the different stages be chosen? What is the optimal number of stages? Is it possible to extend this idea to an infinite number of stages, leading to a continuously adapting, optimal progress variable?

4. **Preferential diffusion effects:** The large diffusivity of hydrogen compared to the other species leads to significant preferential diffusion effects. These effects were shown to have a tremendous effect on the ignition of H_2 containing fuels in non-premixed systems [6]. When preferential diffusion was included, the ignition delay was about 10 times shorter than when equal diffusivities were assumed for all species. Recently, we introduced a first step in the modelling of these effects by using FGM [7,8]. However, more recently, we observed that flame curvature significantly alters the effect of preferential diffusion on ignition behaviour by affecting the local elemental composition [42]. Since the AFT method can adopt itself to such changes, we propose to further investigate this important phenomenon and its modelling with the AFT approach.

The new AFT method described above will be first developed and tested in DNS. Results of DNS with detailed chemistry will serve as a reference for validation. Application of AFT in DNS, however, will also allow to run more demanding cases with, e.g., higher Reynolds number and methane chemistry.

Large-Eddy Simulation

Direct numerical simulation offers the highest accuracy in predicting turbulent combustion, but its tremendous computational cost limits its application to academic canonical problems in small rectangular geometries. Even though the costs are reduced significantly by using tabulated chemistry, DNS is still unaffordable for the modelling of turbulent combustion in real large-scale devices with complex geometries and RANS or LES have to be applied. In LES only the large scales of turbulent motion are resolved. The influence of the smaller scales, which are not resolved, on the large-scale flow is modelled. Since the small flow scales do not have to be resolved, a much coarser computational mesh than in DNS can be used, which enables its application in practical devices.

The main challenge in LES is the modelling of the unresolved phenomena that happen on the sub-grid scale. Especially for combustion simulations, this is a challenge, because the reaction-diffusion structures are typically smaller than the mesh width. Therefore, the interactions of turbulence and chemistry occur mostly in the sub-grid scales and need to be modelled. Much work has been done in recent years on the modelling of these sub-grid scale phenomena [43,44]. FGM or other tabulated chemistry models have been combined with many different approaches to close the unresolved terms in LES. An overview of these approaches is given in a recent review by Fiorina et al. [45]. The use of presumed probability density functions (PDF) offers a good balance between accuracy and computational efficiency. We have used this combined FGM-PDF approach successfully in LES of, e.g., piloted and auto-igniting non-premixed jet flames [8,31], partially-premixed

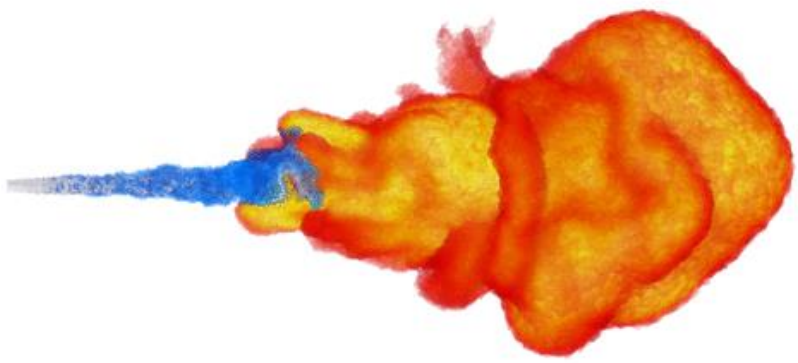

Figure 6: LES result showing instantaneous isosurfaces of n-dodecane (grey), formaldehyde (blue) and CO_2 (orange) mass fractions in a reacting jet 1.5 ms after injection of n-dodecane. Courtesy of H.Y. Akargün, TU/e.

flames in a gas-turbine combustor [38], and diesel spray combustion [34]. A recent LES result of a reacting n-dodecane spray is shown in figure 6.

In this project, we will develop an AFT-LES method and use it to study the combustion process in APC engines. Special attention will be given to the effect of different shapes that can be used for the sub-grid PDF and the modelling of the sub-grid variances of the AFT control variables. Fast numerical methods for online PDF integration will be used. We will also try to develop a new filtered flamelet approach as in [35,36] but now for non-premixed igniting flames. The combination of AFT with transported PDF and stochastic field methods will be investigated. DNS data generated in this project will be used for the development and the *a-priori* and *a-posteriori* validation of these new sub-grid models for APC combustion. The spatial and temporal evolution of the actual PDF determined from DNS results will be compared with model predictions. To that end, the same configurations (periodic jets and unsteady jets) will be simulated by using LES and compared with DNS results. Moreover, the results of the unsteady jet simulations will be validated against experimental results.

After validation of the LES model, we will use it to investigate the effect of injection timing and the location and orientation of the injectors on ignition delay, heat release rate and combustion efficiency. Especially for the DI-H_2-O_2 case, which requires at least two jets, many configurations are possible varying from concentric jets to parallel and impinging jets. The knowledge obtained from these investigations will be used to find the optimal injection scheme for combustion in APC engines. To perform these simulations, we will implement the new AFT model in our in-house LES code and in OpenFOAM, which has the advantage that it can be used for complex geometries. OpenFOAM is an open-source code, which is used by many research groups as a platform to implement and share new models.

Parallel to the AFT-LES development described above, we will work on the application of the developed models to simulations of real full-scale engine geometries. The complete toolchain developed in this project will be integrated in a numerical framework to run such simulations. Application of LES to engine simulations is quite challenging due to the complex geometry with moving parts and opening and closing valves. However, much progress has been made in the last decade and very recently we were able to simulate 60 cycles of a single-cylinder SI engine [46]. While LES has become the standard method for combustion modelling in academic research, it is not as much used in the automotive industry. Therefore, the objective of the development of this LES-AFT modelling toolchain

is twofold:

1. Simulate combustion in an APC engine for model validation with experiments that will be performed on a single-cylinder research engine.
2. Increase the uptake of the project's results by industrial users.

To reach these objectives, the new model developments will be implemented in OpenFOAM, which has been used to simulate reactive flows in internal combustion engines. It includes many physical models and well-developed numerical methods for moving geometries. With this code, we will demonstrate the application of the new AFT combustion model in engine simulations. Moreover, these simulation results will be used to validate the complete model with measurements that will be done on a single-cylinder research engine.

Experimental approach

The numerical work described in the previous sections will be accompanied by experiments in different setups in order to investigate the combustion process in APC engines at both fundamental and more applied level. Moreover, the results of these experiments will be essential for the validation of the newly developed models.

Jet injection experiments

At fundamental level, we will investigate the injection of H_2 and O_2 in argon by performing experiments in the Eindhoven High-Pressure Cell (EHPC). This work will proceed in several steps. As a first step, mixing studies will be performed at room temperature. Molecular hydrogen cannot be visualized by planar Laser-Induced Fluorescence (LIF), but for mixing Rayleigh scattering may be a good alternative (exploiting the contrast in Rayleigh scattering cross section between H_2 and the ambient gas). Moreover, the use of spontaneous Raman scattering (SRS) for species distribution will be evaluated. The major drawback of SRS, its low efficiency, is to some extent alleviated by the high densities at the conditions of interest, and the relatively simple resolution of rotational structure in the H_2-spectrum should provide a simultaneous indication of the local temperature. We will attempt 1-D measurements [47], using a grating spectrograph/ICCD combination together

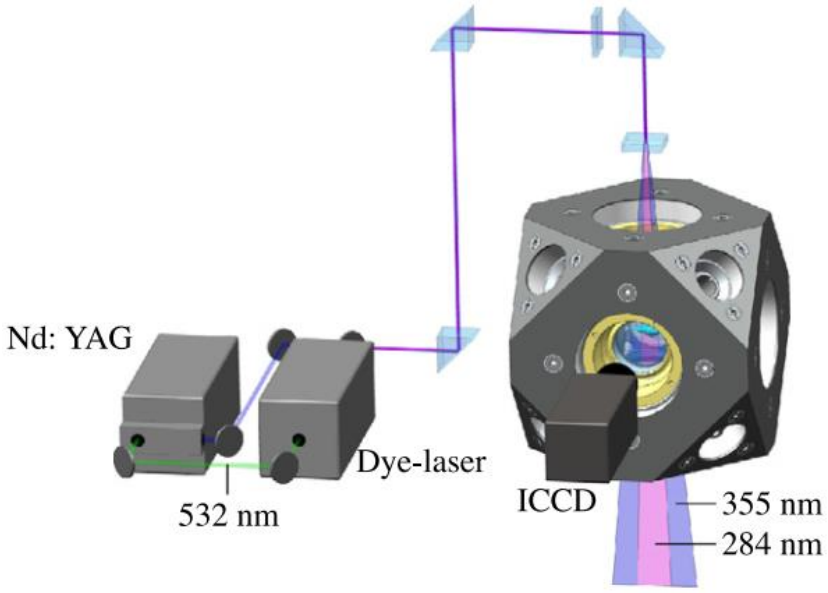

Figure 7: Schematic overview of the EHPC with the applied layout for chemiluminescence and laser-induced fluorescence (from Maes et al., [48]).

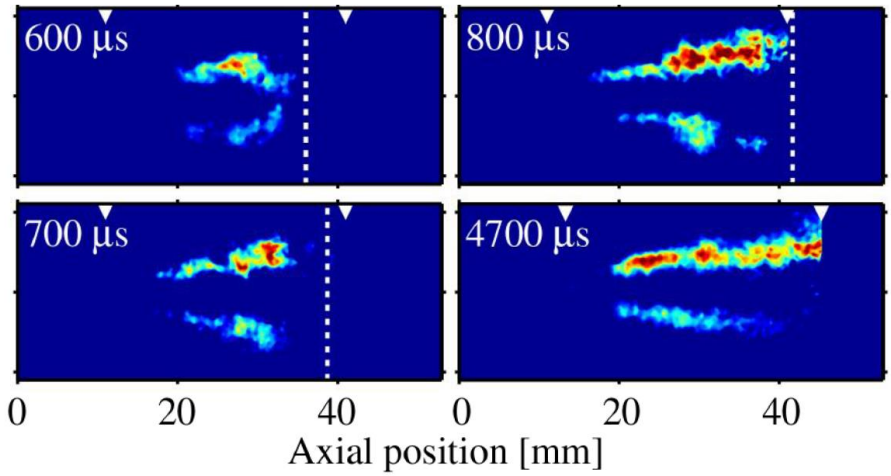

Figure 8: Evolution of OH PLIF structures in a reacting n-dodecane spray (ECN Spray-A) in the EHPC. Courtesy of N. Maes, TU/e.

with a pulsed Nd:YAG laser. The non-reacting mixing experiments can be performed in a separate simplified version of the EHPC. This cold mixing chamber doesn't require preheating of the mixture, which reduces the time to perform an experiment enormously. In this way, we can study the mixing process for many different conditions, gas mixtures, and jet configurations.

In the next step, combustion of reactive jets will be studied in the EHPC. This test rig is specifically intended for liquid fuel spray studies under engine-like conditions, but without moving parts and with wide optical access [48] (see figure 7). It will be available to this research on a time-sharing basis, and will be adapted to gas-phase fuel injection. In the EHPC, engine-like conditions are achieved by means of spark-ignited combustion of a premixed charge. The end gas of this so-called precombustion forms the ambient gas into which the gaseous jets are injected. The composition of the end gas is determined by that of the initial charge, and can be tailored to provide a wide range of ambient conditions for the injections.

The EHPC and its simplified version allow a wide range of optical diagnostics to be applied. Fuel/oxygen jet structure will be studied by means of diffuse back-illumination or Schlieren. The spatial and temporal evolution of the combustion itself will be monitored by imaging the natural OH* luminosity and by planar OH LIF (see figure 8). Based on the results obtained in the cold mixing chamber, suitable diagnostics will be applied to the EHPC as well. In addition, hot O_2 can be visualized by using LIF excited by the 5^{th} harmonic of a Nd:YAG laser. These measurements will give detailed information on the flame structures in unsteady igniting and burning jets under various mixing conditions, which is important for the development and validation of the numerical models.

Engine experiments

In order to validate our numerical efforts on configurations closer to real life application, we plan to conduct experimental engine tests in a single-cylinder research engine. The cooperative fuel research (CFR) engine at the University of California Berkeley will be used for this purpose. The CFR engine at UC Berkeley is the perfect platform to develop APC experiments as it already features APC required systems such as: variable compression ratio, hydrogen and methane port and direct injection supply system (with variable upstream pressure), automated argon and oxygen dilution supply system and intake and exhaust pressure control. If deemed necessary and beneficial for our numerical validation, experiments will be carried out with Noble Thermodynamic Systems' (NTS) multi-cylinder

engine (0.5 MW Caterpillar). The latter will support the testing of more aggressive conditions, closer to actual in the field conditions, such as higher inlet pressure, higher degree of turbulence and larger combustion chamber. A design of experiments exercise will help us define a relevant and reasonable set of experiments to be conducted based upon the specific cases to be validated and the complexity of the experimental setup.

The engine experimental work can be separated in two major periods distinguished by the level of complexity of the work at hand. In the first period testing will focus on the evaluation of DI-H2 operation. During a second period, the work will focus in evaluating oxygen DI and combined fuel/oxygen DI. The experiments with DI of oxygen in the EHPC and the CFR require the design and manufacturing of special injection equipment able to provide accurate and safe control over the oxygen injection event. This work will be carried out by a postdoc at TU/e in collaboration with the team at UC Berkeley, with the support of NTS.

More specifically, the engine experiments will generate in-cylinder pressure data and exhaust gas composition, both accompanied by accurate and well monitored boundary conditions such as exhaust molar composition, mass and molar flow rates, temperatures, pressures and any other parameter required to perform a detailed analysis of the mass, momentum, and energy balances of the system.

Techno-economic analysis

A techno-economic analysis will be provided at the end of this project to assess the near- and long-term potential of this technology to integrate into the global power portfolio. This analysis will, based on numerical and experimental estimates of the system performance, evaluate the internal rate of return in a project integrating the APC, evaluate different cash flow scenarios and compare to the state-of-the-art financial performance of conventional and emerging power generating and energy storage technologies. While this project focusses on the combustion process in the APC engine, as the most challenging part of the system, the techno-economic analysis will also include gas storage and separation units comparing various existing technologies. Among different financial parameters, this analysis will provide to a reasonable measure of accuracy the levelized cost of energy/electricity (LCOE), net present values (NPV) and payback time (PBT). The results of this analysis will be delivered as a report, which may serve as a guidance for policy makers and market regulators in designing future incentives for clean technology integration.

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