

Reduced Convective Combustion Chamber Wall Heat Transfer Losses of Hydrogen-Fueled Engines by Vortex-Stratified Combustion - Part 2: Numerical Analyses

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ABSTRACT

In this second of two parts, the fundamentals of convective wall heat transfer losses are elucidated in the context of the desired objective toward its reduction in a direct-injected, hydrogen-fueled internal combustion engine. A comparative, transient 2D CFD analysis evaluated at 4500 RPM between a combustion chamber design representing current practice and the here-introduced “vortex-stratified combustion” process finds an approximately 50% reduction in the peak convective flux with the latter. The simulation results show that reduced heat flux of the vortex approach is driven by the combination of two effects: The first is finite-time diffusive mixing getting outpaced by the replenishment of pure air being introduced preferentially along the circumference of the combustion chamber due to the Coandă effect; this results in a distinct radial charge stratification during mixture preparation in the compression stroke, with a fuel-concentrated center and essentially pure air at the periphery. The second effect is the forced-segregation of different density reactants during the course of the combustion process caused by large body forces that result from the gravitational acceleration of the rapidly rotating charge, thereby constraining the combustible mixture and the flame to some distance from the walls. Evidence for this is observed by hot, low-density hydrogen being forced to remain near the center and cooler, heavier oxygen being inhibited from migrating from the outer periphery to react with the aforementioned hydrogen, and the distinct curvature of the radial gas temperature profile at a substantially greater distance from the wall than the thermal boundary layer thickness.

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INTRODUCTION

In the first part that precedes this article [1], the authors conduct an extensive survey on hydrogen-fueled ICEs that identify wall-heat transfer as the predominant factor of reduced efficiency and a key factor to its improvement. It introduces a combustion chamber design using a novel “vortex-stratified combustion” approach, aiming to isolate the hot burned gas products from the cold combustion chamber walls using an insulating air layer. Experimental observations from a schlieren optically accessible engine demonstrate the effectiveness of the concept in setting up the vigorous rotational flow field that forms a radial density gradient on the gas mixture before ignition. This gradient is hypothesized to be caused by species stratification that results in a fuel-concentrated core at the center of the combustion chamber and a layer of essentially pure air at the periphery. During combustion, there is visual evidence of the flame propagation being directed radially inward by the effect of centripetal body forces, thus hindering or delaying the contact of hot burned gases with the surrounding combustion chamber walls. This second part now provides the numerical analyses of the flow mechanics involved to correlate and explain the experimental observations of the first part, and most importantly, quantifies the potential reduction in peak convective wall heat flux to be in the order of 50% compared to a combustion chamber design that represents current engine practice

with homogeneous charge mixture and high turbulence but no particularly ordered motion, given identical injection timings, boundary conditions, and all other parameters in the CFD model.

BACKGROUND

Demuyne et al (2009) [2] measured peak heat flux of a CFR SI engine under stoichiometric hydrogen operation to be three times higher than stoichiometric methane at the same power output (the hydrogen case was operated at WOT, but throttled on methane). Total heat loss on an absolute basis is 40% higher for hydrogen. Due to heat release taking place over fewer crank angle degrees on account of the high flame speed, the cooling loss ratio - defined as the total cycle heat loss divided by the released energy during combustion - is about 29% higher. Where the methane case is tested also at stoichiometric and WOT conditions, the hydrogen cooling loss ratio is 52% higher. At $\lambda = 1.5$ ($\phi = 0.67$) the peak heat flux and cooling loss ratio on hydrogen are comparable to that of stoichiometric methane, but power output is only about 75% that of methane.

Kamo, Bryzik and Glance (1987) reported on a low-heat rejection prototype based on a Cummins turbodiesel engine, where ceramic coatings were employed on all combustion-exposed surfaces and the water cooling system was eliminated. Specific heat rejection was

reduced by 38% from the baseline engine, and dynamometer data showed a fuel economy gain of 5-10% over the same speed range at full load. Vehicle data indicated a fuel economy benefit in excess of 20% following a domestic road cycle [3]. Watts and Heywood (1980) calculated that in order to increase the brake thermal efficiency by about 10%, heat transfer must be reduced in the order of 50% from the baseline value in low-speed, full-load conditions of two different automotive SI engines investigated [4]. Oppenheim et al (1996) computed a 24.9% decrease in indicated specific fuel consumption by halving the wall heat transfer [5]. Therefore, reducing heat losses of the magnitude demonstrated in this work has important implications of substantially improving the fuel efficiency of hydrogen-fueled engines employing this vortex-stratified combustion process.

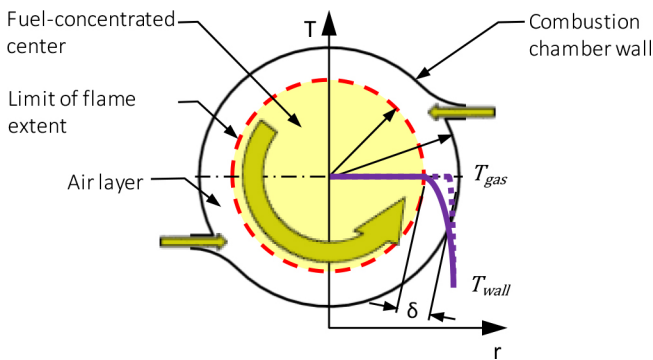


Figure 1. Flow motion of the vortex-stratified combustion chamber, and comparison of burned gas temperature profiles with non-vortex counterpart.

In the combustion chamber of a conventional, homogeneous-charge SI engine - shown schematically in Fig. 1 as having a round cross-section of radius R - the burned gas temperature T_{gas} will take on a nearly constant profile with respect to the radius, with a drastic reduction at the thermal boundary layer close to the wall until matching that of the gas-side wall surface T_{wall} , as sketched qualitatively with the dashed curve. If the combustable charge could be confined to a radius r_x , leaving a distance δ from the wall, the temperature profile would take on a more gradually declining shape as illustrated by the solid curve, beginning at the limiting extent of the flame due to the presence of a fuel-air mixture within flammability limits illustrated by the shaded core. Should δ be greater than the boundary layer thickness and inherent flame quenching distance, a reduction in convective heat flux results. The mechanisms of this phenomenon are explained in the following.

Convective Heat Transfer Fundamentals

All three heat transfer modes of conduction, convection, and radiation are simultaneously active in the working gas, so it is customary to replace the pure convective coefficient with an averaged one that effectively combines the effects of convection, conduction and radiation together. However, Borman and Nishiwaki (1987) state that for SI engines, heat transfer due to gas radiation is small (<10 %) compared to convection [6] and is thus not considered here. The convective heat transfer rate or flux $\dot{Q}_{wall}$ is described by Eq. 1, with A being the surface area:

$$\dot{Q}_{wall} = h \cdot A \cdot (T_{gas} - T_{wall}) \quad (1)$$

The empirically derived convective coefficient h is related to the Nusselt number, which is a function of the Reynolds and Prandtl numbers, where m and n are constants:

$$Nu = \frac{h \cdot l}{k} \propto Re^m \cdot Pr^n \quad (2)$$

$$Re = \frac{\rho \cdot U \cdot l}{\mu} = \frac{U \cdot l}{\nu} \quad (3)$$

$$Pr = \frac{\rho \cdot \nu \cdot C_p}{k} = \frac{\mu \cdot C_p}{k} \quad (4)$$

Heywood [7] cites works that propose the use of the flat-plate forced-convection heat transfer correlation formula:

$$\frac{h \cdot l}{k} = 0.036 \cdot \left(\frac{\rho \cdot U \cdot l}{\mu} \right)^{0.8} \cdot \left(\frac{\mu \cdot C_p}{k} \right)^{0.333} \quad (5)$$

Collection and arrangement of the terms give an expression for the surface area-specific heat flux as:

$$\dot{q}_{wall} = \frac{\dot{Q}_{wall}}{A} \propto \frac{\rho^{0.8} \cdot U^{0.8} \cdot k^{0.667} \cdot C_p^{0.333}}{\nu^{0.467} \cdot l^{0.2}} \cdot (T_{gas} - T_{wall}) \quad (6)$$

Or, in terms of dynamic instead of kinematic viscosity:

$$\dot{q}_{wall} \propto \frac{\rho^{0.333} \cdot U^{0.8} \cdot k^{0.667} \cdot C_p^{0.333}}{\mu^{0.467} \cdot l^{0.2}} \cdot (T_{gas} - T_{wall}) \quad (7)$$

By inspection of the magnitudes of the exponents, it is clear that the largest contributing parameters to wall heat transfer are the temperature delta, as well as the flow velocity and density within the Reynolds number term, so any systematic approach to its reduction should fundamentally be focused in these areas. Addressing the temperature difference on the wall side, extensive research has been done in so-called "adiabatic" engines [3, 8], and current investigations into "low-temperature combustion" (LTC) schemes like HCCI [9], PPC [10] and RCCI [11] are in vogue, partially due to the efficiency gains afforded by reduced wall heat losses from lower burned gas temperatures using highly dilute mixtures typical of these processes.

Charge Density Effect on Turbulence and Heat Transfer

At a given part-load operating point, a hydrogen-fueled engine, by virtue of lean operation, will require less intake air throttling. This will trap a higher mass of fuel-air charge in the cylinder compared to a stoichiometric gasoline case, independent of whether mixture formation is accomplished externally to the cylinders or by direct injection. This will result in higher charge density at the start of ignition. Consequently, turbulence levels and heat transfer coefficients will also be higher by their dependence on the Reynolds number (see Eq. 3) and the density term in Eq. 6 or 7.

LeFeuvre et al (1969) showed that increasing density ratio results in increasing heat flux in a Diesel engine at fixed operating speed, nominal equivalence ratio and injection advance [12]. Alkidas and Myers (1982) showed in a gasoline SI engine that an increase in volumetric efficiency corresponding to an increase of peak gas pressure in from 2363 to 3581 kPa results in peak heat flux increasing 19% to 30% depending on the location of the polled sensor reading in the cylinder head [13]. Demuynck et al (2009) showed that under motored conditions, the measured heat flux in their setup during WOT is about twice that for closed throttle. However, they report that the flux is higher at 75% throttle opening than even the WOT case; the lower cylinder density is more than offset by increased overall turbulence as a result of the butterfly throttle angle upstream from the intake ports.

Heat Transfer Effects from fuel Properties

Hydrogen possesses a faster laminar flame speed than gasoline, between factors of 5-6.5 at stoichiometric fuel-air ratios [14, 15]. At hydrogen-air equivalence ratios of $0.3 < \phi < 0.5$, the laminar flame speed is of comparable magnitude to stoichiometric gasoline-air mixtures. Where the hydrogen equivalence ratio is 0.6, the laminar flame speed is about twice that of stoichiometric gasoline.

Adiabatic flame temperatures are of comparable magnitude for both stoichiometric hydrogen-air and gasoline (analogously isooctane)-air mixtures; Verhelst and Wallner (2009) [15] report values of 2390 K for stoichiometric hydrogen-air and 2276 K for stoichiometric isooctane-air (both values at 300 K and 1 atm initially). The hydrogen-air values are very similar to those from Drell and Belles (1958) [16] and Das (1996) [17]. However, White et al report the adiabatic flame temperature for a stoichiometric gasoline-air mixture to be higher than hydrogen-air at 2580 K [14]. By comparison, the equilibrium adiabatic flame temperature for hydrogen-air at $\phi = 0.5$ is 1643 K per Drell and Belles.

Both flame speed and temperature increase with initial temperature and pressure, especially for near-stoichiometric mixtures, although the pressure effects on flame temperature are minimal at both extremes of equivalence ratios ($0.5 > \phi > 4$) between 0.01 - 100 atm. Nevertheless, experiments have shown that wall heat transfer losses for hydrogen-fueled engines are significantly higher than the same engine operating on stoichiometric gasoline at the same load and speed; an increase is evident even when the hydrogen case operates significantly lean of stoichiometric as shown by several researchers [18, 19]. These results contradict the similar (in stoichiometric) or lower flame temperatures in lean hydrogen combustion, compared to stoichiometric gasoline, even when charge density-induced turbulence and heat release rates are taken into account. Therefore, some other mechanism or mechanisms must be responsible for the higher measured wall heat flux, and focusing upon this area would be the key to reducing the rejection losses and thus contribute to improving the efficiency of internal combustion engines.

Flame Quenching Distance

One mechanism affecting the heat flux is the quenching distance, which is much lower for hydrogen flames than for hydrocarbon fuels like methane, propane and isooctane. Table 1 summarizes the relevant properties of these fuels:

Table 1. Quenching distance between parallel plates for various fuels and equivalence ratios in air at 1 atm, 298 K unless otherwise specified.

Fuel and equivalence ratio	Quenching distance, cm
Hydrogen $\phi = 1$	0.063 [16]
Hydrogen $\phi = 0.5$	0.08 [16]
Methane $\phi = 1$	0.21 [20], 0.23 [21]
Propane $\phi = 1$	0.205 [21], 0.203 [22]
Isooctane $\phi = 1$	0.22 [23] [†]

[†]At 100°C

The quenching distance is not constant but rather a function of both pressure and mixture composition, decreasing with increasing pressure and also with increasing equivalence ratio up to the stoichiometric value, whereupon quenching distances increase with even richer mixtures. Drell and Belles state that it may be assumed that the quenching distance decreases as the temperature of the mixture (and of the surface) is raised [16]. The same pressure and air-fuel ratio dependence are also observed in a wide variety of hydrocarbon fuels [20, 21, 22, 23]

Once all the likely factors to influence the higher observed wall heat transfer in hydrogen-fueled engines compared to gasoline ones are taken into account - flame temperature; heat release rate; trapped charge density; and in-cylinder turbulence levels - it becomes apparent that the key to the wall heat rejection losses in hydrogen-fueled engines lies in the flame quenching distance and this should be the focus of measures toward the reduction of these losses. Shudo, Nabetani and Nakajima (2001) concur that the higher cooling loss for hydrogen combustion could be attributed to a thin temperature boundary layer thickness on the combustion chamber wall due to a shorter quenching distance [24].

VORTEX-STRATIFIED COMBUSTION

In light of this, a sensible approach is to confine the extent of the fuel-air charge and thus the flame to some distance away from the walls, as previous works have attempted by means of fuel injection strategy [25] and the use of air blast injections [26]. The authors introduce and hypothesize by optical engine observations in [1] a novel 2-part mechanism of achieving this: First, by setting up a rotating vortex flow in the combustion chamber and exploiting the Coandă effect, diffusive mixing with fuel is outpaced by the replenishment of pure air being introduced preferentially along the circumference, resulting in a distinct radial charge stratification during mixture preparation in the compression stroke with a fuel-concentrated center and essentially pure air at the periphery. The second effect is the forced-segregation of different density species during the course of the combustion process caused by large body forces that result from the centripetal force acceleration of the rapidly rotating charge, thereby causing the propagating flame front to curl

radially inwards and constraining it at some distance away from the outer walls, as have been observed by [Lapsa and Dahm \(2009\)](#) in experiments using premixed propane in a U-shaped channel [27].

In order to perform a first-order, analytical estimate of the potential for wall heat transfer reduction by means of flame-extent confinement, Fourier's Law used to formulate gas-side thermal conduction could be applied for convection by substituting the conductive coefficient k for the appropriate relation with an effective convective coefficient h , and analogize a solution as a concentric superposition of thermal resistances as shown in [Fig. 2](#), also known as cylindrical shells.

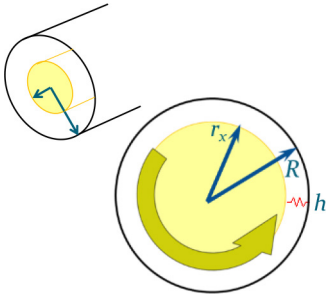


Figure 2. Schematic showing a first-order analytical consideration of heat transfer using the analogy of thermal resistance or cylindrical shells.

In the following relationship, the subscript δ denotes the respective fluid properties in the non-combusting stratification zone and the overbars denote averaged, effective values of all contributing heat transfer modes:

$$\overline{h_\delta} = \frac{\overline{k_\delta} \cdot \overline{Nu_\delta}}{R} \quad (8)$$

Solving the differential equation for Fourier's Law and substituting [Eq. 8](#), where r_x is the limit extent radius of the burned gas:

$$\frac{\dot{Q}}{A} = -k \frac{dT_{fluid}}{dr} \quad (9)$$

$$\frac{\dot{Q}}{2\pi L} \int_{r_x}^R \frac{1}{r} dr = -k \int_{T_{gas}}^{T_{wall}} dT_{fluid} \quad (10)$$

$$\dot{Q} = \frac{2\pi L \overline{k_\delta}}{\ln\left(\frac{R}{r_x}\right)} (T_{gas} - T_{wall}) \quad (11)$$

$$\therefore \dot{Q} = \frac{2\pi L R \overline{h_\delta}}{\overline{Nu_\delta} \ln\left(\frac{R}{r_x}\right)} (T_{gas} - T_{wall}), r_x < R \quad (12)$$

For the same envelope geometry, temperature delta and fluid properties, the difference in heat fluxes between any two compared cases is limited only to the term $\ln\left(\frac{R}{r_x}\right)$. In the case of a homogeneous fuel-air mixture, we take $R - r_x = \delta$ to be the flame quenching distance. With $R = 10 \text{ mm}$ and $r_x = 8 \text{ mm}$ imposed by the vortex stratification process - a value obtained from CFD analysis presented later in this paper - the heat transfer rate is reduced by 71% compared to the homogeneous case. [Eq. 12](#) is useful for another purpose: Consider that the stoichiometric flame quenching distance of methane (see [Table 1](#)) is similar in magnitude to the flame-extent limit of the hydrogen vortex-stratified case just calculated, and the 243% increase of the heat flux $\dot{Q}$ of the homogeneous stoichiometric hydrogen result agrees reasonably well with the factor 3 higher peak heat flux reported by [Demuyne et al \(2009\)](#), noting that the stoichiometric adiabatic flame temperature of methane is in the order of 200 K lower than the hydrogen counterpart.

NUMERICAL ANALYSIS

CFD analyses are performed in ANSYS Fluent (V16.2). In order to minimize solution time, they are performed in 2D rather than 3D space, greatly reducing the number of cells. This is a reasonable approximation given the nature of the flow field. In all cases considered, the models employ the RANS approach due to its low computational expense compared to LES and DNS. In the present study, the pressure-based, coupled solver is used with PRESTO! pressure interpolation and second-order upwind discretization of other variables. The Realizable k- ϵ turbulence model is used here, having been compared and employed extensively amongst other turbulence models against experimental validations in investigations of engine in-cylinder flow featuring under-expanded hydrogen direct injection [28, 29, 30]. Gravity and full buoyancy effects are considered in the calculations.

Especially for convective heat transfer problems, the near-wall modeling significantly impacts the fidelity of numerical solutions. There are two approaches to modeling the near-wall region: one where semi-empirical formulas called "wall functions" are used to bridge the viscosity-affected region between the wall and the fully-turbulent region, and the second termed "near-wall modeling," where the turbulence models are modified to enable the viscosity-affected region to be resolved with a mesh all the way to the wall, including the viscous sublayer [31]. In this work, the former approach is employed with the Enhanced Wall Treatment ϵ -Equation (EWT- ϵ), with pressure gradient and thermal effects options enabled.

[Figure 3](#) shows 3D solid models of the vortex and non-vortex combustion chambers. Only the fluid-exposed surfaces are shown along with the respective locations of the injector and spark plug, without the surrounding engine body. [Figure 4](#) shows the computational domain and meshes of the 2D faces, taken to be the mid-plane cross-sectional cuts of the 3-dimensional parts. The protruding spark plug electrodes are neglected. The outward-opening poppet valve-type hydrogen injectors, which in reality would form a moving annulus, are simplified in the model as being fixed.

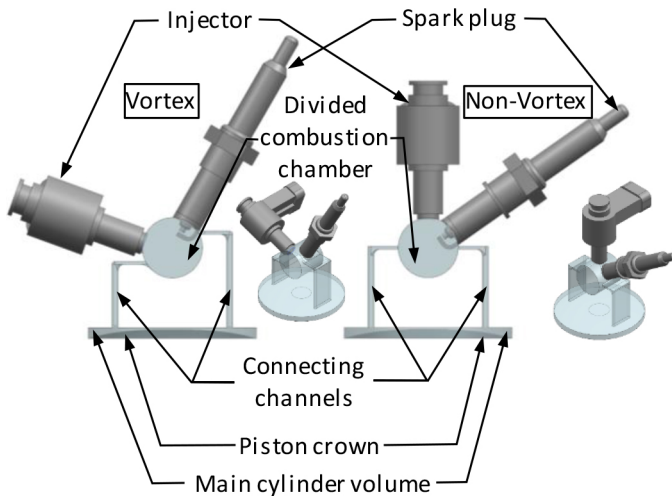


Figure 3. CAD renderings of vortex (left-half) and non-vortex (right-half) divided combustion chambers with connecting channels, injector, sparkplug main cylinder volume and piston crown depicted at TDC.

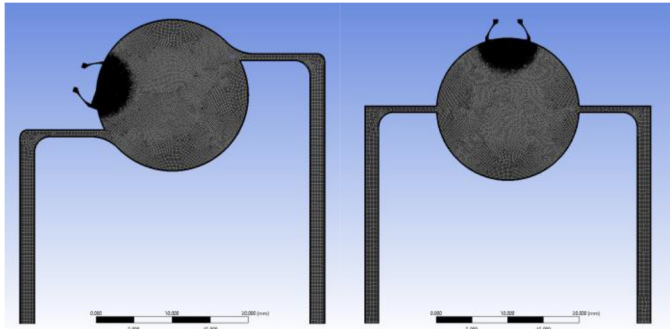


Figure 4. Vortex (left-half) and non-vortex (right-half) combustion chamber meshes showing local refinement in the area around the injector.

Sensitivity analyses of mesh density and timestepping were first preliminarily conducted. Particular refinement is necessary in four zones of the combustion chamber mesh:

- Near the walls;
- Internal gas injector geometry;
- In the area near the modeled spark ignition source;
- In the region of very high velocities of the under-expanded hydrogen injection jets.

The vortex combustion chamber geometry has generally been found to have more rigorous sensitivities to mesh refinement, timestepping and underrelaxation factors. For equal treatment and comparability of results the more conservative settings of either case are applied simultaneously to both the vortex- and non-vortex cases. In fact, the sole difference in the simulations distills only to the geometry.

Rather than performing intricate manual mesh refinements in each of the aforementioned zones, customized for nozzle configuration as done by Scarcelli et al (2011) [30], or using an adaptive mesh refinement (AMR) technique as done by Lin (2010) [32], Sukumaran and Kong (2010) [33] and Le Moine et al (2015) [34] - moreover for the very different bulk flow regimes of each of the vortex- and

non-vortex cases here - the whole combustion chamber uses the same finer mesh near the ignition source, and additional local refinement is reduced to 2 operations applied consistently to both geometries:

- Near wall region;
- Internal injector geometry and under-expanded jet region encapsulated within a sphere of influence of 4mm diameter centered on the injector valve.

For non-injection and ignition/combustion events, a timestep value of $1.85185\text{E-}5$ seconds corresponding to 0.5° crank angle intervals at 4500 RPM proves sufficient, but during injection and ignition/combustion, the interval must be shortened to 0.25° CA ($9.25926\text{E-}6$ seconds). Rather than having different time step intervals between the injection, ignition and combustion events from the rest of the simulated cycle, it was decided to choose a single fixed timestep interval at the more conservative value, that is, $9.25926\text{E-}6$ seconds.

After initializing the model with the default underrelaxation factors and flow Courant number until start of injection, the latter is reduced from 200 to unity for the rest of the simulation. The underrelaxation factors need to be progressively reduced during the course of the simulations for residuals stability, reaching the convergence criteria acceptably rapidly and avoiding floating-point exceptions.

The combined result of the above actions doubles the number of nodes and increases the number of timesteps by 33% over what is considered optimum solely from a sensitivity analysis without local refinement. However, this is a luxury permitted by 2D models where the final meshes only have about 35,000 elements rather than millions in 3D models. Any slowdown in solution time due to the added node and timestep counts is far more than offset in the better convergence behavior, permitting the entire solution to be completed in less than half the total number of iterations and overall faster wall clock time using the same convergence criteria. Furthermore, the differently tailored mesh refinements and timestep intervals that would be required for the vortex- and non-vortex cases greatly increase pre-processing effort and make it impossible to have identical models that compare only the substantive differences due to the respective geometries. This was considered to be of paramount importance over sensitivity optimization and was therefore an area of considerable time spent. All other parameters (e.g., employed physics and their settings/constants; boundary/initial conditions and underrelaxation factors) are kept the same.

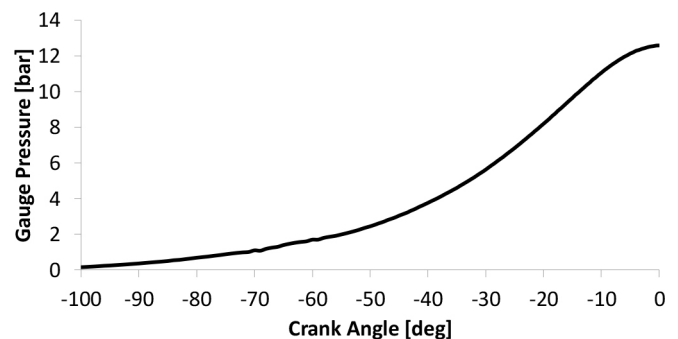


Figure 5. Chamber pressure profile during the compression stroke from ensemble average of experimental measurements.