

# Application of a Flow Field Based Heat Transfer Model to Hydrogen Internal Combustion Engines

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## ABSTRACT

A realistic modeling of the wall heat transfer is essential for an accurate analysis and simulation of the working cycle of internal combustion engines. Empirical heat transfer formulations still dominate the application in engine process simulations because of their simplicity. However, experiments have shown that existing correlations do not provide satisfactory results for all the possible operation modes of hydrogen internal combustion engines.

This paper describes the application of a flow field-based heat transfer model according to Schubert et al. [1]. The model's strength is a more realistic description of the required characteristic velocity; considering the influence of the injection on the global turbulence and on the in-cylinder flow field results in a better prediction of the wall heat transfer during the compression stroke and for operations with multiple injections.

Further an empirical hypothesis on the turbulence generation during combustion is presented. For validation the turbulence model is applied to a simulation methodology based on physical principals to predict the rate of heat release caused by the combustion process.

Measurements of the wall heat flux and the in-cylinder pressure are used for validation.

## INTRODUCTION

As a fuel, hydrogen allows different mixture formation and combustion processes [2, 3]. In particular, the direct injection of hydrogen offers a very high degree of freedom for optimization [4, 5].

Thermodynamic analyses are carried out in order to assess various concepts. The engine process calculation according to the first law of thermodynamics [6]

$$-p \, dV + dQ_B - dQ_W + \sum_i h_i \, dm_i = dU \quad (1)$$

represents a suitable model for the evaluation and the numerical optimization of the working cycle; the change in the internal energy  $dU$  results from the sum of the added enthalpy and the removed enthalpy  $h_i \, dm_i$ , the power output  $p \, dV$ , the heat release due to the combustion process  $dQ_B$ , and the wall heat transfer  $dQ_W$ .

According to Newton's law of cooling the wall heat flux  $q_w$  due to forced convection is the product of a heat transfer coefficient  $\alpha$  and the difference between the local averaged gas  $T_g$  and the wall temperature  $T_w$ :

$$\dot{q}_w = \alpha \left( T_g - T_w \right) \quad (2)$$

In applied engine process calculation, the correlation according to Woschni [7] is widely used to describe the heat transfer coefficient  $\alpha$  in equation (2) because of its simplicity:

$$\alpha = C L_c^{-1/5} \lambda \left( \frac{w_c \rho}{\eta} \right)^{4/5} \quad (3)$$

Here  $C$  represents a constant.  $\lambda$ ,  $\rho$  and  $\eta$  represent various gas properties approximated with polynomials depending on the gas Temperature  $T$ . The characteristic dimension  $L_c$  is the piston diameter  $d$ . Under these simplifications, equation (3) can be rearranged to:

$$\alpha = 130 d^{0.2} p^{0.8} T^{-0.53} w_c^{0.8} \quad (4)$$

The characteristic velocity  $w_c$  is expressed by the mean piston velocity  $c_m$ . Furthermore, the pressure difference between motoring  $p_0$  and firing operation  $p$  is used to describe the influence of the combustion process. In the improved formulation by Huber et al. [8] (further referenced as Woschni/Huber), the IMEP is also taken into account. Hence, the characteristic velocity is defined as:

$$w_c = C_1 c_m + \text{"combustion influence"} \quad (5)$$

Although the correlation according to Woschni/Huber was developed for diesel engines, it is also well suited to describe the wall heat transfer of hydrogen internal combustion engines because of similar pressure gradients during combustion [9]. However, it does not provide satisfactory results for stoichiometric operation and for operation with higher turbulence levels caused by direct injection.

The role of turbulence in heat transfer was explicitly considered for gasoline engines by Borgnakke et al. [10]. Morel and Keribar [11] refined that model later; among other things they studied the effects of swirl and squish on the wall heat transfer. Further, they added a spatial resolution to the heat transfer model by calculating the wall heat transfer coefficient for different areas in the combustion chamber separately.

Based on these works, Schubert et al. [1] recently decided to employ elaborate methods to more realistically describe the characteristic velocity in modern direct injection diesel engines. The problem due to an increased wall heat transfer caused by turbulence generated through the direct injection of the fuel is also well known in diesel engines.

The focus of this paper is the application of this flow field model for hydrogen internal combustion engines. Due to the additional more accurate description of the gas properties required, further improvements, especially for the stoichiometric operation, are expected.

## IMPROVED HEAT TRANSFER MODEL

Schubert et al. [1] and their predecessors adopted the description of the heat transfer coefficient required in equation (2) from the boundary layer theory. When Prandtl numbers are close to unity and Reynolds numbers are not too far above transition, the laminar flow Reynolds-Colburn analogy [12] can be used:

$$St = \left( \frac{c_f}{2} \right) Pr^{-2/3} \quad (6)$$

Thereby  $St$  is the Stanton number,  $c_f$  is a friction coefficient and  $Pr$  the Prandtl number. On the other hand, the Stanton number is defined either by the fluid's Nusselt number  $Nu$ , the Reynolds number  $Re$  and the Prandtl number  $Pr$  or by a convective heat transfer coefficient  $\alpha$ , a density  $\rho$ , a specific heat  $c_p$ , and a characteristic velocity  $w_c$ :

$$St = \frac{Nu}{Re Pr} = \frac{\alpha}{\rho c_p w_c} \quad (7)$$

Substitution of these two equations results in the favored formulation of the heat transfer coefficient  $\alpha$  in the form:

$$\alpha = \frac{1}{2} \rho c_p w_c c_f Pr^{-2/3} \quad (8)$$

When the turbulent momentum exchange and the energy exchange are proportional to the increase of molecular transport and the turbulent Prandtl number is close to one, the Reynolds-Colburn analogy can also be used for turbulent flows. Assuming a turbulent flow over a smooth flat plate, the friction coefficient  $c_f$  can be approximated by the turbulent Reynolds number  $Re$ , according to [12]:

$$c_f \cong 0.0592 Re^{-1/5} \quad (9)$$

The turbulent Reynolds number  $Re$  itself is defined as:

$$Re = \frac{w_c L_c}{\nu} \quad (10)$$

The further required kinematic viscosity  $\nu$  is defined as:

$$\nu = \frac{\eta}{\rho} \quad (11)$$

By substitution of the equations (9, 10 and 11) and under the assumption of a constant Prandtl number, equation (8) can be rearranged to:

$$\alpha = C L_c^{-1/5} c_p \eta^{1/5} (w_c \rho)^{4/5} \quad (12)$$

From the definition of the Prandtl number  $Pr$  it can be seen that the thermal conductivity  $\lambda$  is proportional to the product of dynamic viscosity  $\eta$  and the specific heat capacity  $c_p$ :

$$Pr = \frac{\eta c_p}{\lambda} \quad (13)$$

With this information in mind, it becomes obvious that the model approach used by Schubert et al. [1] - equation (12) - shares the same principles as the correlation according to Woschni [7] - equation (3). Therefore, anticipated improvements should come from the more accurate calculation of the required gas properties, a more complex description of the characteristic velocity and the spatial resolution by calculating the wall heat transfer coefficient for different areas in the combustion chamber separately.

To aid understanding, equation (12) is broken down into terms for the gas transport properties, the characteristic velocity and the characteristic dimension. The influence of hydrogen as fuel on all these terms is discussed in the following subsections. Furthermore, the effect of the combustion process on the wall heat transfer is analysed.

**GAS PROPERTIES** – In a first step towards a model improvement, the theoretical influence of hydrogen on the global gas properties (specific heat capacity, thermal conductivity, dynamic viscosity and density) required either by equation (3) or equation (12) is discussed.

**Specific heat capacity** - The specific heat capacity  $c_p$  for mixtures of ideal gases can be calculated using the well known NASA polynomials taken from [14]. These polynomials are functions of the temperature and the mixture composition. As shown in Figure 1, the influence of the temperature is rather weak compared to that of the actual mixture composition. This is because of the very high specific heat capacity of hydrogen compared to that of air.

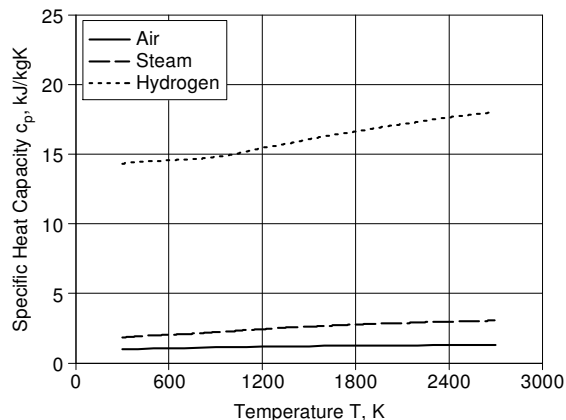


Figure 1: Specific heat capacity of various gases

**Thermal conductivity** - The pure species thermal conductivities are computed, as given by Peters and Warnatz [15]. The combination averaging formula suggested by Mathur et al. [16] is used for the mixture-averaged thermal conductivity. Figure 2 shows the strong influence of hydrogen on the thermal conductivity  $\lambda$  for various air/hydrogen mixtures and the approximation by Woschni [17]:

$$\lambda = 3.17 \cdot 10^{-4} T^{0.772} \quad (14)$$

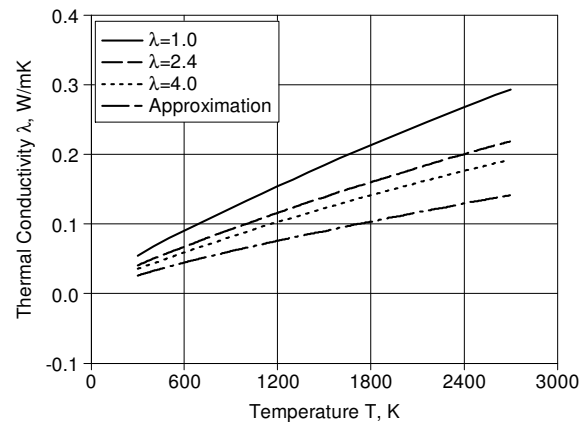


Figure 2: Thermal conductivity of various gas mixtures for various air/fuel ratios compared with the approximation according to Woschni

**Dynamic viscosity** - The dynamic viscosity  $\eta$  of the gas is obtained according to the formulation of Hirschfelder et al. [18]. The mixing law of Wilke [19] is applied for calculation of the mixture viscosity. Figure 3 shows the weak influence of hydrogen on the dynamic viscosity for various air/fuel ratios and the approximation by Woschni [17]:

$$\eta = 0.612 \cdot 10^{-6} T^{0.609} \quad (15)$$

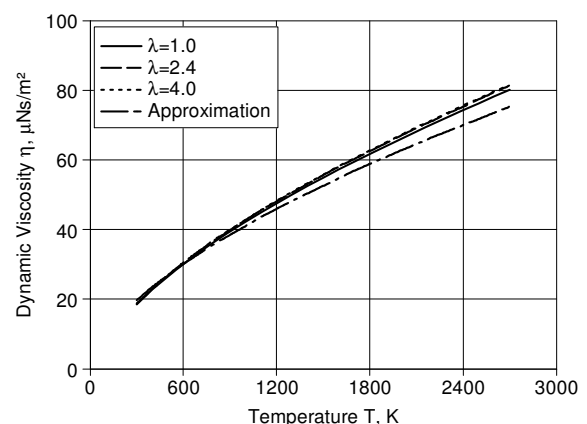


Figure 3: Dynamic viscosity of various gas mixtures for various air/fuel ratios compared with the approximation according to Woschni

Density - Based on the ideal equation of state, Woschni sets the density  $\rho$  proportional to the global in-cylinder pressure  $p$  and the global in-cylinder temperature  $T$ :

$$\rho = C \frac{p}{T} \quad (16)$$

This assumption does not seem valid for hydrogen combustion as the gas constant  $R$  changes greatly during the combustion process. However, the average density  $\rho$  is well-known within the thermodynamic analysis.

Suggested approach – The following suggestions are made for the calculation of the required gas properties from the above considerations:

- Hydrogen has a strong influence on the thermal conductivity and therefore the formula doing without that term is favoured.
- The global average density and global average specific heat capacity are already required for the thermodynamic analysis in equation (1) and should be available.
- Hydrogen only has a weak influence on the global dynamic viscosity of the mixture, which is further raised to a small power in equation (12). A polynomial of 3<sup>rd</sup> degree is used to approximate the exact solution. As shown in Figure 4, the coefficients are chosen in such a way that the values below 1800 K are consistent with those of the reactants and those above 1800 K are consistent with those of the products.
- Only the global gas temperature is taken into account for the calculation of the gas properties, although it is well known that temperature compensation takes place within the boundary layer. A given gas temperature automatically leads to a equivalent wall temperature because of similar cooling conditions in modern engines. Therefore, an explicit consideration of the boundary layer temperature seems unnecessary.

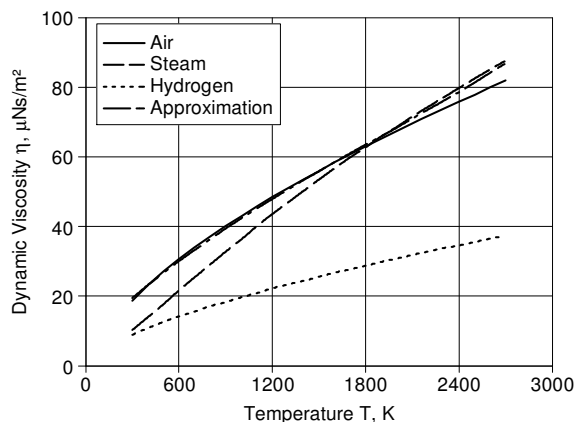


Figure 4: Dynamic viscosity of various gases compared with an approximation by a polynomial of 3<sup>rd</sup> degree

CHARACTERISTIC VELOCITY – The charm of the approach by Schubert et al. [1] lies in the more complex description of the characteristic velocity. This is based on the model by Morel and Keribar [11]:

$$w_c = \sqrt{w_x^2 + w_y^2 + 3 u'^2} \quad (17)$$

In equation (17),  $w_x$  and  $w_y$  represent velocity components parallel to a surface and  $u'$  is the turbulent velocity fluctuation. Assuming a homogeneous isotropic turbulence throughout the combustion chamber seems to be accurate enough, and thus the turbulent velocity fluctuation  $u'$  is given by the global turbulent kinetic energy  $k$ :

$$u' = \sqrt{\frac{2}{3} k} \quad (18)$$

Velocity components - The individual areas and the respective velocity components (axial velocity  $w_a$ , radial velocity  $w_r$  and tangential velocity  $w_t$ ) shown in Figure 5 have already been thoroughly discussed in [1].

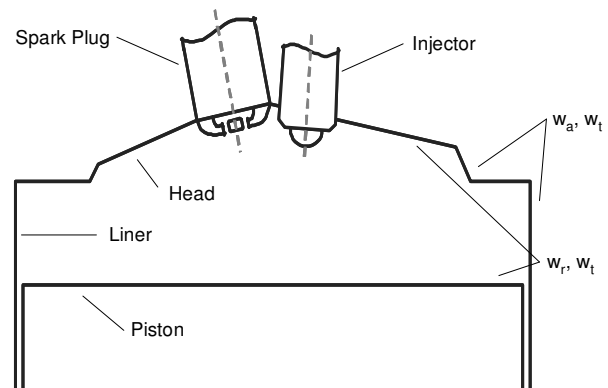


Figure 5: Different areas for calculating the heat transfer and the velocity components for characteristic velocity on the individual areas

Due to the flat-piston design, the angular velocity  $\omega$  is described by only one equation instead of two [1]:

$$d(I \omega) = M_{in} + M_{inj} - M_f - M_{out} \quad (19)$$

The change of the angular momentum  $d(I \omega)$  results from the increase of the momentum  $M_{in}$  due to the mass flow in the cylinder and the decrease in momentum  $M_f$  and  $M_{out}$  due to friction on the combustion chamber walls and the mass flow out of the cylinder. For the time being the additional influence of the injection  $M_{inj}$  is suggested as:

$$M_{inj} = C_{inj} dm_B w_{inj} \frac{d}{2} \quad (20)$$

Thereby,  $C_{inj}$  is a constant,  $dm_B$  the injected fuel mass,  $w_{inj}$  the speed of the injected stream and  $d$  the cylinder diameter. The influence of the injection on the flow field also needs to be considered. The squish flow only has a weak influence on the in-cylinder flow field because of the engine design. Moreover, no swirl variations were carried out.

**Turbulent kinetic energy** - The global k- $\epsilon$  model applied to determine the turbulent kinetic energy  $k$  is based on Borgnakke et al. [10]:

$$dk = \frac{2}{3} (1+a) k \frac{d\rho}{\rho} - C_d \epsilon + dk_{inj} \quad (21)$$

Thereby, the first term represents turbulence production due to compression and the second term describes the decrease of turbulence due to dissipation. The influence of the fuel injection on the turbulent kinetic energy is expressed, as with [10], by the cylinder pressure  $p$ , the cylinder mass  $m$ , the change of mass  $dm_B$ , the density of the fuel  $\rho_B$ , and the pressure of the fuel  $p_B$ :

$$dk_{inj} = \frac{1}{2} \frac{dm_B}{m} \frac{2(p_B - p)}{\rho_B} \quad (22)$$

The dissipation rate is calculated by using the well-known approximation by Taylor [10] with the third root of the cylinder volume for the turbulent length scale:

$$\epsilon = \frac{k^{3/2}}{\sqrt{V}} \quad (23)$$

The turbulent kinetic energy at inlet closes is calculated according to [23] and is of special interest along with variations in the engine speed:

$$k_E = \left( \frac{\sqrt{2} d^2}{2 d_v h_v \cos \beta} c_m \right)^2 \quad (24)$$

Here  $d$  is the cylinder diameter,  $d_v$  is the valve diameter,  $h_v$  is the valve lift,  $\beta$  is the seat angle, and  $c_m$  is the mean piston velocity.

The application of the model is shown in Figure 6. A weak rise of the turbulent kinetic energy during the compression stroke can be seen there. A strong boost is produced by the injection of hydrogen at 40 °CA BTDC. After the injection, a steep decay is noticeable. The comparison with the mean turbulent kinetic energy of a 3D-CFD simulation shows a good congruence. Comparisons of 3D-CFD simulation with results from optical measurements for the mixture formation have shown satisfactory results of sufficient quality [13]. Therefore, it is assumed that the values are representative for the turbulent kinetic energy although no direct measurements are possible.

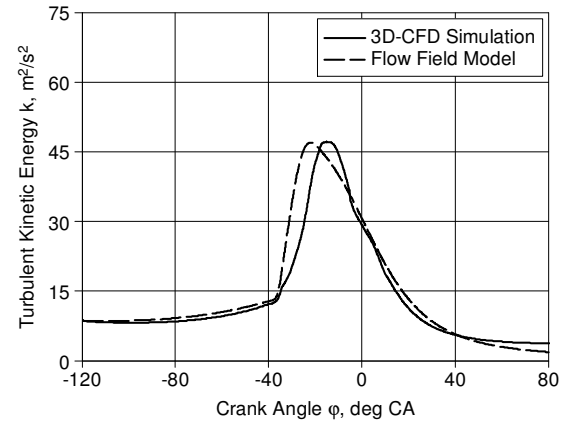


Figure 6: Comparison of turbulent kinetic energy of the turbulence model according to equation (21) with a 3D-CFD simulation [13]

**CHARACTERISTIC DIMENSION** – The characteristic dimension  $L_c$  is adapted in order to achieve a good correlation between measurements for motoring operation and the model, as shown in Figure 7. Thus, it is clear that the flow field-based model yields a better result than the correlation by Woschni/Huber. But it also can be noted that this model represents the centre of gravity of the characteristic curve much better.

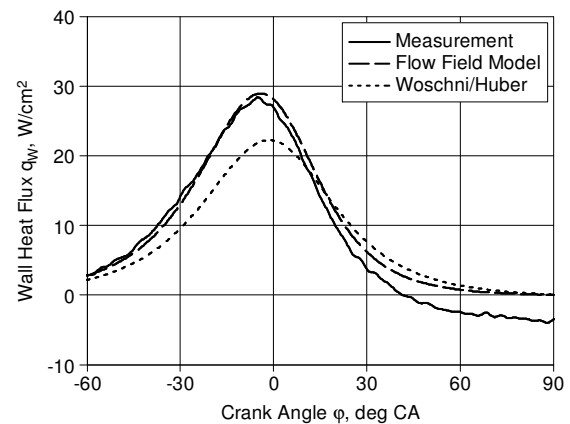


Figure 7: Comparison of measured heat flux and the results of Woschni/Huber and the flow field based model, 2000 rpm, motoring operation

The approximation for the characteristic dimension is expected to be adequate as it has only a weak influence on the heat transfer, being raised to a small power in equation (9). In this context it is important to point out that the heat transfer coefficient is acquired separately for the three different areas of the combustion chamber defined in Figure 5. Therefore, three characteristic dimensions pertaining to the three elementary surfaces are required. These characteristic dimensions are related to the geometrical dimensions of the combustion chamber and proportional to the suggestions made by Morel and Keribar [11].