

Determination of Supersonic Inlet Boundaries for Gaseous Engines Based on Detailed RANS and LES Simulations

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ABSTRACT

The combustion of gaseous fuels like methane in internal combustion engines is an interesting alternative to the conventional gasoline and diesel fuels. Reasons are the availability of the resource and the significant advantage in terms of CO₂ emissions due to the beneficial C/H ratio. One difficulty of gaseous fuels is the preparation of the gas/air mixtures for all operation points, since the volumetric energy density of the fuel is lower compared to conventional liquid fuels. Low-pressure port-injected systems suffer from substantially reduced volumetric efficiencies. Direct injection systems avoid such losses; in order to deliver enough fuel into the cylinder, high pressures are however needed for the gas injection which forces the fuel to enter the cylinder at supersonic speed followed by a Mach disk. The detailed modeling of these physical effects is very challenging, since the fluid velocities and pressure and velocity gradients at the Mach disc are very high. A detailed simulation of these effects in CFD calculations of real engine geometries is numerically challenging and computationally expensive. The main goal of this study is hence to develop inlet boundary conditions which can accurately reproduce the most important physical mechanisms without increasing the complexity of a real engine simulation significantly.

To this end, two and three-dimensional underexpanded flows for a single-orifice injector were numerically investigated in STAR-CD. The two dimensional setup was used to investigate the spatial and temporal resolution requirements. Based on these findings a three-dimensional setup, with the same nozzle diameter as in the real engine was created and the flow field simulated using RANS and LES approaches. The results showed very good agreement with an empirical correlation concerning the position of the Mach disc for pressure ratios of 16.5 and 32. The numerical data was statistically post-processed and then used as a basis for derivation of inlet conditions which reproduce velocity, turbulence and CH₄ mixture fraction fields downstream of the Mach disc.

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INTRODUCTION

In the recent years a number of emission regulations were introduced [9]. The main goal is to reduce carbon dioxide, NO_x and particle emissions.

To meet future regulations for internal combustion engines concerning CO₂, one can either increase the efficiency or substitute the conventional fuel (Petrol and Diesel). Natural gas is such a fuel which allows decreasing relative emissions not only by increasing the efficiency but also reduces relative carbon dioxide emission due to the higher hydrogen/ carbon ratio in the methane. The efficiency can be increased since natural gas has a high octane number (130) [9] which allow higher compression ratios.

Beside these qualities natural gas engine have many other advantages: compared to oil resources are presently abundant and in addition CH₄ shows significant potential to be produced by renewables. Due to the high energy density of natural gas the driving range is of the same order as for conventional fueled vehicles. During the combustion of natural gas, particle emissions are relatively low which leads to reduced local air pollution. In order to improve the combustion process in internal combustion engines (ICE), CFD simulations are nowadays routinely used to gain deeper insight into the physical processes in internal combustion engines. The conventional approach to simulate ICEs is based on RANS turbulence modeling, which calculates averaged quantities. In the last years Large Eddy simulations are more

and more used to investigate also the cyclic behavior between individual engine cycles. An overview concerning the recent state of the art in LES engine modeling can be found in the recent review paper of Rutland [28]. One of the most challenging aspects of CFD simulations in engines lies in the modeling of the fuel injection: for liquid fuels the challenge is to model the spray (which includes atomization, secondary break-up and evaporation, heat and mass transfer), whereas for gaseous fuels the high pressure ratio results in a supersonic underexpanded jet which must be appropriately described numerically.

Since the physical properties of an underexpansion are important for modeling the gaseous injection, a short review is given here. The sudden expansion of the gas injected at high pressure can be observed outside of the nozzle above a certain pressure ratio, which depends on the pressure ratio between nozzle and combustion chamber. As a result the expansion waves are reflected as compression waves which lead to a vertical shock downstream of the nozzle exit.

Three dimensional axisymmetric underexpanded flows have been studied in detail for almost a century; most often by means of Schlieren imaging or shadowgraphy. An empirical correlation relating the location of the Mach disk to the pressure ratio was proposed in [2]. Later this correlation was verified analytically by balancing the entropy [32]. Beside the location of the Mach disk also the structure of the underexpanded flow is well known. The most important structures beside the Mach disk are the jet boundaries, the barrel shocks and the reflected shock. The dimension of the Mach disk, the location thereof as well as the size of the reflected and the barrel shocks are dependent on the geometry of the nozzle. The influence of the nozzle on the jet was examined by Otake et al [22, 23].

In the literature several approaches to simulate the physical processes during the gaseous injection in ICEs can be found. One possible way to model this physical effect is to fully resolve the supersonic underexpansion and include the nozzle geometry into the simulation. This method was e.g. employed by Kim et al. [14], Zhang et al [33] and Gerke et al. [10]. However the meshing procedure is very complicated and the computational costs are very high. An alternative to fully resolved calculations has been proposed by Mather and Reitz [16], where the barrel shock structure are approximated using a one-dimensional compressible flow model. The 3D calculation uses prescribed quantities down-stream of the Ma disk where the flow is subsonic. The major advantage of this approach is the reduced calculation time, since the supersonic flow does not have to be resolved with the computational mesh. More recently, according to Otake et al. [22, 23], the correlation for the diameter of the Mach disk, has been found to be dependent on the nozzle geometry. Similar models were also published by Oulette et al. [24, 25] and Andreassi et al [3]. A different approach was followed by Baratta et al. [4], who used a Lagrangian - Eulerian approach to simulate the gaseous injection of a poppet-valve injector. The parameters of the injected particles are set based on a detailed simulation

of the injection including the nozzle flow. The results showed good agreement in the CH_4 distribution. However, no comparisons were presented in [4] for the turbulence and velocity fields. Another method proposed by Johnson et al. [13] uses detailed computations to derive inflow boundary data; the profiles obtained are then prescribed on coarser grids. The main disadvantage of this model is the sensitivity with respect to the chamber condition: for the time-varying pressure levels in engines, a large number of preliminary computations may be required.

The general idea in this paper is to create artificial inlet boundary conditions which are able to reproduce the methane concentration, the velocities and the turbulence of the flow after the Mach disc and the reflected shocks. Especially the reflected shocks around the Mach disc have a significant influence on the flow field downstream the nozzle. This can be seen in work of Giordano et al. [11] where iso-contours of the Mach number are plotted in a slice through a circular supersonic jet.

The parameters for artificial inlet boundary conditions in this work are derived based on fully resolved simulations, which also include the reflected shocks. Therefore the proposed method takes this influence into account. In addition the numerical and mesh requirements for the artificial jet inlet conditions are very low with the advantage that it is easily applicable in real engine simulations. Since the grid doesn't need to be refined also the computational time is not strongly affected.

In this work a circular underexpanded methane jet flow has been numerically studied using both RANS and Large Eddy Simulation for a pipe diameter of $d = 1 \text{ mm}$ and two pressure ratios of 16.5 and 32.

In a first step, the influence of different model parameters such as: grid size, time step size and temporal discretization order on the solution has been analyzed by means of a two dimensional RANS calculation.

Based on the findings a three-dimensional setup, with the same nozzle orifice diameter as in the real engine, was created and the flow field simulated with RANS and LES. The resulting data has subsequently been used to derive parameters for the flow velocity and angle, the density, turbulence as well as temperature levels of an artificial inlet boundary condition. The inlet boundary is then applied to a simple box mesh with a coarse resolution (i.e. representative of in-cylinder resolutions) and the results for the methane concentration, the velocity and the turbulence were compared to the high resolution simulation data and to empirical correlations from the literature.

MATHEMATICAL METHODOLOGY

In this work is based on the numerical tool STAR CD v4.18. The time in the LES calculations are discretized with a third order implicit Euler scheme and for the pressure-velocity coupling a SIMPLE algorithm was used. For the RANS simulations a first order implicit scheme was used for

the temporal discretization. The chosen coupling algorithm was a PISO type.

The underexpanded flow of the injection is governed by the transient compressible Navier-Stokes equations. The continuity, momentum and the energy equation of the Navier-Stokes equation written in cartesian form are given here:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \quad (1.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_i} \quad (1.2)$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial}{\partial x_j} (\rho h u_j + F_{h,j}) = \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} \quad (1.3)$$

Where τ_{ij} are the stress tensor components:

$$\tau_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (1.4)$$

With s_{ij} being the rate of strain tensor,

$$s_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1.5)$$

and μ the dynamic viscosity of the fluid.

The gas properties of air and methane were assumed to be ideal. Therefore the ideal gas law can be included in the set of governing equations:

$$\rho RT = p \quad (1.6)$$

The thermodynamic and transport properties for the gases were assumed to be constant.

Turbulence Modeling

By applying the Reynolds averaging on the Navier-Stokes equation, the turbulences are averaged over time. By this averaging the so called Reynold averaged Navier Stokes (RANS) equations are resulting. The momentum equation of the RANS is written as following:

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \bar{u}_i \frac{\partial \bar{u}_i}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_i} + 2\mu \frac{\partial}{\partial x_i} \bar{s}_{ii} - \frac{\partial}{\partial x_i} (\rho \bar{u}_i' u_i') \quad (1.7)$$

The Reynold stress tensor $-\rho \bar{u}_i' u_i'$ is undefined, leaving the set of equations underdetermined. In order to close the equation the Reynolds stress tensor has to be modeled. The

most common modeling approach is the eddy viscosity model, which assumes a proportional relation between the Reynolds stress tensor and the mean deformation rate:

$$-\rho \bar{u}_i' u_i' = \mu_t s_{ij} - \frac{2}{3} \left(\mu_t \frac{\partial u_k}{\partial x_k} + \rho k \right) \delta_{ij} \quad (1.8)$$

For the RANS simulation a SST $k-\omega$ model was used for modeling the kinetic energy in the present work. This two-equation eddy viscosity model uses the $k-\varepsilon$ model in the flow field far away from the wall. Close to the walls it uses the $k-\omega$ model. The combination of these two models allows to use the model which is most appropriated for each flow situation [20]. Michel [21] and Bartosiewicz et al [5] achieved good results by using the SST $k-\omega$ model for similar flow problems.

For the $k-\varepsilon$ model the eddy viscosity is modeled as following,

$$\mu_t = f_\mu \frac{C_\mu \rho k^2}{\varepsilon} \quad (1.9)$$

where k is the turbulence kinetic energy and ε the turbulence dissipation rate. f_μ is a damping function and C_μ an empirical coefficient for which the recommended values from Ouelette et al. [24] have been chosen. The turbulence kinetic energy and the turbulence dissipation rate have to be solved for each time step with transport equations.

Instead of the turbulence dissipation rate the specific dissipation rate ω is used for the $k-\omega$ model.

$$\mu_t = \rho \frac{k}{\omega} \quad (1.10)$$

Accordingly to k and ε also ω is calculated with a transport equation.

For the Large Eddy Simulation (LES) large non-linear interactions are resolved and the small ones are modeled. For the implementation of LES a filter which separates the modeled and the resolved part is needed. The width of this filter is related to the volume of each cell. Similar to RANS the sub-grid scale stresses (τ_{sgs}) needs to be modeled. In the present work the sub-grid scales stresses (τ_{sgs}) were modeled with the $k-l$ model which is a one-equation eddy viscosity model and the eddy viscosity defined as: $\mu_t = C_2 \bar{\rho} \Delta k_{sgs}^2$. The transport equation for k_{sgs} given here:

$$\frac{\partial \bar{\rho} k_{sgs}}{\partial t} + \frac{\partial \bar{\rho} <u_j> k_{sgs}}{\partial x_j} = -\tau_{sgs,ij} <s_{ij}> - C_1 \bar{\rho} \frac{k_{sgs}^{3/2}}{\Delta} + \frac{\partial}{\partial x_j} \left[C_2 \bar{\rho} \Delta k_{sgs}^{1/2} \frac{\partial k_{sgs}}{\partial x_j} \right] \quad (1.11)$$

C_k is an empirically determined constant. By using the $k-l$ model with LES good results were reported by Rutland [28].

Mach Disc Location: Validation Data

For the three dimensional circular underexpanded flow several existing correlations allow for a quantitative validation of the predictions. As already mentioned above, these correlations have been found both empirically as well as analytically. E.g. Adamson et al [2] experimentally determined that the relative location of the Mach disk only depends on the pressure ratio as follows:

$$\frac{L_M}{D} = 0.667 \left(\frac{p_0}{p_\infty} \right)^{\frac{1}{2}} \quad (1.12)$$

Where L_M is the location of the Mach disk, D the diameter of the pipe, p_∞ is the free stream pressure and p_0 the stagnation pressure in the reservoir.

Young et al [32] later on the other hand derived a correlation by balancing the entropy, and proposed the following correlation:

$$\frac{L_M}{D} = C(\gamma) \left(\frac{p_0}{p_\infty} \right)^{\frac{1}{2}} \quad (1.13)$$

Where the coefficient C is depended on the specific heat ratio γ in the following way:

$$C(\gamma) = \frac{1}{\sqrt{2.2}} \left[\gamma(\gamma+1) \right]^{\frac{1}{4}} \left(\frac{\gamma+1}{2\gamma} \right)^{\frac{1}{2(\gamma-1)}} \left(\frac{4\gamma}{(\gamma+1)^2} \right)^{\frac{\gamma}{2(\gamma-1)}} \quad (1.14)$$

When evaluating this numerical coefficient for different gases it can be recognized that the coefficient is very weakly dependent on the specific heat ratio. In fact the error of the experimental measurements is always greater, therefore no dependency was observed by Adamson et al [2].

SIMULATION-SETUPS

Two Dimensional Mesh

The model parameter study was done on a planar two dimensional setup, since the computational costs are much lower compared to a three dimensional setup. The SST - RANS turbulence model was used for all 2d simulations. The varied parameters were the time step size and the grid size. The two dimensional model was built with a channel height of $h_{ch} = 1$ mm. In order to save computational costs, only half of the domain was modeled and symmetry conditions applied. For the outer most surface on the left side (stream upwards) an absolute pressure of $p_0 = 33$ bar was set. Where for the one on the right side (down-stream) an absolute pressure of $p_\infty = 2$ bar was defined resulting in a pressure

ratio of $p_r = 16.5$. All remaining surfaces were defined as walls. The reservoir and the channel itself were initialized with methane at $p_0 = 33$ bar, while the remaining domain was initialized with $p_\infty = 2$ bar and air as fluid.

In order to validate the grid independency four different mesh sizes were used. The coarse mesh had a cell size of $\Delta x = 200$ μm in the underexpanded flow region. The medium mesh was modeled with a cell size of $\Delta x = 100$ μm in the underexpanded flow region. The medium-fine mesh had a cell size of $\Delta x = 66.667$ μm in the underexpanded flow region. Finally the fine mesh had a cell size of $\Delta x = 50$ μm . Four different time step sizes were tested to validate the solution independency. The finest grid ($\Delta x = 50$ μm) was used for this variation. The time step sizes were: $\Delta t = 1\text{e-}06$ s, $\Delta t = 5\text{e-}08$ s, $\Delta t = 6.3\text{e-}10$ s and $\Delta t = 2\text{e-}10$ s. The detailed settings with all the remaining parameters are listed in [Table 1](#).

Table 1. Parameters for the simulation setups

Density	Ideal gas law
Momentum equation RANS	First order upwind
Momentum equation LES	Second order central
Turbulence kinetic energy and dissipation	Second order monotone and reconstruction scheme
Temperature	First order upwind
Wall boundaries	Non-slip
Outlet boundary	Pressure
Inlet boundary	2, 3d setup => pressure, simple box => velocity

Three Dimensional Mesh

In a next step a three dimensional setup was created to calculate highly resolved validation data of the supersonic methane injection in the investigated engine. Therefore the geometry is based on the investigated prototype injector with a nozzle diameter of 1 mm ([Figure 1](#)).

The computational mesh in total consists of 9.6 million cells. For the pipe and the region of the underexpanding flow a cell size of $\Delta x = 50$ μm was chosen, which serves as a very highly resolved reference case. The time step size was set constant equal to $\Delta t = 4.0\text{e-}08$ s. The temporal and spatial resolutions were chosen very conservatively to ensure good quality validation data. The turbulence was modeled using SST-RANS and one equation $k-l$ LES turbulence models. The numerical parameters are summarized in [Table 1](#) and for the temporal discretization a third order Euler implicit method has been used.