

Prediction of the Nozzle Flow and Jet Characteristics at Start and End of Injection: Transient Behaviors

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ABSTRACT

This paper reports investigations on diesel jet transients, accounting for internal nozzle flow and needle motion. The calculations are performed with Large Eddy Simulation (LES) turbulence model by coupling the internal and external multiphase flows simultaneously. Short and multiple injection strategies are commonly used in internal combustion engines. Their features are significantly different from those generally found in steady state conditions, which have been extensively studied in the past, however, these conditions are seldom reached in modern engines. Recent researches have shown that residual gas can be ingested in the injector sac after the end-of-injection (EOI) and undesired dribbles can be produced. Moreover, a new injection event behaves differently at the start-of-injection (SOI) depending on the sac initial condition, and the initial spray development can be affected for the first few tens of μs . To investigate these phenomena, LES of end-of-injection and start-of-injection processes have been carried out on a single hole injector, in order to provide insights in to the physics. Detailed needle motion data and orifice morphology have been measured using x-ray synchrotron source at Argonne National Laboratory. Simulations are validated against available x-ray data of the internal flow and near nozzle exit region. Results are able to realistically capture the injection rate ramp-up, the initial gas discharge followed by liquid injection, the realistic liquid tip penetration and the EOI dribbles, provided all the boundary condition details are properly included in the simulations. Such information is invaluable towards developing simulation tools for enabling and improving low temperature combustion concepts with multiple injection strategies.

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INTRODUCTION

Research on fuel injection technology, sprays and combustion is continuously motivated by the increase in the global energy demand, especially for the transportation sector. Direct injection engines are using higher and higher injection pressures, up to 3000 bar for compression ignition engines. Flow physics become complicated under these conditions, especially due to the small length and time scales that govern the relevant processes. For e.g., high flow velocities can lead to phase change resulting in cavitation. Liquid compressibility cannot be neglected due to the high pressure gradients. Also heat transfer becomes relevant due to the continuous operation of these injectors. Fast transients due to short injection durations are also of utmost importance as both direct injected gasoline and diesel engines often adopt multiple injections, and possibly injection rate shaping, to cope with emission limits and fuel efficiency targets. The transient part of spray behavior is most of the time the dominant part of an injection event. In diesel common rail systems, commanded pulse duration can easily be as short as 200 μs , for pilot or post injections, targeting injected mass as low as 1 mg/

shot. Furthermore, the minimum dwell time between two consecutive injections has been progressively reduced, approaching nowadays 200 μs for solenoid injectors [1].

As near nozzle region is concerned, most of the research has been devoted to the steady state part of a fuel jet, focusing on the steady liquid break-up, air entrainment, and mixing. Little information is available on the transient behavior during both opening and closing phases. The shape of injection ramps affects initial spray penetration and mixing. During the first 100 μs after Start-of-Injection (aSOI) liquid penetration is shorter and evaporation rate is altered because residual hot gases can be left in the nozzle sac [2]. As a matter of fact, after the main injection pulse, fuel dribbles out of the holes and ambient gas is ingested into the sac, replacing the volume of the extra liquid expulsion [3, 4, 5, 6]. In addition, dribbles create locally fuel-rich pockets within an overall fuel-lean region near the injector, the combination of which may contribute to soot and unburned hydrocarbon emissions [7]. The impact extends to consecutive sprays in multiple injection strategies [8].

Diagnostics and measurements techniques are extremely complex for these type of analyses in real scale nozzles. Computational Fluid Dynamics (CFD) offers several appealing advantages and provides complementary results which can further enhance our understanding of the experimental observations. However, several complexities in the area of nozzle flow and sprays still limit their usage. Large variability of scales makes the two-phase flow modeling particularly difficult and computationally demanding. Some numerical methods track the liquid-gas interface explicitly like Level-Set (LS) or some formulations of Volume of Fluid (VOF) methods. In general, all these methods require a very fine grid, assume incompressible phases, neglect phase change, and may still be limited to relatively low Reynolds number flows. Also detailed two-phase simulation is often limited to only external jet domain, and complex geometries or moving boundaries are generally quite challenging [8, 10, 11]. Other methods use a diffuse-interface modeling approach with the advantage of easier inclusion of the energy equation, with complex equation of states for the fluids, mass transfer due to phase change and compressibility. Depending on the scales being resolved and the grid resolution, both single-fluid [12, 13, 14, 15] and multi-fluid [16, 17] formalism have been used in the literature to describe the two-phase system. Concerning the mass transfer model, significant improvements have been demonstrated if non-condensable gases are accounted for in the multi-phase model [18].

Due to the high Reynolds number involved in practical diesel injections (Re is greater than 500,000 in the present cases) addressing these problems is extremely challenging even using High Performance Computing (HPC) resources. In addition, because of the large variations in the length and time scales involved in the internal flow compared to the outward spray, the concurrent simulation of the internal and external domains is extremely demanding.

In this paper, LES results of the end-of-injection (EOI) behavior will be discussed, first showing the dribble phenomenon associated with gas ingestion for two injection conditions. Leading on from this, start-of-injection (SOI) cases will follow and two sac initialization methods, i.e., empty vs. full, will be shown and discussed. The internal and external flow is computed simultaneously in one simulation using the single-fluid VOF method outlined in the next section. This approach is deemed essential for capturing the correct physics, since the flow-field inside the injector influences the external jet behavior.

SIMULATION METHOD

Governing Equations

The compressible Navier-Stokes equations, which express the conservation of mass, momentum, energy and species, for a single-fluid mixture are as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} \quad (2)$$

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_j}{\partial x_j} = & -p \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \\ & + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D h_k \frac{\partial Y_k}{\partial x_j} \right) \end{aligned} \quad (3)$$

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho Y_i u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_i}{\partial x_j} \right) + \sum_{k,k \neq i} S_{ik} \quad (4)$$

where ρ is the mixture density (or pseudo-density), u is the velocity, p is the pressure, and σ_{ij} is the mixture shear stress tensor assumed to behave as Newtonian. Y_i denotes the mass fraction of species i . The energy equation (3) is formulated in terms of specific internal energy e of the mixture. T is the mixture temperature, and h_k is the specific enthalpy of species k . In addition, λ is the thermal conductivity and D is the mass diffusion coefficient expressing the diffusion of a component in the mixture. D is assumed constant for each component, therefore the sum of equations (4) for all components i reduces to the continuity equation (1). Continuity is solved to obtain the mixture density, and at the same time all the species transport equations are solved for the species mass fractions. A reconciliation procedure at the end of each loop ensures that any discrepancy due to round-off error is adjusted by renormalizing the species mass fractions to satisfy global continuity. Lastly, S_{ik} express synthetically the source terms related to species mass transfer due to cavitation/condensation, calculated according to the Homogeneous Relaxation Model (HRM) [13, 19] (cf. next subsection).

The multi-phase system is assumed to be a multi-component two-phase mixture comprising of

- the liquid fuel (subscript 1, or liq),
- and multiple gaseous species, i.e.,
 - fuel vapor (subscript 2, or vap)
 - non-condensable gas (subscript 3),
 - other gaseous species, like ambient chamber species (subscripts 4, ...).

The mixture has a variable density given by the weighted average of the single components densities. Gas phase densities are determined using the equation of state for an ideal gas:

$$\rho_i = p / R_i T \quad (5)$$

where R_i is the gas constant and T is the temperature. The liquid phase is considered compressible. The following barotropic equation of state is used:

$$\rho_{liq} = \rho_{liq,0} \cdot e^{\frac{p-p_0}{K}} \quad (6)$$

where K is the liquid bulk modulus, and subscript 0 refers to an arbitrary reference condition.

The sum of all gas species will be referred to with the subscript g . The mixture density ρ is expressed through the following equation:

$$\rho = \sum_i (\alpha_i \rho_i) = \alpha_g \rho_g + (1 - \alpha_g) \rho_{liq} \quad (7)$$

where α_i is the volume fraction of each component. Volume fractions α_i and mass fractions Y_i are related through:

$$\rho_i \alpha_i = Y_i \rho \quad (8)$$

Using [equations \(7\) and \(8\)](#), the cumulative void fraction α_g takes the form

$$\alpha_g = \frac{Y_g / \rho_g}{\sum_i (Y_i / \rho_i)} = \frac{Y_g / \rho_g}{1 / \rho} \quad (9)$$

This cumulative void fraction includes voids generated by phase change (cavitation), expansion of non-condensable gases, and mixing with ambient gas.

In this implementation, the void fraction α_g is not calculated with an explicit transport equation, as found in other VOF formulations, but the interface is resolved only using the grid. Individual species mass fractions Y_i of each fluid is tracked throughout the domain, by first solving the related species [equation \(4\)](#). Then the void fraction is calculated using [equation \(9\)](#). This approach results in a diffused-interface modeling. As an example, the liquid break-up is modeled as diffusion and through the aid of a sufficiently fine grid. This approach, compared to geometric interface reconstruction methods employed in other VOF approaches, offers the advantages of easy coupling with energy and turbulence equations, inclusion of phase change, and modeling of complex and moving geometries at high Reynolds numbers.

Phase Change

Mass transfer due to phase change can occur at the liquid/gas interface. In general, in a multi-component mixture, it can occur between the liquid fuel and its vapor, or it can potentially occur when gas is released from or absorbed into the liquid solution. Different species are involved in the two cases and different mechanisms are involved.

Liquid-vapor Mass Transfer Model

The model for mass exchange between liquid and vapor (true cavitation) is based on the HRM model as developed by Bilicki and Kestin [19]. The model assumes a simple first order rate equation for the evolution of the instantaneous vapor quality x towards its

equilibrium value $\bar{x}$ over a given time-scale Θ . This synthetic approach has been proved to be able to represent not only cavitation but also flash boiling [13]. These are phase change processes driven by a pressure drop. Usually, the process is referred to as ‘cavitation’ when a tiny amount of superheating is required to evaporate the liquid and the process is very fast, whereas ‘flash boiling’ is used when a higher degree of superheating is achieved, and the process takes a relatively long time. The HRM model expresses in a synthetic way the extremely complex process by which the two phases exchange heat and mass. The rate equation takes this form:

$$\frac{dx}{dt} = \frac{\bar{x} - x}{\Theta} \quad (10)$$

The instantaneous non-equilibrium vapor quality x is:

$$x = \frac{Y_{vap}}{Y_{vap} + Y_{liq}} = \frac{m_{vap}}{m_{vap} + m_{liq}} \quad (11)$$

The equilibrium vapor quality $\bar{x}$ is a function of the thermodynamic properties at the local pressure, i.e., $\bar{x}(p, h)$ is expressed by the following equation with bounds at zero and unity:

$$\bar{x} = \frac{h - h_{l,sat}}{h_{v,sat} - h_{l,sat}} \quad (12)$$

where h is the actual fluid enthalpy of liquid and vapor mixture, excluding air content, and $h_{l,sat}$ and $h_{v,sat}$ refer to saturated liquid and vapor, respectively. The time-scale Θ is evaluated using an empirical fit [20]:

$$\Theta = 3.84 \cdot 10^{-7} \alpha^{-0.54} \phi^{-1.76} \quad (\text{units of s}) \quad (13)$$

$$\phi = \left| \frac{p_{sat} - p}{p_{crit} - p_{sat}} \right| \quad (14)$$

where α is the gas phase volume fraction, and subscripts ‘sat’ and ‘crit’ denote saturation and critical pressures, respectively. Correlation provided by combining [equations \(13\) and \(14\)](#) has been determined in experiments of flashing flows of water in pipes with upstream pressures of in excess of 10 bar. In the absence of specific values for other liquids and conditions, it has been applied in the present form in this study for representing fuels. The time integration of the rate [equation \(10\)](#) allows to compute the source terms S_{1-2} and S_{2-1} ($= -S_{1-2}$) in [equations \(4\)](#). Additional details are given in [18].

Liquid-air Mass Transfer Assumption

The model also accounts for the presence of non-condensable gas in the mixture (third component), however, the related species mass transfer source term is neglected, i.e., $S_{1-3}=0$ in [equation \(4\)](#) and the time scale of the injector flow events are assumed to be very

rapid for significant mass transfer of contaminant gas to occur between a bubble and the surrounding liquid. The mass transfer of air from the liquid solution to the gaseous form (gaseous cavitation), and vice versa, is neglected. Indeed, mass transfer due to diffusion or dissolution is extremely slow compared to the time scales involved in the main flow [18, 21], especially during SOI or EOI transients. In the current implementation, the amount of air added to the liquid fuel is introduced directly in gaseous phase, homogeneously mixed with other components. In other words, we have not introduced a specific model for air adsorption and release from the solution. As a result, as pressure in the fluid drops, air promptly expands, because it is already assumed to be in gaseous form. Conversely, if a cloud of expanded air exists and pressure rises back, gas will be compressed, but not reabsorbed in the liquid medium.

An effective constant amount of non-condensable air in gaseous form is assumed mixed with the liquid. In the current work, the value is set to $Y_3 = 2 \times 10^{-5}$ by mass, according to our previous studies [18, 22], and the assumption is based on an analysis of the characteristic time-scale of air mass diffusion in the liquid solution.

Sub-Grid Models for Filtered Equations

Large Eddy Simulation (LES) has been performed covering the inner nozzle region and the outside near nozzle exit region. The code uses a modified cut-cell Cartesian method for generating the grid at run time [23]. Within this framework, the filter size Δ and shape are fixed by the computational cell size and shape, therefore the filter type is a box. The set of equations (1), (2), (3), (4) are recast according to the LES decomposition into resolved fields and sub-grid fields, i.e., for any flow variable: $\phi = \bar{\phi} + \phi'$, where ϕ is any scalar. For compressible flows Favre averaging is conveniently applied, yielding: $\bar{\phi} = \bar{\rho\phi}/\bar{\rho}$. The procedure results in additional sub-grid scale (SGS) terms that need to be modeled. As far as the momentum equation is concerned, following Pomraning and Rutland [24], the dynamic structure (DS) model exploits the significant similarity between the SGS and the Leonard stresses that has been observed in real as well as numerical experiments. The sub-grid stress tensor, $\tau_{ij} = \bar{\rho}(\tilde{u}_i\tilde{u}_j - \hat{u}_i\hat{u}_j)$, in the DS model is provided by:

$$\tau_{ij} = 2k_{sgs}\bar{\rho}\frac{L_{ij}}{L_{kk}}, \quad L_{ij} = \tilde{u}_i\tilde{u}_j - \hat{u}_i\hat{u}_j \quad (15)$$

where the Leonard stress tensor L_{ij} can be calculated from the resolved velocity field. The hat symbol ($\hat{\cdot}$) designates the test level filter, which is larger than the grid level filter. In this implementation it is created from the center cell and the neighboring cells. The DS model also involves an additional transport equation for the sub-grid turbulent kinetic energy, $k_{sgs} = (\tilde{u}_i\tilde{u}_i - \hat{u}_i\hat{u}_i)/2$, which takes the form:

$$\frac{\partial \bar{\rho}k_{sgs}}{\partial t} + \frac{\partial \bar{\rho}k_{sgs}\tilde{u}_j}{\partial x_j} = -\tau_{ij}\bar{S}_{ij} - \bar{\rho}\varepsilon - \frac{\partial}{\partial x_j} \left(\frac{\mu}{Pr_{sgs}} \frac{\partial k_{sgs}}{\partial x_j} \right) \quad (16)$$

The sub-grid dissipation rate is given by:

$$\varepsilon = \frac{C_\varepsilon k_{sgs}^{1.5}}{\Delta} \quad (17)$$

where the model constant C_ε is set equal to 1. As a consequence of the non-eddy viscosity nature of the dynamic structure model, the SGS energy diffusion due to turbulent viscosity is not present in the transport equation (16): i.e., $Pr_{sgs} = 1$. However, other sub-grid terms resulting in the energy and species conservation equations are modeled using an eddy viscosity concept. As an example, a turbulent diffusion concept is used and the turbulent diffusion is given by

$$D_t = \frac{C_k \Delta k_{sgs}^{0.5}}{Sc} \quad (18)$$

Here, C_k is a model constant set to 0.5 and Sc is the turbulent Schmidt number set to 0.71. Further details about this implementation are provided in [25, 26].

Numerical Method

The overall set of equations is solved using the finite volume method. All variable values are co-located at the cell center and the Rhie-Chow algorithm [27] is used to prevent pressure field decoupling (checker-boarding). First, the conservation equations of mass and momentum are solved using a pressure-velocity coupling iteration method, specifically the Pressure Implicit with Splitting of Operators (PISO) method of Issa [28]. Other transport equations, such as the energy and the species, are solved after the momentum predictor and the first corrector have been completed. Previous studies on nozzle flow simulations using this algorithm for a mixture model can be found in [29]. Spatial discretization is second-order accurate using central differencing schemes for all quantities wherever is possible. A minmod type of flux limiter is used to capture sharp gradients as well as to maintain high accuracy in the smoother regions [29]. Grid refinements are managed through time-dependent fixed embedding located in the key regions. Time integration is first order accurate running fully implicit Euler scheme, with fine time-stepping controlled by a CFL below 0.2. This multiphase flow model has been implemented in CONVERGE code. Validation studies of the mixture model and its implementation within the LES framework have been shown in [30, 31, 32].

DIESEL JET TRANSIENT SIMULATIONS

In this paper, we study the transient behavior of diesel fuel jets issuing from single-hole injectors, with focus on the initial and final part of an injection event. The internal and external flow is computed seamlessly in one simulation, using the CFD method outlined in the previous section. A combination of complex physics (multi-phase, compressibility, phase change due to cavitation) and uncertainties in boundary conditions (accuracy of the internal geometry, moving boundaries, etc. ...) make the prediction of these flows a recognized challenging task [10]. Nevertheless, we present in the next sections two analyses on EOI and SOI transients. The potential of continuous internal and external simulations and the main findings concerning injector transient behavior is discussed.

END OF INJECTION DYNAMICS

The multi-phase model is applied to simulate single-hole mini-sac diesel injector nozzles, for which synchrotron x-ray imaging data, collected at the Advanced Photon Source (APS) at Argonne National Laboratory, are available [3, 33]. In the experimental campaign, different injection pressures (from 500 bar to 1500 bar), back-pressures (from 1 bar to 20 bar) and orifice diameters (from 110 μm to 180 μm) have been investigated. Overall, it has been observed that the amount of ingested gas increases with the increase of the orifice diameter and the injection pressure. Conversely, the ingested gas amount decreases increasing the ambient back-pressure.

Here, we present the simulation of two conditions selected among the above mentioned dataset. One refers to the maximum expected ingested gas situation, i.e., injection pressure = 1500 bar, chamber pressure = 1 bar, and orifice diameter = 180 μm . The second one refers to an intermediate condition with less dribble and gas ingestion, i.e., injection pressure = 500 bar, chamber pressure = 10 bar, and same orifice diameter = 180 μm . A summary of conditions and fuel properties, along with the main injector features is given in Table 1.

Table 1. Nozzle features and operating conditions.

• Nozzle geometry:		
Orifice outlet diameter, D_{out}	0.180 mm	
Orifice length, L	1.0 mm	
Inlet edge rounding, R	0.050 mm	
k-factor	2.4	
Sac volume, V_{sac}	0.15 mm ³	
• Fuel properties:		
Type	diesel	
Liq. density, $\rho_{\text{liq},0}$ (eq. 6)	848 kg/m ³ (300 K)	
Liq. bulk modulus (eq. 6)	1.9×10 ⁹ Pa	
Fuel inlet temperature	300 K	
Liquid viscosity, μ_{liq}	variable with T (2.5×10 ⁻³ Ns/m ² @ 300 K)	
Saturation pressure, p_{sat}	variable with T (1000 Pa @ 300 K)	
Non condensable gas mass fraction, Y_{air}	2×10 ⁻⁵	
• Operating conditions:		
	CASE # 1	CASE # 2
Injection pressure, P_{inj}	1500 bar	500 bar
Chamber pressure, P_{out}	1 bar	10 bar
Chamber temperature, T_{out}	300 K	
Wall temperature	300 K	

Cases Description and Setup

Needle lift data are available from x-ray phase contrast imaging with a time resolution of 25 μs . Figure 1 shows the measured lift profiles for both cases # 1 and # 2. It is clear that the needle lift is higher for case # 1 which is expected since the injection pressure is also higher.

In terms of absolute timing from the electrical opening command, the needle closure occurs in between 2150 μs and 2175 μs for case # 1, and in between 1875 μs and 1900 μs for case # 2. For numerical purposes we assume the needle valve closes below 10 μm . This defines the numerical EOI timing as 2140 μs and 1892 μs for the two cases,

respectively. These points in time are used to express the time relative to the EOI of each case. Plots in Figure 1 use this referencing definition for the time axis. It will also be used throughout the following.

The injection duration used in the experiments [3, 33] is extremely long for the purpose of our numerical study on the EOI behavior. Simulating the whole process would have required excessive computational resources, therefore we devised a simulation methodology for directly focusing around the EOI. We skipped the initial and central part of the injection event, and started the calculation at 300 μs before EOI timing. The chart in Figure 1 shows the needle seat minimum flow area on the secondary y-axis, calculated as the frusto-conical cross section of minimum area between the needle valve and the seat. At the beginning of the simulation, the needle flow passage area is still very high compared to the orifice area (0.025 mm²), therefore no needle throttling is applied yet. The needle-seat flow area remains larger than the hole exit area until approximately 30 μs before EOI.

Results (shown later) demonstrate that starting the calculation from this relatively high lift at 300 μs before EOI we can reach steady jet conditions before the effective flow ramp-down starts. The objective of reducing the computational time is fulfilled, and a good estimate of the initial flow pattern for the simulation of the transient EOI behavior is provided as well. Simulations are then extended up to 400 μs after the EOI timing to ensure that all the relevant transient dynamics is captured.

The flow is simulated as a single domain before the closure, and we switch to two disconnected domains thereafter. The minimum cell size is 5 μm , and it has been maintained throughout the simulations. Needle lift profiles are applied to the moving surfaces. The main focus for the gridding strategy has been on the sac, orifice, and near nozzle exit regions. Grid is temporally refined and changed for better adapting to the relevant dynamics. A view of the computational grid for the EOI cases is shown in Figure 2. The region around the orifice is discretized with the finest cell size (5 μm) throughout all the ramp-down phase and it is retained after the needle closure. The assessment of the grid resolution for LES is discussed in [32]. It is shown that the grid is sufficiently fine in the sac, in the orifice core and in the near exit region up to 4-5 mm.

Despite a fine 3D grid is employed, the Werner and Wengle [34] wall model is used at all wall boundaries, since the cell size is not fine enough for direct boundary layer resolution. Pressure and temperature are specified at the inlet boundary. The outlet chamber is 20 mm long and 16 mm large, hence, it is smaller than the real one, but its size has been calibrated to be large enough to accommodate all the jet development in the time interval of interest. The bottom surface of the chamber is closed and the jet will eventually impinge on it. The side walls are open and the static pressure is applied as the boundary condition. The near nozzle region, below 10 mm, is unaffected by the choice of the chamber size, yet the savings in terms of total number of cells are substantial. Overall, the mesh size ranges from 10 to 16 million cells over a simulated period of 700 μs and the cost of one simulation is about one month of wall-clock time on 256 cores.