Simplified computer code for modelling fuel jet

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Abstract. This paper presents a simplified mathematical model used in computer code for modelling the fuel jets. The used equations describe a fuel jet with minimum physical phenomena (jet atomization, droplets vaporization, droplets interaction with gases, and droplets collisions). It was considered that the fuel jet does not react with the surrounding gases. The thick spray regime is analysed and a collision function is deduced. A multi-component non-reacting turbulent flow is taken into consideration. The method used for solving the equations of the model is a combination between Eulerian fluid and Lagrangian particle calculation. The calculated results (jet penetration and mixing-fractions) is compared with experimental data.

1. Introduction
This paper presents a study of the dynamics and evaporation of droplets in a non-reacting spray. The main purpose of the code is to develop a simple model for those regions within a spray where the droplets occupy a significant fraction of the total volume of the two-phase mixture. These spray regimes have been termed the thick spray and churning spray regimes, and an understanding of these regimes are important for a variety of applications. Formation of the fuel-air mixture accomplished by injecting a fuel spray into the air and is the main process in most combustion systems.

The study developed for modelling the fuel sprays in the Diesel engine and in the direct-injected, stratified charge engine. In addition, the physical processes that are important in thick sprays are also important for many other applications in which two-phase flows are involved.

Four spray regimes is identified, and in each, we will classify the physical effects that could be important. These four regimes called, churning, thick, thin, and very thin.

Very thin sprays regime developed far to the nozzle, is characterized by a reduced number of isolated small drops (due to evaporation), that has a negligible mass and volume compared to the gas. The drops exchange mass, momentum and energy with the gas, but this not altered the gas state. Many physical effects can be ignored in the very thin spray.

Thin sprays regime, is closer to the nozzle, and in this regime, the droplet field has negligible volume, but significant mass, due to gas. The assumption of negligible volume means that the droplets are isolated, and the collisions are unimportant. The new physical effect added in this regime is the interaction between gas and drop.

Thick spray regime occurs within a spray where the drops have a significant volume. The volume fraction of the two-phase mixture is big, between 0.5 and 0.8 according to some authors. The new effects added is the interaction between drops. Named collision this effect can produce coalescence, braking of droplets and elastic collision with distortion of the droplets shape.

Churning Flow develop close to the spray nozzle, and the volume fraction is close to unity. The
spray is formed by a colon of liquid phase or as sheets, filaments, or lattices, the liquid phase is no disperse in the gas phase. The geometry of the spray jet is that of liquid phase. The process of transitions from the liquid column to the thick spray regime called atomization. The main physic process in churning flow regime is the break-up of the liquid jet.

Many authors have studied the jet formation process and over time, they have developed numerous models [1-3]. The most models are analytical for the very thin and thin regime, and semianalytical and phenomenological for the thick and churning regime.

The model presented in this paper aims to be as simple as possible, but it can capture the main phenomena present in the study of fuel jets in the Diesel engines. For very thin and thin spray we used analytical models, for the thick regime we used a semianalytic model and for churning flow, we used a phenomenological approach, with the stated aim of obtaining a code that does not require a very large computational effort.

2. Equations of the model

The equations used are those generally used for modelling fuel jets [1, 3]. The fuel jet is probabilistically modelled as a flow of droplets with an initial distribution that moves in the gaseous phase. Fuel droplets interact with the gaseous phase and between them, evaporate, but do not react. Drop atomization was phenomenological modelled using the Hiroyasu proposed correlations [4] for the break-up length.

The basic equations used to describe the fuel jet model are:

- Equations of jet, equations (1) and (2):

\[
\frac{\partial f}{\partial t} + \nabla \cdot (f u_p) + \frac{\partial}{\partial r_p} (f R_p) + \frac{\partial}{\partial T_p} (f T_p) = Q
\]

\[
Q = \frac{1}{2} \int \int \left[ f(x,u_{p1},r_{p1},T_{d1},t) f(x,u_{p2},r_{p2},T_{p2},t) \pi(r_{p1} + r_{p2}) \right] \left[ u_{p1} - u_{p2} \right] E_{12} (x,u_{p1},r_{p1},u_{p2},r_{p2},t) \]

\[
\{ \sigma(u_p,r_p,T_{d1},u_{p1},r_{p1},T_{p1},u_{p2},r_{p2},T_{p2},x,t) - \delta(r_p - r_{p1}) \delta(u_p - u_{p1}) \delta(T_p - T_{p1}) - \delta(r_p - r_{p2}) \delta(u_p - u_{p2}) \delta(T_p - T_{p2}) \} du_{p1} dr_{p1} dT_{p1} du_{p2} dr_{p2} dT_{p2}
\]

(2)

- Gas continuity equation (3):

\[
\frac{\partial \theta}{\partial t} + \nabla \cdot \theta u_g = 0
\]

(3)

- Gas momentum equations (4), (5), (6):

\[
\frac{\partial}{\partial t} u_g + u_g \cdot \nabla u_g = -\frac{1}{\rho_g} \nabla p + \frac{1}{\theta} \nabla \cdot \theta u_g \nabla u_g + \frac{1}{\theta \rho_g} M_p
\]

\[
\theta = 1 - \sum_k \frac{4/3 \pi r_k^3}{\theta} \delta(x - x_{pk})
\]

\[
M_p = -\sum_k D_k (U_g)(U_g - u_{pk}) \delta(x - x_{pk})
\]

(5)

(6)

- Particle velocity, equation (7):

\[
u_{pk} = dx_{pk} / dt
\]

(7)

- Particle momentum equations (8) and equation (9):
\[ f_{pk} = D_k [U_g] (U_g - u_{pk}) - D_k (u_g - u_{pk}) \quad (8) \]

\[ m_k \frac{d}{dt} u_{pk} = m_k g - \frac{m_k}{\rho_k} \nabla p + D_k (u_g - u_{pk}) + f_{pk} \quad (9) \]

In the equations (1)-(9), \( u_{pk} \) is the \( k \) particle (droplet) mean velocity and \( m_k, \rho_k \) is its mass and density. \( u_g \) is the gas mean velocity, \( f_{pk} \) is a force acting to the particle due to the turbulence, \( U_g = u_g + u_g' \) is instantaneous gas velocity \( u_g' \) is the turbulent component of the gas velocity, \( F_p \) is the force acting on a particle, \( R_p \) is the rate of radius variation, \( T_p \) is the temperature of an arbitrary droplet in the spray \( D_k \) denote the drag function, \( M_p \) is the momentum exchange with the particles, \( p \) is the pressure, and \( \mu_k \) is the kinematic viscosity. \( fdr_p du_p dxdT_p \) is the probable number of droplets at \( x \) position, in the space \( dx \) with \( u_p, F_p, R_p, \phi \) is the probability function of change made by collision and \( \theta \) is the fraction of the volume occupied by the gas or void fraction. In equation (2) the index 1 and 2 indicate the corresponding parameter of the tow interacting droplets, \( \sigma \) is the transition probability function for collisions, \( E_{12} \) is the collision efficiency and \( \delta \) is the Dirac function.

- **Collisional effect**

  Collisional effect expressed by the equation (2) is taken into account due to \( E_{12} \) collision efficiency and \( \sigma \) the transition probability function for collisions and

  Collision efficiency \( E_{12} \) is the ratio of collisional volume of two droplets in the presence of the surrounding gas and the collisional volume in vacuum expressed by \( \pi (r_{p1} + r_{p2})^2 |u_{p1} - u_{p2}| \).

Theoretical study [2] investigate the trajectories of a small drop carried by the gas flow around large droplet. The air flow around the large droplet was taken to be aerodynamic type \( \rho_g |u_g - u_{p1}| r_g/\mu_g >> 1 \) or viscous \( \rho_g |u_g - u_{p1}| r_g/\mu_g << 1 \). The assumption used for the study is that the small droplet did not modify the gas flow around the large droplet and the droplet is small enough that its drag coefficient can be calculated from Stokes low. The results are expressed using one dimensionless parameter, as in equation (10):

\[ K = \frac{2}{9} \frac{\rho_g |u_{p1} - u_{p2}| r_{p2}^2}{\mu_g r_{p1}} \quad (10) \]

For aerodynamic flow around of largest droplet, \( E_{12} \) is represented in equation (11):

\[ E_{12} = \frac{K^2}{(K + 1/2)^2} \quad (11) \]

For viscous flow around of largest droplet, \( E_{12} \) is, equation (12):

\[ E_{12} = [1 + 3/4 \ln (2K/(K - 1.214))]^{-2} \quad K > 1.214 \]

\[ E_{12} = 0 \quad K \leq 1.214 \quad (12) \]

*Transition probability function for collisions* \( \sigma \) is the probable number of droplets implicated in a
collision at position $x$ and time $t$, with the parameter in the interval $\Delta r_p, \Delta u_p, \Delta T_p$. $\sigma$ depend on the same parameter like $E_{12}$, and supplementary on the surface tension coefficient.

The result of two droplets collision according to the study is permanent coalescence, coalescence followed by the break-up and possible satellite droplets, shattering. The theoretical study and experiments reveal that the ratio of surface tension forces and inertial forces is the most important parameter for collision characterisation. The relative magnitude of this forces ratio is the Weber number, $We_L = \rho u_p^2 |r_{p1} - r_{p2}| / a$. For the collision followed by the break-up, it is possible to determinate, similar with $E_{12}$, a parameter $E_{\text{coal}}$ named coalescence efficiency and a critic impact parameter $b_{\text{crit}}$. The relation deduced is presented in equation (13) [2]:

$$\frac{b_{\text{crit}}^2}{(r_{p1} + r_{p2})^2} = 2.4f \left( \frac{r_{p2}}{r_{p1}} \right) \frac{1}{We_L}, \quad r_{p1} \leq r_{p2}$$

$$f \left( \frac{r_{p2}}{r_{p1}} \right) = f(\gamma) = \frac{[\gamma^2 + 1 - (\gamma^3 + 1)^{2/3}](\gamma^3 + 1)^{1/3}}{\gamma^6(1 + \gamma)^2}$$

$$b \leq b_{\text{crit}} \quad E_{\text{coal}} = \min \left( 2.4f(\gamma) \frac{1}{We_L} \cdot 1 \right)$$

- Particle mass equations due to evaporation

The evaporation of a droplet is influenced by neighbouring droplets, but it is usually assumed that the droplets behave as if they were isolated from each other in a gas environment.

We assume that the overall jet behaviour is obtained by summing the behaviour of isolated droplets dynamics inserted into the hot gas flow. Fuel vapour that leaves into the gas by convection and diffusion. Hot gases transfer the heat to colder droplets, affecting the droplet temperature change, and the velocity and phase change from liquid to vapour. It is assumed that the droplets are spherical. It is also assumed that the liquid fuel temperature is uniform throughout the droplet and that the pressure drop in the gas is negligible.

The droplet mass $m_k$ is influenced by the evaporation rate. The evaporation rate is calculated considering non-stationary evaporation of a steady-drop spherical drop according to the formulations deduced by O'Rourke [1] and has the following form from equation (14):

$$\frac{dm_k}{dt} = \left( 1 - \frac{y_0}{\gamma^*} \right) \frac{2 + 0.6(Re^*Sc^*)^{1/3}}{2 + 0.6(Re^*Pr^*)^{1/3}} \frac{q_{\text{ev}}Le^*}{y_i(h_i - h_{i*}) + y_0(h_0 - h_{0*})}$$

The index 1 refers to species 1 (composed of droplets), index 0 refers to the liquid mixture around droplets, the index * refers to the surface conditions of droplets, those that do not have the upper index refers to local conditions.

The dimensions involved in the equation (14) have the following calculation relationships (15)-(17):

$$y_i = \frac{\rho_i}{\rho} \quad y_0 = 1 - y_i$$

$$h_{i*} = h_i(T_k) \quad h_{0*} = h_0(T_k)$$
\[ \gamma_i^* = \frac{W_i}{pW_0 - W_i} - W_0 \]  

(17)

\( T_k \) is droplet temperature (considered constant inside the droplet) and \( P_v(T) \) is the pressure of the fuel vapour.

The value of the fluid parameter at the droplet surface is in equation (18):

\[ \rho^* = \frac{p}{R_y T_k \left( \frac{y_i^*}{W_i} + \frac{y_0^*}{W_0} \right)} \]  

(18)

\( c_p^* = y_i^* c_{p,i}(T_k) + y_0^* c_{p,0}(T_k) \)  

(19)

\[ h = y_i^* h_i + y_0^* h_0 \]  

(20)

\[ h^* = y_i^* h_i^* + y_0^* h_0^* \]  

(21)

The transport coefficients are:

\[ D^* = \frac{D_{01} T_k^3}{p} \]  

(22)

\[ \mu^* = \frac{x_i^* \mu_{01} T_k^2}{x_i^* + \Gamma_{10} x_0} + \frac{x_0^* \mu_{00} T_k^2}{x_0^* + \Gamma_{00} x_i} \]  

(23)

\[ K^* = \frac{x_i^* K_{01} T_k^2}{x_i^* + \Gamma_{10} x_0} + \frac{x_0^* K_{00} T_k^2}{x_0^* + \Gamma_{00} x_i} \]  

(24)

\[ \Gamma_{ij} = \frac{1}{4} \sqrt{2} \left[ 1 + \frac{W_i}{W_j} \right]^{1/2} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{W_i}{W_j} \right)^{1/4} \right]^{1/2} \]  

(25)

In equations (22)-(25) \( \mu_{01}, \mu_{10}, K_{01}, K_{00} \) and \( D_{01} \) are constant coefficients, and \( x_i^*, x_0^*, y_i^*, y_0^* \) are molar fractions;

\[ x_i^* = \frac{1}{1 + \frac{W_1 y_0}{W_0 y_i}} \quad x_0^* = 1 - x_i^* \]  

(26)

The heat flux changed by the drop with the environment \( q_i \) from equation (9) can be determined with the following relation (27):
\[ q_k = 2\pi r_k K'(T - T_k) \left( 2 + 0.6 (Re^*)^{1/2} (Pr) \right) \frac{1}{B_E} \]  \hspace{1cm} (27)

\( B_E \) is the mass correction factor and is calculated with the equation (28):

\[ B_E = \frac{1 - y_i}{1 - y_j} \]  \hspace{1cm} (28)

Energy equation for droplet is presented in equation (29):

\[ m_k \frac{dH_k}{dt} = L(T_k) \frac{dm_k}{dt} + q_k \]  \hspace{1cm} (29)

the specific enthalpy of the liquid droplet is \( H_k \) and \( L(T_k) \) the latent heat of vaporization is calculated with the equation (30):

\[ L(T_k) = h'_i - H_k \]  \hspace{1cm} (30)

3. Numerical solutions of the equations
To numerically solve the coupled spray equation and gas phase mass, momentum, and energy equations, three distinct methods have been used.

The first method is used for the full spray equation. The portion of droplets space is subdivided into computational cells. Each cell is an \( n \)-dimensional rectangle (\( n \) is the number of dimensions of droplets) and is fixed in space for all time. For each time moment \( t \), the value of the distribution function \( f \) in every centre of cells is stored, and derivatives of \( f \) function are approximated by finite-differences of these stored values. The Eulerian form of technique scheme is used for calculation of the dynamics of the gas phase (void fraction).

The second method is used for solve de momentum equation. Equations are solved for selected moments of the distribution function \( f \). The moment equations is obtained from the spray equation multiplied by functions of the radius, drop velocity or temperature, and the results are integrated over all droplets coordinates. The equations used are mass, momentum, and energy equations for the liquid, although other moments could be considered. The moment equations, are solved by finite-difference techniques similar to those used for the gas-phase equations. The exchange rates are evaluated by assuming for the droplets distribution function a form with adjustable parameters that are obtained through knowledge of its moments.

The third method is the parcel methods. This method is used to solve numerically the continuous distribution of droplets that is approximated using a finite number of computational parcels. Each parcel represents a number of drops of identical size, velocity, and temperature. The parcel trajectories in drop space are drop characteristic paths. The dynamics of the gas phase is usually calculated by a Eulerian scheme, and each parcel exchanges mass, momentum, and energy with the gas in the computational cell where it is currently located.

The computer code is inspired by the basic methodology of the parcel method [3]. The unsteady equations solved in cylindrical coordinates assuming symmetry about the axis of the spray. The droplets and gas momentum equations are solved by a coupled and implicit method that exceed time-step restrictions due to the close-coupling of small drop and gas phase velocities. Turbulence is treated with the Sub-Grid Scale model. To calculate the effects of drop collisions we have added an algorithm. Compressibility is included by using a modified ICE technique. The moment equations that we solve are in conservative form. The effects of vaporization and unsteady drop heating can be calculated.

The flow region is subdivided into computational cells of rectangular cross-section in the \( r, z \) plane.
To eliminate factors of $2\pi$ in the finite-difference equations, each cell is formed by rotating its rectangular cross section through a unit azimuthal angle. A specific computational cell is shown in figure 1, which also presents the locations of the variables stored for that cell. We will use $x$ and $y$ instead of $r$ and $z$ because $r$ is droplet radius. The flux component is evaluated using the velocity in the middle of the edge of every computational cell. All other variables are located at the centre of the cell and is supposed to be constant in that cell.

The computational cycle begins by introducing new particles into the mesh as a result of the injection. The all particles are then transported using the explicit equation (31):

$$\frac{x_{pk}^{n+1} - x_{pk}^n}{\Delta t} = u_{pk}^n$$  \hspace{1cm} (31)$$

Each computational injected particle must have:

- an initial velocity $u_{pk}$ , $u_{pk}$ at the nozzle exit:

$$u_{pk} = C \left( \frac{2\Delta p}{\rho_p} \right)^{0.5}$$  \hspace{1cm} (32)$$

$$\text{Max}(v_{pk}) = V \tan\left( \frac{\alpha}{2} \right), \quad \tan\left( \frac{\alpha}{2} \right) = C \left( \rho_s / \rho_p \right)^{1/2}$$  \hspace{1cm} (33)$$

in equation (32), (33) $\Delta p$ is pressure drop across the nozzle, $\alpha$ initial spray angle,

- a radius $r$, the radius of each particle is then chosen from a uniform random distribution:

$$f_r(r) = 6 \frac{D_{32}}{D_{32}} \exp \left( \frac{-6r}{D_{32}} \right).$$  \hspace{1cm} (34)$$

$D_{32}$ is Sauter mean diameter, $Q$ is the rate of injection, that verified the equation (35):
\[
\sum_{k=1}^{K} N_{pk} m_k = Q \Delta t
\]  

- a number of particles in the group \( N_{pk} \) and a number of computational particles injected per cell per time step are \( k \), equation (1):

\[
f(r, x, u_p, t) = \sum_{k} N_{pk} \delta(r - r_k) \delta(x - x_k) \delta(u_p - u_{pk}) \approx \frac{\Delta N}{\Delta r \Delta x \Delta u_p}
\]

After moving the droplets, we calculated the collision, in order to redistribute the particle.

The Calculation is performed for the pair of parcels, if and only if they are in the same computational cell and the drops associated with each parcel are considered to be uniformly distributed in the computational cell. In that condition, we can calculate the collision frequency \( \nu \) of a drop with all droplets:

\[
\nu = \frac{N_i}{V_{ij}} \pi (r_1 + r_2)^3 |u_{pk} - u_{pj}| E_{ij}
\]

\( N_i \) is the number of droplets in their associated parcel; and \( V_{ij} \) is the volume of the cell. The probability \( P_n \) that a droplet undergoes \( n \) collisions with droplets follows a Poisson distribution:

\[
P_n = e^{-n} \frac{n^n}{n!}, \quad P_0 = e^{-n}
\]

\( n = \nu \Delta t, \ \Delta t \) is the computational time step and \( P_0 \) is zero probability collisions. Chosen a random number \( N N \in (0,1) \) it is possible to have:

- \( NN < P_0 \) no collision probability,
- \( NN \geq P_0 \) collision probability;

If \( NN \geq P_0 \) we chose a second random number \( MM \in (0,1) \), that number determines the type of the collision \( b = \sqrt{MM} (r_{pl} + r_{pj}) \) is the collision impact parameter \( b \).

If \( b < b_{crit} \), (equation 13) coalescence occurs, and the result of every collision is coalescence.

If \( b \geq b_{crit} \), then we not have coalescence and is possible to have many droplets.

If coalescence occurs the number of coalescence \( n \), for every droplet in the parcel is calculate by finding the value of \( n \) for which:

\[
\sum_{p=0}^{n-1} P_p \leq NN < \sum_{p=0}^{n} P_p
\]

If the particle position and dimension has changed, the void fraction, \( N_{pk} \) and \( k \), in that cell need upgrade in accordance.

For each regular cell the void fraction is, equation (40):

\[
\theta_{ij}^{n+1} = 1 - \frac{4 \pi}{3V_{ij}} \sum_{k} N_{pk} r_k^3
\]

the continuity equation (41) is:
\[
\frac{\theta^{n+1} - \theta^n}{\Delta t} + \nabla \cdot \theta^{n+1} u_g^{n+1} = 0
\]

(41)

We split the time and first calculate intermediate gas and particle velocities, accounting explicitly for all force, except for particle interactions and turbulence:

\[
\frac{u_{g}^{2T} - u_{g}^{T}}{\Delta t} = \left( g - \frac{1}{\rho_g} \frac{\partial p^n}{\partial x} \right) \Delta t S^T - u_{g}^{2T} S^T + R^T
\]

(42)

Drag function \( D_k \) and particle interaction terms \( R^{2T}, S^{2T} \) equations (43), neglecting turbulence \( (u'g = 0) \) are calculated with intermediate velocities:

\[
\begin{align*}
R^{2T} &= \frac{1}{\rho_g \theta^{n+1} V_{mcel}} \sum_k \frac{N_{pk} D_k^{2T}}{1 + \Delta t \frac{D_k^{2T}}{m_k}} \left( u_{pk}^{n} - u_{g}^{T} \right), \\
S^{2T} &= \frac{1}{\rho_g \theta^{n+1} V_{mcel}} \sum_k \frac{N_{pk} D_k^{2T}}{1 + \Delta t \frac{D_k^{2T}}{m_k}}, \\
F^n &= u_{g}^{n} \cdot \nabla u_{g}^{n} - \frac{1}{\theta^{n+1}} \nabla \cdot \theta^{n+1} \mu_g \nabla u_{g}^{n}.
\end{align*}
\]

Using both gas and particle velocities it is possible to calculate final drag function \( D^{2T} \) with the influence of the turbulence:

\[
\begin{align*}
\frac{u_{pk}^{2T} - u_{pk}^{n}}{\Delta t} &= \frac{D_k^{2T}}{m_k} \left( u_{g}^{2T} + u_{g}^{T} - u_{pk}^{2T} \right), \\
\frac{u_{g}^{2T} - u_{g}^{T}}{\Delta t} &= \left( g - \frac{1}{\rho_g} \frac{\partial p^n}{\partial x} \right) \Delta t S^{2T} - u_{g}^{2T} S^{2T} + R^{2T}
\end{align*}
\]

(44)

Conveniently written the momentum equation is solved with the relation (45):

\[
\begin{align*}
\frac{t_{g}^{n+1} - u_{g}^{2T}}{\Delta t} &= -\frac{\Delta t}{\rho_g} \left[ \frac{1 + (\rho_g / \rho_p) \Delta t S^{2T}}{1 + \Delta t S^{2T}} \right] \frac{\partial}{\partial x} \left( p^{n+1} - p^n \right) 
\end{align*}
\]

(45)

In the last iteration, the particle velocities are updated to the final value, using the equation (46):

\[
\frac{u_{pk}^{n+1} - u_{pk}^{2T}}{\Delta t} = g - \frac{1}{\rho_g} \frac{\partial p^n}{\partial x} + \frac{D_k^{2T}}{m_k} \left( u_{g}^{n+1} - u_{g}^{2T} - u_{pk}^{n+1} + u_{pk}^{2T} \right)
\]

(46)

The code uses the coupled ICE and momentum exchange calculation and eliminates the Courant sound speed restriction on the computational time step, and time-step restrictions due to the close-coupling of gas and drop velocities. Still, the program have many restrictions on the time step size.

The convective terms in the gas momentum equations are differenced explicitly or partially
explicitly, and hence, we must observe the Courant condition based on the gas velocity:

$$\max \left( \frac{|u| \Delta t}{\Delta x} + \frac{|v| \Delta t}{\Delta y} \right) < \frac{1}{2} \quad (47)$$

A similar time-step criterion arises because the turbulent diffusion terms are differenced explicitly, equation (48):

$$\max \left( \frac{D \Delta t}{\Delta x^2} + \frac{D \Delta t}{\Delta y^2} \right) < \frac{1}{2} \quad (48)$$

A hybrid upwind-implicit difference scheme is used for the convective terms of the gas mass, energy, and vapour mass equations. An interpolated donor-cell scheme is used with $\alpha$ interpolation parameter. Intermediate values of $\alpha$ give linear combinations of the interpolated donor-cell scheme and pure upwind or donor-cell differencing is used. Numerical stability was achieved for $\alpha=1/2$.

There are two time-step restrictions to obtain accurate calculations of mass, momentum, and energy exchange. To distribute accurately the exchanged mass, momentum, and energy, the time step must be a small fraction of the residence time of a parcel in a cell:

$$\max \left( \frac{|u| \Delta t}{\Delta x}, \frac{|v| \Delta t}{\Delta y} \right) < \frac{1}{2} \quad (49)$$

The finite-difference equations used to calculate mass and energy exchange between the drops and gas are implicit for each droplet's radius and temperature, but explicit in their dependence on the gas temperature and vapour concentration. Thus, for accuracy, the total energy that is used to vaporize all drops in a computational cell in one-time step should be some small fraction of the energy that is available for vaporization:

$$\frac{\rho_l}{\rho_v} \frac{3R \Delta t}{B \cdot r} < \Delta \quad (50)$$

Additional time-step restrictions arise when drop collisions are important. As has been discussed previously, to accurately calculate collisions, the computational time step must be small compared to the collision times between drops of nearly equal size. In practice, it is difficult to estimate these collision times a priori due to a lack of knowledge of the relative velocities between drops. The best procedure is to lower the time step until the computed results do not change appreciably.

4. Results and comparisons
The program was developed in the Matlab MathWorks development environment. It has a classic structure with a main function and many related functions. The basic functions that implement the computational algorithm have been written by the author. In addition to this, we used a large number of functions from Matlab environment, for deal whit large data and graphical processing of the results.

Initially, the code was written directly into Matlab, which works implicitly as an interpreter, after errors corrections it was compiled into C using the development environment facilities. The graphical interface is not developed; it has several options for loading the input data from text files with a defined structure and options for displaying some control values for monitoring the progress of the work. Graphical processing of results and comparison wit experimental data use a library of interpolation function [5].
This application is developed for modelling fuel injection in the Diesel engine. For calibrations of the constants and validation of the result, a comparative analysis with experimental is very important. We used experimental data from Sandia National Laboratories available through the Engine Combustion Network (www.ca.sandia.gov/ecn) for validating the jet and combustion models. For simulation, we used Spray-A configuration. This configuration is very similar to what is generally encountered in Diesel engines: pressure, temperature and the fuel used n-dodecane (C12H26).

The condition of simulation is gas pressure 5.92 MPa; gas temperature 900 K, injector nozzle diameter 90 μm; fuel injection pressure 150 MPa; fuel temperature 363 K; injection mass 3.46 mg, N2 100%, oxygen 0% [6]. The condition in the constant-volume vessel is non-reacting conditions that properly assess the spray models. Turbulence was modelled with the subgrid-scale model approach. Simulations were carried out in an axisymmetric 2D mesh, 0.1 mm min mesh size, close to the nozzle, to properly describe the momentum exchange between gas and liquid in that region.

Thermophysical properties of n-dodecane and ambient gases must be known in order to perform correct calculations. These properties significantly change with temperature, and that must be taken into account. NASA polynomials were used in this case, since they are known to provide accurate results in the simulation temperature range. NASA coefficients were taken from Burcat’s database [4].

In figure 2, is compared processed and averaged experimental data that were obtained by Raleigh-scattering technique [6], with the computed distribution of mixture fraction. The results of the model seem to be in good agreement with the experimental data. Of course, we can see the uniformity in the mixture fraction shape predicted by the model. Probably the turbulence model is not very performant, and the collisional model not provided sufficient effect on spray evolution like in the experiment.

![Figure 2](image.png)

**Figure 2.** Mixing fraction comparison with D32=3μm.

Figure 3 compares experimental data in term of liquid and vapours penetration with the experimental data. As if we can see in figure 2 the penetration calculated by the model is a little underpredicted. The liquid penetration has good predictability for the zones far for the nozzle, and have a poor resolution near injection orifice. This is expected because our model does not have a real model for the churning flow regime (atomization).
5. Conclusions
Even if it is a simple model that contains many simplifications and approximations, it is capable to
describe with sufficient accuracy the main phenomena and processes that take place in the fuel jets.
The model shows a good predictability. Calculated and measured data presented in figure 2 and
figure 3 have similar trends and very closes values.
The code developed as proposed is a simple one that is efficient in terms of the use of computing
resources and time, so we think it is appropriate to be integrated into a more complex model that can
simulate the process of combustion in Diesel engines
Of course, simulation can be improved in terms of both models and numerical schemes. As it
turned out from the analysis made, at least a better models for turbulence and collision would be
needed.

6. References
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