

Mathematical models and numerical algorithm for the dynamics of gas-droplets flows investigations using high performance computing

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Abstract. *The paper presents the mathematical model of the dynamics of gas-droplets flows taking into account such processes as droplets evaporation, deformation and break-up. Dispersed phase of droplets description is based on the "quasi-particles" Lagrange formalism. The Dukowicz model for the droplet evaporation, TAB approach for droplet deformation and WAVE-model for droplet break-up description are used. The numerical algorithm of quasi-particles equation of motion integration is presented. The main features of parallelization technique are discussed. The special attention is paid to the consideration of numerical algorithm details connected with the description of the procedure of quasi-particle track intersection with cell face finding. Verification results of test case about water droplet motion under the action of drag and gravity forces are presented.*

Keywords

Gas-droplets flow, quasi-particle, Dukowicz evaporation model, TAB deformation model, WAVE break-up model

1 Introduction

Operating of a number of energy-converting plants and chilling units is based on the dynamics of sprays. Fuel injection in diesel engine combustion chamber or water injection for the cooling of the ambient air in conditioners are the examples of the processes which are described by the mathematical models of gas-droplets flow.

Due to the growing importance of the technical restrictions conditioned by the ecological, financial and many other factors, manufactures of the mentioned devices are forced continuously to improve the mixture formation processes. In this context, the numerical simulation and optimization of mixture formation process is today becoming more and more important. One advantage of using simulation models is that in contrast to experiments, results can often be achieved faster and cheaper.

Much more important is the fact that despite the higher uncertainty compared to experiments, the numerical simulation of mixture formation especially using high performance computing can give much more extensive information about complex multi-phase processes than experiment could ever provide. Furthermore, numerical simulation can be used to investigate processes that take place at time and length scales or in places that are not accessible and thus cannot be investigated using experimental techniques.

In the case of high-pressure diesel injection for example, the spray break-up near the nozzle is mainly influenced by the flow conditions inside the injection holes [1]. However, because of the small hole diameters (less than 200 μm for passenger cars) and the high flow velocities (about 600 m/s and more), the three-dimensional turbulent and cavitating two-phase flow is not accessible by measurement techniques.

Outside the nozzle in the very dense spray measurements of the three-dimensional spray structure (droplet sizes, velocities etc.) become even more complicated, because the dense spray does not allow any sufficient optical access of the inner spray core. In these and other similar cases numerical simulations can give valuable information and can help to improve and optimize the processes of interest. Note however that the mathematical models should be calibrated on the basis of natural experiments.

The paper is dedicated to the brief description of mathematical models and parallel numerical algorithm that are to be realized in the numerical software for the gas-droplets flows dynamics computations using high performance computing in three-dimensional statement. The processes of droplets motion under the action of different forces, deformation in a flow, evaporation and break-up are taken into account. For the gaseous phase flows modeling the numerical techniques and author's software [2] will be used.

2 Mathematical models of gas-droplets flows dynamics

For the modeling of two-phase gas-droplets flows the combined approach is used when the gaseous phase is described with the Euler formalism equations [2] and the dispersed (droplet) phase – in Lagrange formalism. In other words the motion equations for dispersed phase are solved along the particles trajectories. Mathematical description of dispersed phase dynamics is based on the Lagrange formalism of "quasi-particles" – the representatives of droplets assemblies with identical physical properties.

Such approach is used today in a number of engineering commercial packages for computations of sprays, for example, ANSYS CFX, ANSYS FLUENT, FIRE, KIVA. Among the native authors one should no doubt note the investigations of scientific groups of Drs. S.M. Frolov (N.N. Semenov Institute of Chemical Physics, see [3], for example) and N.N. Smirnov (Moscow State University, see [4], for example).

Interaction of quasi-particles with gaseous phase is realized in the form of source terms to the equations of gaseous phase mass, impetus and energy conservation (see Section 4).

2.1 Equation of droplets motion

The equation for a single droplet impetus conservation can be written in the following form:

$$m_p \frac{d\mathbf{U}_p}{dt} = \mathbf{F}_{drag} + \mathbf{F}_{grav} - \mathbf{F}_{arch}, \quad (1)$$

$$\mathbf{F}_{drag} = 0.5\rho_g A_p C_D |\mathbf{U}_g - \mathbf{U}_p| (\mathbf{U}_g - \mathbf{U}_p), \quad \mathbf{F}_{grav} = m_p \mathbf{g}, \quad \mathbf{F}_{arch} = \rho_g \mathbf{g} V_p,$$

where m_p , A_p , V_p and \mathbf{U}_p – mass, midsection, volume and droplet velocity vector, ρ_g and \mathbf{U}_g – gas density and gas velocity vector, C_D – drag coefficient, \mathbf{g} – acceleration gravity vector. Hereinafter subscript p corresponds to the droplet parameters, subscript g – to the gaseous parameters.

Drag coefficient C_D is determined by the empirical Schiller and Naumann law with Torobin and Govin correction due to the droplets inertia [5] for the flow around rigid sphere by the incompressible fluid:

$$C_{D0} = \begin{cases} \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687}) & \text{if } \text{Re}_p < 10^3 \\ 0.44 & \text{if } \text{Re}_p \geq 10^3 \end{cases}, \quad \text{Re}_p = \frac{\rho_g |\mathbf{U}_{rel}| d_p}{\mu_g},$$

where d_p – droplet diameter, μ_g – ambient air dynamic viscosity coefficient and $\mathbf{U}_{rel} = \mathbf{U}_g - \mathbf{U}_p$ – relative droplet and gas velocity vector. Furthermore it is planned to take into account the following corrections for C_D calculation: (a) droplet deformation in the flow (see Section 2.2) [6]; (b) flow compressibility around the droplet [7]; (b) internal flow circulation in droplet [8].

Integration of (1) gives the droplet velocity vector components and consequently provides the calculation of its trajectory by the equation:

$$\frac{d\mathbf{r}_p}{dt} = \mathbf{U}_p, \quad (2)$$

where \mathbf{r}_p is a droplet radius-vector. For the numerical integration of (1) the semi-explicit scheme is used, for (2) – explicit Euler scheme:

$$\frac{\mathbf{U}_p^{n+1} - \mathbf{U}_p^n}{\tau} = \frac{3}{4} C_D \frac{\rho_g}{\rho_p} \frac{1}{d_p} |\mathbf{U}_g^n - \mathbf{U}_p^n| (\mathbf{U}_g^n - \mathbf{U}_p^{n+1}) + \left(1 - \frac{\rho_g}{\rho_p}\right) \mathbf{g}, \quad \frac{\mathbf{r}_p^{n+1} - \mathbf{r}_p^n}{\tau} = \mathbf{U}_p^n,$$

where upper subscripts $n+1$ and n correspond to the new and old time layer, τ – interval of integration in time.

2.2 The model for droplet deformation

If there exists the relative motion of gas and droplet the latter deforms and obtains the form similar to the oblate spheroid. Mathematical model of droplet deformation as well as the corresponding numerical algorithm were introduced in [9] and are based on the Taylor analogy (Taylor Analogy Break-up, TAB-model). The main principle of the analogy is that the oscillating droplet is associated with the system of a pointed mass on a spring that is acted by the external force (see Fig. 1).

The force that causes the mass oscillating corresponds to the aerodynamic force that deforms the droplet. The restoring force corresponds to the surface tension force that tends to keep the spherical shape of the droplet and minimize its deformation. Damping force accords with the friction force inside the droplet determined by the droplet liquid viscosity coefficient μ_p .

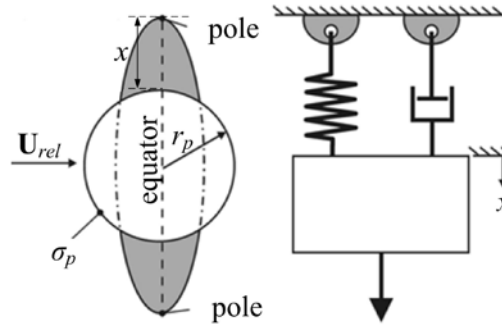


Fig. 1. Taylor analogy between deformed droplet and the pointed mass on the spring [1]

The equation which in dimensionless form describes the droplet diameter oscillating in time is the following:

$$\frac{d^2 y}{dt^2} = \frac{C_F}{C_b} \cdot \frac{\rho_g}{\rho_p} \cdot \frac{|\mathbf{U}_{rel}|^2}{r_p^2} - C_k \frac{\sigma_p}{\rho_p r_p^3} y - C_{damp} \frac{\mu_p}{\rho_p r_p^2} \frac{dy}{dt}. \quad (3)$$

Here r_p – radius of the spherical droplet at rest, ρ_p and σ_p – density and surface tension coefficient of the droplet, $y = x / (C_b \cdot r_p)$ – dimensionless displacement, C_F , C_k , C_{damp} and C_b – constants of the model. The standard values of the constants for the deformation model: $C_F = 1/3$, $C_k = 8$, $C_{damp} = 5$, $C_b = 1/2$. Considering that within the time integration interval the coefficients in (3) are constant the equations for droplet equator oscillation can be solved analytical [9]:

$$y(t) = C_F We_g / (C_k C_b) + e^{-\frac{t}{t_{relax}}} \cdot [A \cdot \cos(\omega t) + B \cdot \sin(\omega t) / (\omega \cdot t_{relax})],$$

$$A = y_0 - \frac{C_F}{C_k C_b} We_g, \quad B = \frac{dy_0}{dt} t_{relax} + y_0 - \frac{C_F}{C_k C_b} We_g, \quad We_g = \frac{\rho_g |\mathbf{U}_{rel}|^2 r_p}{\sigma_p},$$

$$\frac{1}{t_{relax}} = \frac{C_{damp} \mu_p}{2 \rho_p r_p^2}, \quad \omega^2 = C_k \frac{\sigma_p}{\rho_p r_p^3} - \frac{1}{t_{relax}^2}, \quad y_0 = y(0) = 0, \quad \frac{dy_0}{dt} = \frac{dy(0)}{dt} = 0.$$

Through t_{relax} the character time of oscillations relaxation is denoted, ω – frequency of droplet surface oscillations, We_g – gas Weber number.

Although there is a possibility of the existence of several oscillation modes TAB-model describes the main mode which is the most significant [9]. Note also that the TAB-model actually describes not only droplet deformation but also droplet break-up which occurs if $y > 1$.

2.3 The model for droplet evaporation

As a model for evaporating droplets the known Dukowicz model [10] is used. The basis of the model is the analogy between heat- and mass-transfer processes in the vicinity of the droplet surface.

The following assumptions are made:

- (a) the flow near the droplet is spherically symmetrical;
- (b) the quasi-stationary layer of liquid vapor exists near the droplet surface;
- (c) temperature in the droplet is distributed uniformly;

- (d) the gas properties around the droplet are constant;
(e) vapor and liquid on the droplet surface are in thermodynamic equilibrium.

The rate of droplet temperature change T_p is determined from the energy balance equation. Heat applied to the droplet goes to its heating and evaporation:

$$m_p C_p \frac{dT_p}{dt} = Q + L \frac{dm_p}{dt}, \quad (4)$$

where C_p and L – specific capacity and latent heat of the droplet liquid and Q – heat flux from the gas to the droplet:

$$Q = \alpha S_p (T_\infty - T_p).$$

Here α – heat exchange coefficient, S_p – area of total droplet surface, subscript ∞ corresponds to the parameters far from the droplet. Droplet mass balance equation is written in the form:

$$\frac{dm_p}{dt} = Q \frac{f_{vs}}{q_s}, \quad (5)$$

where q_s – specific heat flux to the droplet surface, f_{vs} – specific vapor flux from the droplet surface. Subscript s corresponds to the parameters in the droplet surface, subscript v – to the vapor parameters. If you know the values of heat flux to the droplet surface Q and the ratio f_{vs}/q_s using (4) and (5) you can determine the mass and temperature droplet at any time moment.

The ratio of vapor mass flux and heat flux are connected with the following relationship:

$$\frac{f_{vs}}{q_s} = \frac{\rho_g D_g}{\lambda} \cdot \frac{1}{1 - Y_{vs}} \cdot \frac{\nabla_s Y_v}{\nabla_s T},$$

where D_g – diffusion coefficient, λ – heat-conduction coefficient, Y_{vs} – mass fraction of the vapor on the droplet surface, $\nabla_s Y_v$ – vapor mass fraction derivative in the direction normal to the droplet surface, $\nabla_s T$ – near droplet temperature derivative in the direction normal to the droplet surface. The analogy between heat- and mass-transfer processes is reduced to the relationship:

$$\frac{h_g - h_s}{h_\infty - h_s} = \frac{Y_v - Y_{vs}}{Y_{v\infty} - Y_{vs}},$$

where h – specific enthalpy. For the ratio $\nabla_s Y_v / \nabla_s T$ taking into account the droplet surface boundary conditions one can obtain:

$$\frac{\nabla_s Y_v}{\nabla_s T} = \frac{C_p}{Le} \left[\frac{h_\infty - h_s}{Y_{v\infty} - Y_{vs}} - h_{vs} + h_{gs} \right]^{-1}.$$

Taking the Lewis number equal to 1 we obtain the final expression for fluxes ratio:

$$\frac{f_{vs}}{q_s} = - \frac{B_Y}{h_\infty - h_s - (h_{vs} - h_{gs})(Y_{v\infty} - Y_{vs})}, \quad B_Y = \frac{Y_{vs} - Y_{v\infty}}{1 - Y_{vs}}.$$

2.4 The model for droplet break-up

Today a great variety of models such as TAB, E-TAB, KH-RT, Reitz-Diwakar model et al. with different conditions of applicability are used for the numerical investigation of sprays and single droplets break-up (see the review in [11], for example). One of the most popular is the WAVE-model proposed in [12], [13]. WAVE-model is based on the linearized analysis of the Kelvin-Helmholtz instability of the stationary round jet penetrating into the quiescent ambient incompressible gas.

The result of such analysis is the dispersion relation that connects the rate of initial disturbances of the jet surface growth Ω with the wave length of the disturbance Λ . Approximation of the results obtained by the numerical analysis of the dispersed relation provides the following expressions for Ω and Λ :

$$\Omega = \left(\frac{\sigma_p}{\rho_g r_p^3} \right)^{0.5} \cdot \frac{0.34 + 0.38 \cdot We_g^{1.5}}{(1 + Oh)(1 + 1.4 \cdot Ra^{0.6})}, \quad \Lambda = 9.02 \cdot r_p \cdot \frac{(1 + 0.45 \cdot Oh^{0.5})(1 + 0.4 \cdot Ra^{0.7})}{(1 + 0.87 \cdot We_g^{1.67})^{0.6}}, \quad Oh = \frac{\mu_p}{\sqrt{\rho_p r_p \sigma_p}}, \quad Ra = Oh \cdot We_g.$$

It is supposed in WAVE break-up model that during the character break-up time τ_a the droplet radius decreases to the stable radius r_{stable} :

$$\frac{dr_p}{dt} = -\frac{r_p - r_{stable}}{\tau_a}, \quad \tau_a = \frac{3.726 \cdot b_1 \cdot r_p}{\Lambda \Omega},$$

where b_1 – model parameter. The condition of break-up beginning in WAVE-model is the excess by the droplet radius the value of the stable radius r_{stable} which actually depends on the flow parameters:

$$r_{stable} = \begin{cases} b_0 \Lambda & \text{if } b_0 \Lambda \leq r_p, \\ \min \left[\left(\frac{3\pi r_p^2 |\mathbf{U}_{rel}|}{2\Omega} \right)^{1/3}, \left(\frac{3r_p^2 \Lambda}{4} \right)^{1/3} \right] & \text{otherwise, occurring once.} \end{cases}$$

The recommended value of parameter b_0 is 0.61. Parameter b_1 is defined less precisely because it depends on the injection conditions and takes the value from 10 to 30.

It is known however that WAVE-model gives poor results in the vicinity of the injector hole. In particular the model doesn't provide the sufficient liquid vapor concentration. That is why the standard WAVE-model was modified and it was supplemented by the additional mechanism of stripping mode droplet break-up. It is considered in the modified model that the break-up droplet parts with the radius r_{stable} are formed with some periodicity beginning with the droplet exit from the injector hole.

Mathematically such periodicity as well as the number of the break-up droplet parts are determined by several empirical criteria. The stripping break-up mode provides the increase of inter-phase mass-exchange area and consequently the rise of vapor concentration to the experimental values.

3 Numerical algorithm and parallelization

In this section the procedure of quasi-particles equations of motion integration during one gas dynamics time step Δt taking into account all the physical processes described above is considered. The certain possibility exists that during time step some quasi-particle will intersect the faces of several computational cells.

In such cases as one can see from the above mathematical models descriptions the parameters of inter-phase interaction between droplets in quasi-particles with the ambient gas will change from cell to cell. Such cases consequently should be caught and processed. Besides one should provide the uniform injection of quasi-particles to the computational domain.

So the ideology of gas dynamics step Δt subdividing to the substeps is introduced and each substep the new quasi-particles are injected to the computational domain in the correspondence with the specified injectors mass flow rates (see Fig. 2).

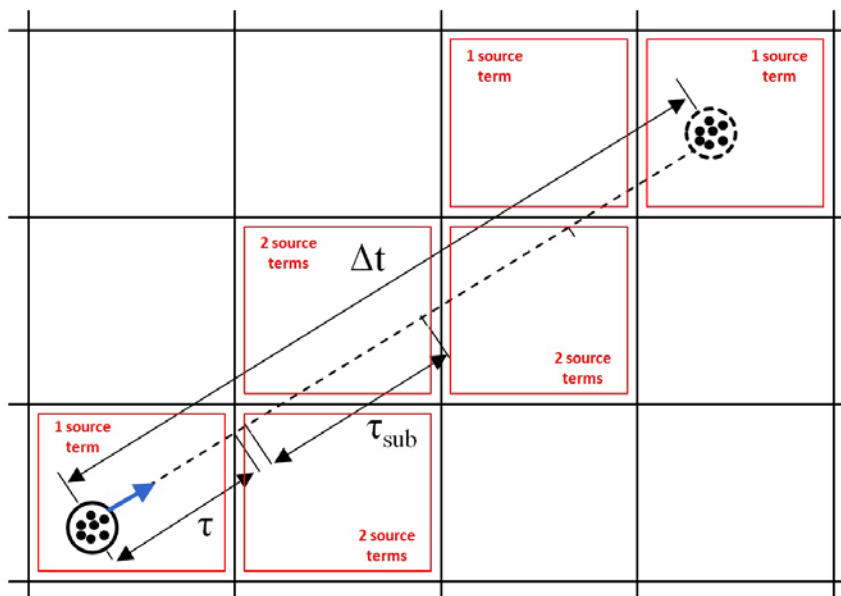


Fig. 2. The ideology of substeps and source terms for description of inter-phase interaction

Thus the algorithm of quasi-particles motion is a substeps cycle each iteration of which contains the processing of each quasi-particle that is another cycle over the all quasi-particles. Within the substep the quasi-particle is integrated until the special time variable associated with the quasi-particle reaches the substep value. During the integration the quasi-particle pass from one cell to another is possible either on one computational unit or between different units.

The quasi-particle equation of motion integration is based on the physical processes splitting approach. First of all (i) the new quasi-particle position is determined with the use of velocity vector from the previous time step, then sequentially the calculations of (ii) droplet deformation, (iii) droplet break-up, (iv) droplet evaporation and (v) quasi-particle new velocity vector are carried out though as the input parameters for the computational block responsible for each following physical process computation the changed quasi-particles parameters from the previous block are come. After all physical processes calculation for the quasi-particle during certain time interval the source terms calculation is performed to define the inter-phase gas – droplets interaction (see Fig. 2 and the next Section).

The next stage of the algorithm is the analysis of what computational cell the quasi-particle enters. It is also possible that during the time integration period quasi-particle reaches the computational domain boundary. In such a case the analysis of specified boundary condition is carried out. It is also important to note that at this stage the identification of quasi-particles that got to the cells of different computational units or that are totally evaporated during current integration period is performed.

The programming realization for such situation processing includes the array with the size equal to the quasi-particles number for each computational unit filled in with zero elements. If the quasi-particle is to be send to another unit or removed at all the unity element is placed to the corresponding place in the array. The next iteration of the quasi-particle motion algorithm is ended with the exchange function call for all quasi-particles for which the unity element in the array is set.

The desirable property of the developed numerical method is its working capacity for unstructured meshes which are considered as sets of convex polyhedrons. Such requirement issues a challenge of quasi-particle track with cell faces intersection finding (see Fig. 3).

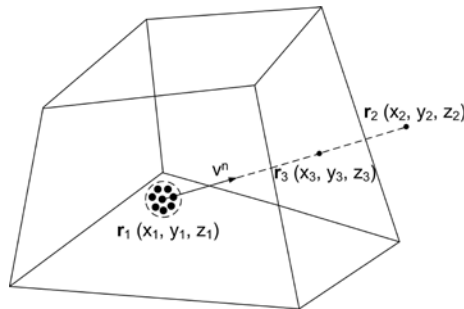


Fig. 3. To the algorithm of the finding of the quasi-particle track intersection with the cell face

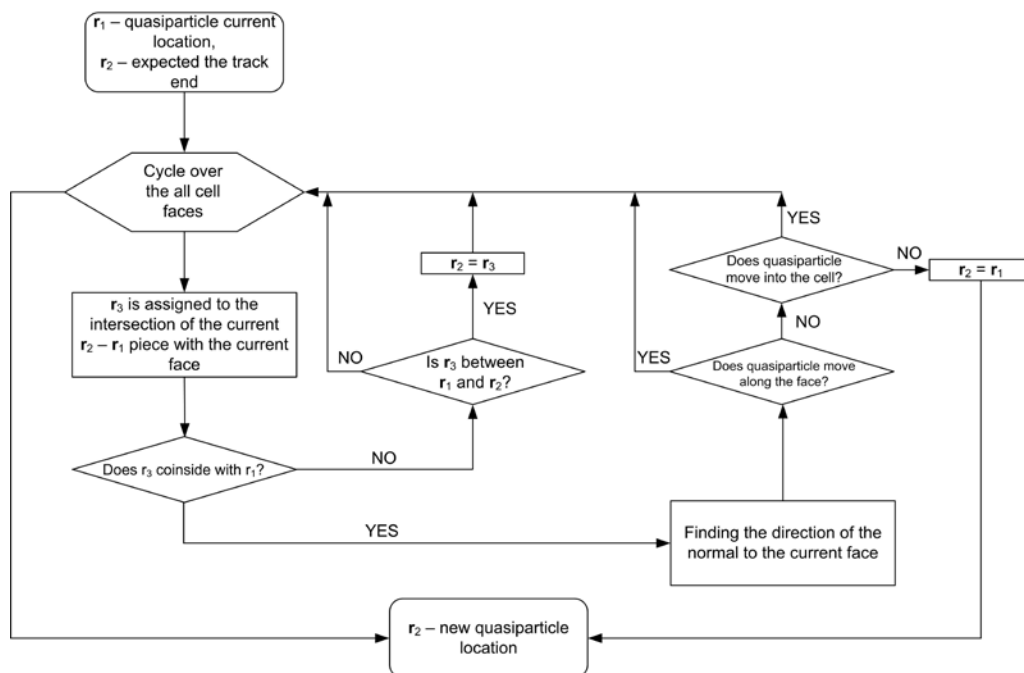


Fig. 4. The algorithm of the finding of the quasi-particle track intersection with the cell face block-scheme

Fig. 4 presents block-scheme of the algorithm of quasi-particle track intersection with the cell face finding. The peculiarity of the algorithm is taking into account special cases when quasi-particle is on the cell face for example at the initial time moment when the quasi-particle is injected to the computational domain from the injector. In such case the special procedure of small displacement of quasi-particle location is realized. The displacement is performed to the center of the cell where quasi-particle should be keeping in mind the velocity vector direction.

4 Inter-phase interaction source terms

Consider the source terms that determine the gas – quasi-particle interaction and should be added to the conservation laws in gas phase. In accordance with the algorithm of quasi-particle motion calculation presented in the previous Section the elementary source term from one quasi-particle in the computational cell is determined on some time interval with the length τ . Denote the time interval on which the elementary source term is calculated as $(t; t+\tau)$. Then

$$\Delta t = \sum \tau,$$

where Δt – gas dynamics time step. Then for each computational cell all the elementary source terms from different quasi-particles for this cell are summed.

For the continuity equation the elementary source term which is determined by the influence of quasi-particle with mass m in a cell with volume V is:

$$I_{mass} = \frac{m(t) - m(t+\tau)}{V \Delta t}. \quad (6)$$

Note that the summation of all the elementary mass source terms (6) on the gas dynamics time step gives the total gas mass change in the cell which can take place due to the process of droplets evaporation.

For the impetus equation the elementary source term is written in the vector form in the following manner:

$$\mathbf{I}_{impetus} = \frac{m(t)\mathbf{v}(t) - m(t+\tau)\mathbf{v}(t+\tau)}{V \Delta t} + \frac{1}{V} \left[\frac{m(t) + m(t+\tau)}{2} \right] \mathbf{g} \frac{\tau}{\Delta t},$$

where \mathbf{V} – vector of quasi-particle velocity and \mathbf{g} – gravity acceleration vector. The change of quasi-particle's velocity on the time interval $(t; t+\tau)$ is connected with the force inter-phase interaction of quasi-particle with gas taking into account the possible droplets diameter change in the process of evaporation and break up.

The action of gravity force is also considered. The quasi-particle mass which can change during integration period is taken equal to the averaged quasi-particle mass on the interval.

For the energy equation the elementary source term is written in the following manner:

$$I_{energy} = \frac{1}{\Delta t V} \left[\frac{m(t)\mathbf{v}(t)^2}{2} - \frac{m(t+\tau)\mathbf{v}(t+\tau)^2}{2} \right] + \frac{\Delta I_1 + \Delta I_2 + \Delta I_3}{\Delta t V},$$

where the term ΔI_1 is connected with the energy consumed to the quasi-particle heating, ΔI_2 – with the energy obtained from the quasi-particle evaporation and ΔI_3 – with the energy of generated vapor.

Consider more detailed each of these terms. Energy which gas loses for the heating of the droplets with specific capacity at constant pressure $C_{part}(T)$ from the temperature $T(t)$ to the temperature $T(t+\tau)$ is:

$$\Delta I_1 = C_{part} \left(\frac{T[t] + T[t+\tau]}{2} \right) \left[\frac{m(t) + m(t+\tau)}{2} \right] (T[t] - T[t+\tau]).$$

For the droplets evaporation the following gas energy is obtained:

$$\Delta I_2 = L \left(\frac{T[t] + T[t+\tau]}{2} \right) (m[t] - m[t+\tau]),$$

where $L(T)$ – the latent heat of the droplet substance. Finally, the energy of the generated vapor is determined as:

$$\Delta I_3 = C_{vap} \left(\frac{T[t] + T[t+\tau]}{2} \right) (m[t] - m[t+\tau]) \left(\frac{T[t] + T[t+\tau]}{2} \right),$$

where $C_{vap}(T)$ – vapor specific capacity at constant pressure.

5 Test case

The method of droplets motion dynamics calculation was verified with the use of experimental data about different diameter water droplet motion under the gravity and drag forces action from the rest [14] (see Fig. 5).

The initial droplet acceleration due to the gravity force is balanced after some time by the increased drag force occurred with the presence of relative gas and droplet velocity. Note that for the visualization of quasi-particles the open source ParaView system is used. The quasi-particles properties are stored to the files with .csv format.

6 Conclusions

In the paper the mathematical model for the gas-droplets flows investigation is proposed. The model is based on the Lagrange formalism of quasi-particles. The whole mathematical model includes the equation of particles motion and submodels for droplets deformation (TAB approach), evaporation (Dukowicz model) and break-up (WAVE-model). The numerical method for quasi-particles calculation is introduced to the software for gaseous phase flow investigation in Euler statement [2].

The description of the parallel numerical algorithm for the quasi-particle equation of motion integration is presented. The algorithm is based on the physical process splitting technique. Attention is paid to the problem of quasi-particle track intersection with the cell face finding for the correct modeling of quasi-particle motion through the grid.

The developed models, algorithms and code are verified on the problem of water droplet motion with the presence of gravity.

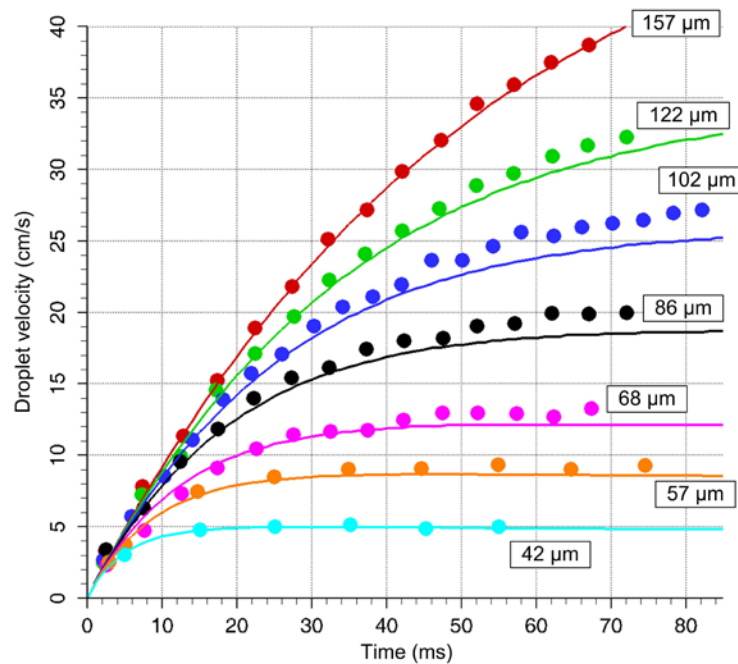


Fig. 5. Comparison of experimental [14] (dots) and calculated (lines) velocity dynamics for different diameter droplets

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