Stochastic model of the near-to-injector spray formation in Diesel-like conditions

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Abstract

The stochastic model of spray formation in the vicinity of the injector has been described and assessed by comparison with measurements in Diesel-like conditions. In this mesh-free model, the 3D configuration of continuous liquid core is simulated stochastically by ensemble of spatial trajectories of specifically introduced stochastic particles. Each trajectory of such particle corresponds to one realization of the liquid core geometry. The stochastic process is based on assumption that due to a high Weber number, the exiting continuous liquid jet is depleted in the framework of statistical universalities of a fragmentation under scaling symmetry. The parameters of such stochastic process are presumed from the physics of primary atomization. The spray formation model is consists in computation of spatial distribution of the probability of finding the non-fragmented liquid jet in the near-to-injector region. This model is combined with KIVA II computation of atomizing Diesel spray in two ways. First, simultaneously with the gas phase RANS computation, the ensemble of stochastic particles is tracking and the probability field of their positions is calculated, which is used for sampling of initial locations of primary blobs. Second, the velocity increment of the gas due to the liquid injection is computed from the mean volume fraction of the simulated liquid core. Another novelty in the model presented is that unsteadiness of the injection velocity is taken into account in breakup simulation. The critical Weber number, indicating when the atomization model is activated, is computed on the bases of the increment in time of the injection velocity, when the last one is decreasing, and thereby leads to supplementary breakup. We show that by such a numerical procedure, the measurements reported by Arcoumanis et al. (time-history of the mean axial centre-line velocity of droplet, and of the centre-line Sauter Mean Diameter), are fairly well predicted.

Introduction

When a high-speed liquid jet is discharged into stagnant dense air, it disintegrates into filaments and drops due to interaction with the gas. In Diesels, the vapour issued from liquid fragments mixes with the turbulent gas flow and chemically reacts. If the produced spray is not well-atomized, the combustion process is incomplete. This leads to power loss, to additional consumption of the fuel, and to increased formation of pollutions. In order to identify the mechanism of spray formation in Diesel-like conditions, many experimental studies were performed (see [1-10], for example). These studies have shown that several interdependent phenomena may instigate simultaneously the complex process of breakup; among them the dominant phenomena are: turbulence [1]-[4]; cavitation pockets [5-8] within injection holes, drop shedding [9], and unsteadiness of the injection velocity [10]. During the last twenty years, the knowledge obtained from experiment was included into classical break-up models ([11]-[13], [14], [15], [16], [17]-[18]). These models are based on statistical representation of spray, as an ensemble of proliferating round spheres, which are injected initially from the nozzle exit. The next step in simulation of spray formation consists in primary atomization modeling. The numerical approaches, which are often referred to as the direct simulation of primary atomization, are based on integration of the Navier-Stokes equations with identification of the gas-liquid interface at each time step. In this technique, the liquid fragments break apart, when a progressively stretched filament becomes of order of the typical size of the numerical cell. These approaches, reviewed recently in [19], can become a major tool for understanding the physics of primary atomization. However, when the Weber number is high, the computational expense associated with resolution of length scales of breaking ligaments is very high. Hence application of those approaches in practical conditions, in a whole domain of atomizing spray, is limited by the Weber and the Reynolds numbers. Consequently, alongside with the direct numerical simulation of primary atomization, there is an interest for the engineering community in developing of primary atomization modeling in a phenomenological way, using physical knowledge and intuition. One of these approaches was proposed in [20] for air-blast atomization. The feature of this approach is that it is a mesh-free approach: in the very close-to- injector domain, the distribution of probability that the continuous liquid jet is broken, is simulated by trajectories of stochas-

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tic particles (each trajectory implies one realization of the liquid core geometry). The parameters of such stochastic process are presumed from the physics of primary atomization, and the process itself is based on the statistical universalities of fragmentation under scaling symmetry [21-22]. These probabilities are computed simultaneously with the gas phase computation, and, also simultaneously, with sampling of initial locations of primary blobs, according to the probability field. In the present paper, we develop further this model, targeting the spray formation in Diesel-like conditions: the model is linked with the RANS computation of flow with sprays; the unsteadiness of the injection velocity and the flow contraction due to cavitation within injection hole are taken into account in the breakup simulation.

Stochastic model of the liquid core configuration

When the Weber number of a high-speed liquid jet spreading into stagnant compressed gas is very high, the exact prediction of each elementary fragment pinched off from the jet, is a too difficult task. However the frequency of detachments of liquid elements is high. Then it is natural to abstract a simple "effective" scenario of fragmentation, regardless of details of the elementary break-up realization, but representing its essential features statistically through physical parameters of break-up. The main steps in our model are as follows.

1. At each time, the liquid core has random geometrical configuration. Each geometrical configuration of the liquid core is determined by spatial trajectory of the stochastic particle referred to as "floating cutter" or FC-particle.

2. At different times, these configurations represent an ensemble of independent realizations. The FC particles are injected one after another; each particle proceeds along its own path, which ends after a length of time determined by kinetic energy transfer from the gas flow to the liquid. The one-point distribution, $f(\mathbf{x},t;r)$, defined such that $f(\mathbf{x},t;r)d^3r$ is the probability that the radial position of interface, r, at axial position x and at time t is in the space element d^3r about r is given by $f(\mathbf{x},t;r)=\langle\delta(r(\mathbf{x},t)-r_{FC}\rangle$, where r_{FC} is the radial position of the FC particle and $\delta(r(\mathbf{x},t)-r_{FC})$ is the Dirac function. The spray around the non-depleted liquid core is assumed to be thin (the droplet field has negligible volume, but significant mass in comparison to the gas). Thereby the position of blobs to be formed in the near-injector region can be sampled from the computed distribution $f(\mathbf{x},t;r)$.

3. Concerning the radial position of a given FC particle at different axial positions, we assume that $r_{FC,x}$ is modified in a step by step manner by a cascade process, in which $r_{FC,x+\Delta x}$ is produced from $r_{FC,x}$ by multiplication by a random independent variable : $r_{FC,x+\Delta x}=r_{FC,x}e^{\ln\alpha}$. Here the random multiplier α $(0\le\alpha\le1)$ is governed by the probability density distribution $q(\alpha)$, $\int_0^1 q(\alpha)d\alpha=1$. The problem is that this multiplicative process, often referred to as fragmentation under scaling symmetry ($r\to\alpha r$), requires $q(\alpha)$, which is, in principal, unknown. However in such fragmentation, with a constant frequency T^{-1}, the population balance equation, describing continuous evolution with time of the particle-size distribution, can be reduced , at large times, exactly to the Fokker-Planck equation [21, 22]:

$$\frac{\partial f(r,t)}{\partial t}=-\frac{\langle\ln\alpha\rangle}{T}\frac{\partial}{\partial r}r\,f+\frac{\langle\ln^2\alpha\rangle}{2T}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}r\,f \qquad (1)$$

Here $f(r,t)$ is the normalized distribution function, $\int_0^\infty f(r)dr=1$, and only two first logarithmic moments of α may intervene in the evolution of $f(r,t)$, and also $\langle\ln\alpha\rangle/\langle\ln^2\alpha\rangle=\langle\ln r\rangle/\left\langle\left(\ln r-\langle\ln r\rangle\right)^2\right\rangle$. According to (1) in Ito interpretation (on Ito versus Stratonovich interpretation of the stochastic equation see [23], for example), the stochastic equation for radial position of the FC-particle is:

$$r_{FC,x+u_l\,dt}=r_{FC,x}+\left[\frac{\langle\ln\alpha\rangle}{T}+\frac{\langle\ln^2\alpha\rangle}{2T}\right]r_{FC,x}\,dt+\sqrt{\frac{\langle\ln^2\alpha\rangle}{2T}}\,r_{FC,x}\,dW(t) \qquad (2)$$

where $r_{FC,x=0} = R_{inj}^{eff}(t)$ is given by the effective radius of injector, and $dW(t)$ is the Winner stochastic process with $\langle dW(t)\rangle = 0$, $[dW(t)]^2 = 2dt$ [23].

4. In the down-stream direction x, each FC particle is moving with axial velocity equal to the effective inlet velocity of the liquid jet $u = U_{inj}^{eff}(t)$. The effective radius of injector and the effective velocity of injection is computed using the flow contraction coefficient C_C [24], which is based on the cavitation number CN: $C_C = \left\{0.62\sqrt{1+\frac{1}{CN}},\ 1;\ CN \geq 3\right\}$. The expressions are: $U_{inj}^{eff}(t) = \frac{U_{inj}^{exp}(t)}{C_C}$, $R_{inj}^{eff}(t) = \sqrt{C_C}\,R_{inj}^{geom}$, where $U_{inj}^{exp}(t)$ is the given injection velocity.

5. Three parameters, $\langle \ln\alpha\rangle$, $\langle \ln^2\alpha\rangle$ and T, have to be determined in (2) according to the mechanism of break-up. In the stochastic modeling of the secondary atomization in [25], the suggestion was : $\frac{\langle \ln^2\alpha\rangle}{\langle \ln\alpha\rangle} = \ln\left(\frac{r_{cr}}{l_0}\right)$, where l_0 is the size of the mother drop subjected to the fragmentation under scaling symmetry, and r_{cr} is the typical size of finally produced droplets. In the present study, it is assumed that interaction between the accelerated liquid jet and the gas gives rise to the Rayleigh-Taylor instability, and then the drops are produced from crests on the free surface. Introducing from [11] the most unstable wavelength λ_{RT} of the Rayleigh-Taylor instability, one writes: $\langle \ln\alpha\rangle = const\cdot\ln\left(\frac{r_{crit}}{\lambda_{RT}}\right)$, $\langle \ln^2\alpha\rangle = \langle \ln\alpha\rangle\cdot\ln\left(\frac{r_{crit}}{\lambda_{RT}}\right)$, with the constant chosen to be equal to 0.1. The typical size r_{cr} is defined by $We_{cr} = \rho_{gas}\langle U_{inj}^{eff}\rangle^2 r_{cr}/\sigma = 1$ and expression for λ_{RT} are taken from [11]. The life time for each FC-particle, $T(t) = 1/\nu_{bup}$, is determined by: $\nu_{bup}(t) = \frac{1}{10}\sqrt{\frac{\rho_{gas}}{\rho_{fuel}}}\frac{U_{inj}^{eff}(t)}{R_{inj}^{eff}(t)}$.

In Fig. 1, we show the distribution of probability $prob(x, r)$ to have a continuous non-fragmented liquid close to injector. The initial conditions in this simulation are taken from [17]. The probability distribution is calculated by positions of all FC-particles containing in the computational domain at a given moment. Meanwhile, the inverse to this distribution will show the probability of positions of drops to be newly formed, with their total mass equal to the injected one. The size of newly produced drops is sampled from χ-squared distribution: $\frac{1}{R^*}\exp\left(-\frac{r}{R^*}\right)$, where R^* is the mean from distribution of radial position of FC-particles at a given distance from the nozzle.

Implementation into KIVA II; model of secondary atomization, and results

In the vicinity of injector in the KIVA II code, we subdivide each momentum cell of volume V into a number of identical small cells of volume v_{FC}. This supplementary sub-mesh is used for realization of the model (1.-5.), in order to compute the rate of subgrid momentum gain to the gas phase per unit volume due to the spray injection. The time step for FC-particle is taken as $\Delta t_{FC} = v_{FC}^{1/3}/U_{inj}^{eff}(t)$. On each KIVA II time step, we compute the volume fraction of the liquid core in the given momentum cell: $\theta = \sum prob_{ik}\cdot v_{FC}/V$ and the velocity increment of the gas due to the liquid injection : $\delta u_g = \delta\left(\theta\cdot U_{inj}^{eff}\right)$.

The secondary atomization model, which is used, is described in [25]. This model is activated when the Weber number of the considered blob is greater than the critical Weber number. In the present study, we propose a new modification of this condition. When the injection velocity is decreasing, $\frac{dU_{inj}^{eff}}{dt} < 0$, the previously injected liquid mass has higher velocity than the mass injected at the considered moment. This provokes the supplementary break-kup. Therefore we introduce the new expression of the Weber number, which has to be compared with the critical

one: $We = \max\left[\rho_{fuel}\left|\delta_t U_{inj}^{eff}\right|^2 r/\sigma,\ \rho_g\left|u_g - u_p\right|^2 r/\sigma\right]$, where $\delta_t U_{inj}^{eff}$ is the injection velocity increment in time. With the model described above, we performed computations of atmospheric spray ($U_{inj} = 0 \div 260\, m/s$, $R_{inj} = 0.009\, m$, $t_{inj} = 0.85\, ms$, $m_{inj} = 3.2\, mg$), which was studied experimentally in [17]. Fig. 2 - Fig.4 represents the comparison between computation and measurements of the liquid core tip penetration, of the centreline Sauter Mean Diameter and of the mean axial centreline velocity of droplet. An agreement with experiment can be seen.

Conclusion

The stochastic model of spray formation in the vicinity of the injector has been described and assessed by comparison with measurements in Diesel-like conditions. In this mesh-free model, the 3D configuration of continuous liquid core is simulated stochastically by ensemble of spatial trajectories of specifically introduced stochastic particles. Each trajectory corresponds to one realization of the liquid core geometry. The stochastic process is based on assumption that due to a high Weber number, the exiting continuous liquid jet is depleted in the framework of statistical universalities of a fragmentation under scaling symmetry. The parameters of such stochastic process are presumed from the physics of primary atomization. The spray formation model, based on computation of spatial distribution of the probability of finding the non-fragmented liquid jet in the near-to-injector region, is combined with KIVA II computation of atomizing Diesel spray in two ways. First, the probability field, from which the initial locations of primary blobs are sampled, is computed simultaneously with the gas phase RANS computation. Second, we compute the rate of sub-grid momentum gain to the gas phase per unit volume due to the spray injection. Another novelty in our simulation concerns accounting for unsteadiness of the injection velocity and for the flow contraction due to cavitation within the injection hole. The injection velocity is computed using the flow contraction coefficient. The critical Weber number, which indicates when the atomization model is activated, is computed on the bases of the increment of the injection velocity, when the last one is decreasing and consequently, leads to supplementary breakup. We show that by such a numerical procedure, the measurements reported by Arcoumanis et al. (time-history of the mean axial centre-line velocity of droplet, and of the centre-line Sauter Mean Diameter), are fairly well predicted.

References

1. Wu P.K., Tseng L.K. and Faeth G.M., *Atomization and Sprays*, vol. 2, pp. 295-317 (1992).
2. Wu P.K. and Faeth G.M., *Atomization and Sprays*, vol. 3, pp. 265-289 (1993).
3. Faeth G.M., Hsiang L.P. and Wu P.K., *Int. J. Multiphase Flow*, vol. 21, pp.99-127 (1995).
4. Stahl M., Gnirß M., Damaschke N. and Tropea C., ILASS-2005, Orleans, France (2005).
5. Stahl, M.; Damaschke, N.; Tropea, C., ICLASS-2006, Aug. 27-Sept. 1, Kyoto, Japan (2006).
6. Chaves H. and Ludwig C., ILASS 2005, Orléans 5-7 September (2005).
7. Badock C., Wirth R., Fath A., Leipertz A., *Int. J. Heat and Fluid Flow*, vol. 20, pp. 538-544 (1999).
8. Arcoumanis C., Badami M. and Gavaises M., SAE Pap. 2000-01-1249 (2000).
9. Sallam K.A., Dai Z. and Faeth G.M., *Int. J. Multiphase Flows*, 28, 427-449 (2002°.
10. Domann, R., Hardalupas, Y., In: Proceedings of 42nd AIAA, Reno, Nevada (2004).
11. Reitz R.D., *Atom. Spray Tech*., 3, 309–337 (1987).
12. Beale J.C., Reitz R.D., *Atomization and Sprays* , 9, 623–650 (1999).
13. Habchi C. and Baritaud T., SAE Pap. 9700881 (1997).
14. Yi Y. and Reitz R., *Atomization and Sprays*, V.14, N°1, 53-80 (2004).
15. Tanner, F.X., *Atomisation and Sprays*, 14, 211–242 (2004).
16. Huh K.Y. and Gosman A.D., Proceedings of ICMF, Sept. 24-27, Tsukuba, Japan (1991).
17. Arcoumanis, C., Gavaises, M., French, B., SAE paper 970799 (1997).
18. Arcoumanis, C., Gavaises, M., *Atomization and Sprays*, V.8, 307-347 (1998).
19. Gorokhovski M. and Herrmann M., *Annual Revues in Fluid Mechanics*, 40:343–66 (2008).
20. Gorokhovski M., Jouanguy J. and Chtab-Deportes A., *Fluid Dynamics Research.* 41, 035509 (2009)
21. Gorokhovski M.A. and Saveliev V.L., *J. Phys. Fluids*, vol.15, n°1, January, 184-192 (2003).
22. Gorokhovski M.A. and Saveliev V.L., *J. Phys. D: Appl. Phys.* 41, 085405 (2008).
23. Nurick, W.H. Journal of Fluids Engineering, 98, 681–687 (1976).
24. Risken H. (1989), The Fokker-Planck Equation, 2nd ed., Springer, Berlin, 472p
25. Apte S., Gorokhovski M. and Moin P., *J. of Multiphase Flow*, 29, 1503-1522 (2003).

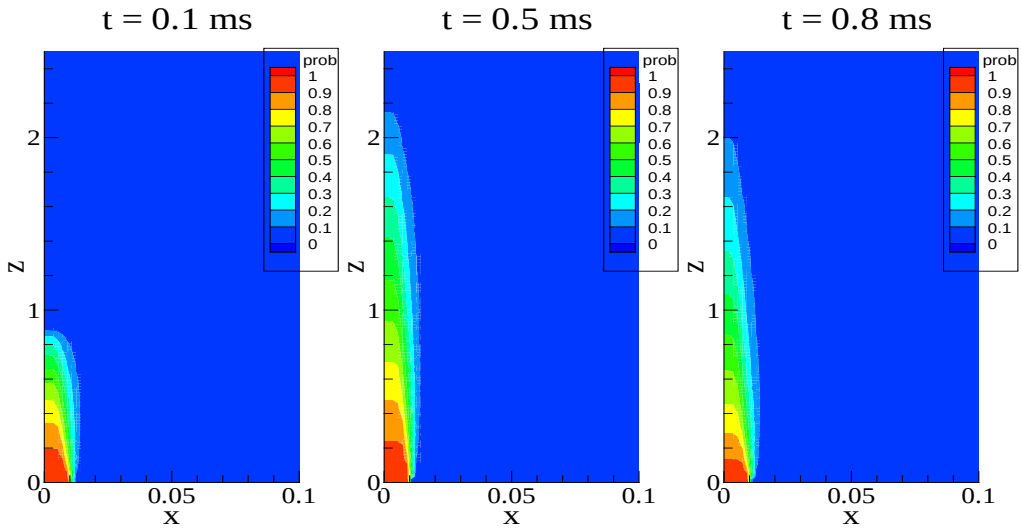

Figure 1. Example of the probability distribution of a continuous non-fragmented liquid close to injector (initial conditions from [17])

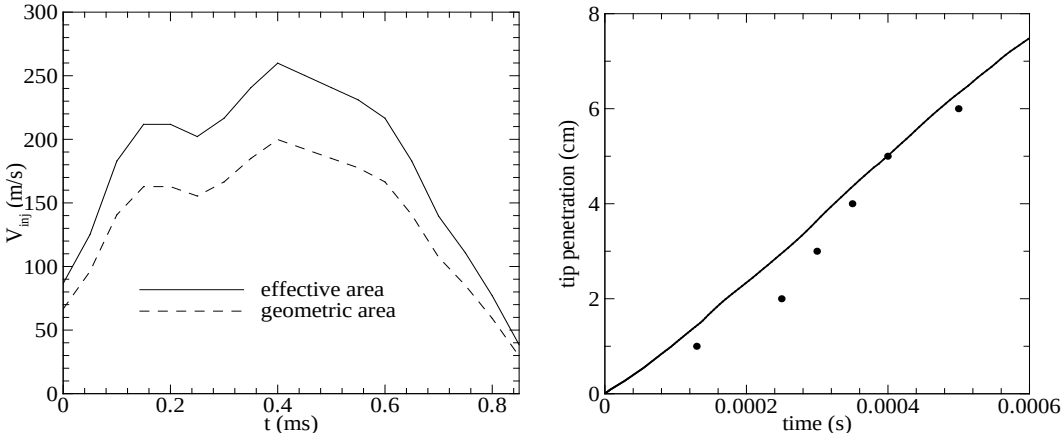

Figure 2. On the left: the injection velocity from [17] and its recomputed value by the effective area. On the right: comparison of the computed tip penetration with the measured in [17]

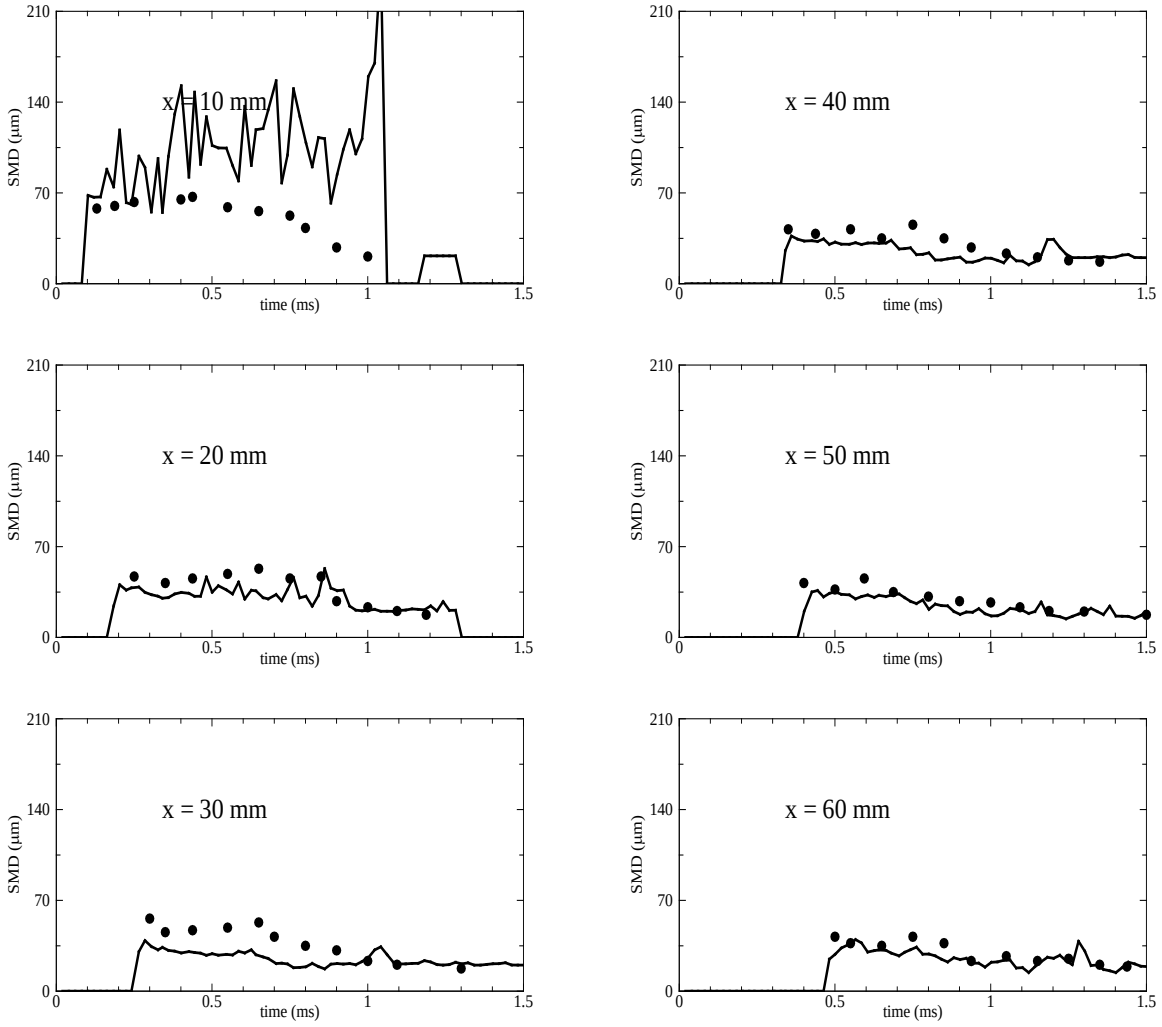

Figure 3. The computational temporal evolution of the centerline droplet SMD versus measurements in [17] at 10, 20, 30, 40, 50 and 60 mm below the injection hole.

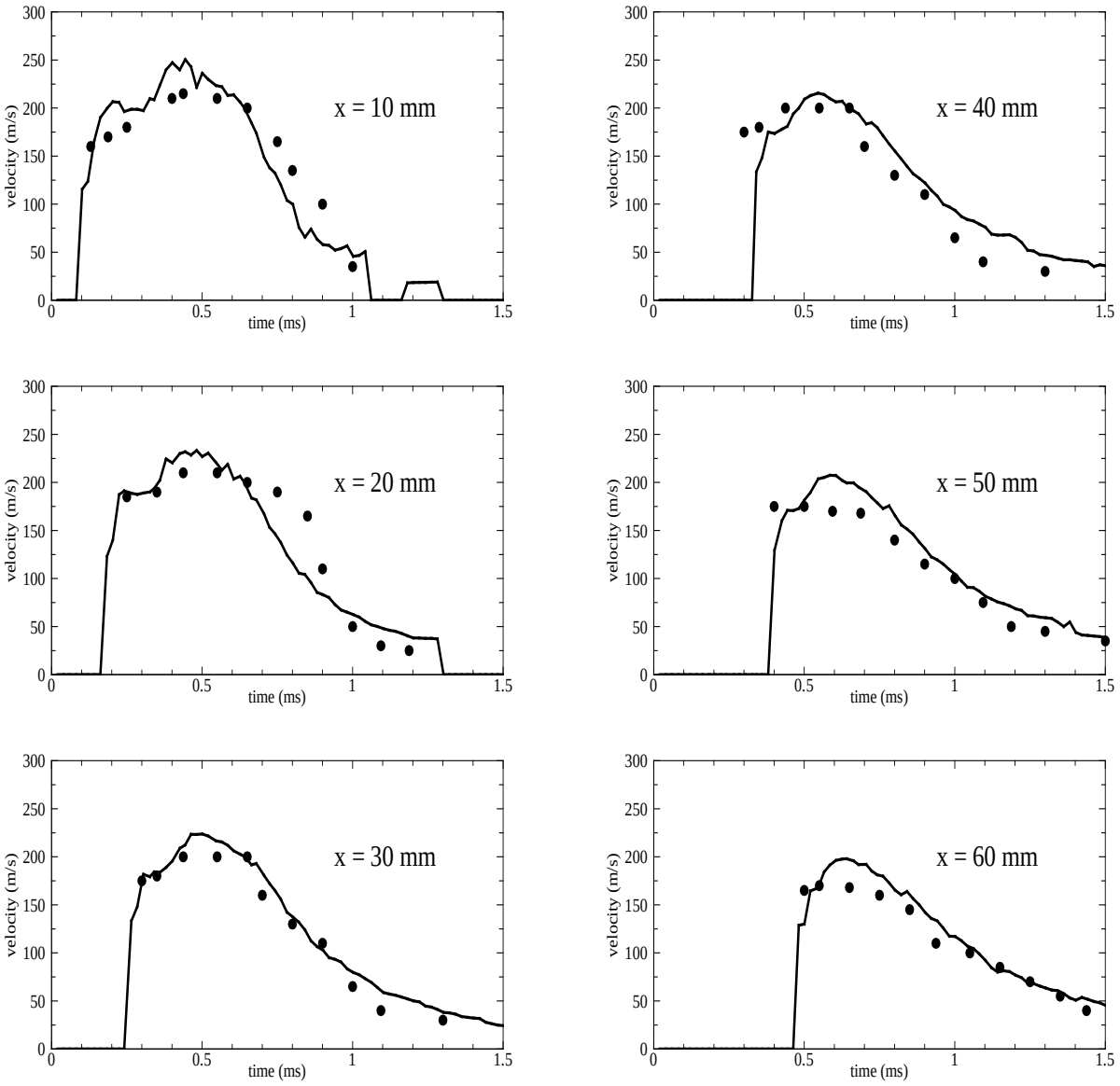

Figure 3. The computational temporal evolution of the the mean axial centreline velocity of droplet versus measurements in [17] at 10, 20, 30, 40, 50 and 60 mm below the injection hole.