# Computational Simulation for the Fragmentation Regimes by Using Droplet Breakup Model

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Submission date:- 20/6/2018 Acceptance date:-28/6/2018 Publication date:- 6/8/2018

#### **Abstract:**

There are no numerical research paper attempts to simulate the break-up mechanism of droplets in the spray development . In particular, the work described here refers to study and quantify the breakup of droplets regime and their effects on the spray behavior. With this purpose, the model parameters results, based on droplet break-up model proposed by Reitz and Diwakar [1] and momentum flux calculations are performed. The parameters that are used in the droplet break-up model are stored in the code as properties. These properties are saved in every computation cell. The parameters are Weber number, break-up time and stable droplet diameter. The numerical simulation is implemented as Eulerian-Eulerian approach .The spray moments theory is used for the liquid phase. Finally the study is implemented in a conceptual model to investigate the possible benefits of the droplet break-up model. A good agreement for the numerical results are compared with the experimental data for the spray tip penetration.

Keywords: - Eulerian modeling, Droplet break-up, Weber number, Spray.

Nomenclature		Gree	Greek symbols	
a	diameter	ρ	density	
	The drop number density function.	μ	Dynamic viscosity	
	probability density function	σ	The surface tension	
	Reynolds number		Subscripts	
	Time	b	Break time	
	velocity	t	Turbulent	
	Weber number	Γ	gamma number size distribution	
U	the moment-average velocity	k	turbulence kinetic energy	

### **1. Introduction**

The distribution of droplets after the breakage process is a crucial parameter for the sequence of phenomena leading to atomization and combustion in self-ignition engines. Indeed, the size of the droplets determines the speed with which they vaporize, thus influencing the combustion process. The determination of this parameter is delicate because it is necessary to distinguish fragments directly from the initial drop of those from fragmentation secondary drops.

The results of the literature are contradictory on the results obtained during the "bag breakup" scheme. In the case of "Transitional breakup" and "shear breakup", some authors [2], [3], [4] conclude, however, that final distribution of droplets satisfies the universal distribution of Simmons (1977a, b) [5] and [6], with MMD / SMD = 1, 2

In the case of the injection of a liquid under supercritical or transcritical conditions, the characteristics of the atomization process are considerably modified [7], [8]. Indeed, in these particular conditions, the liquid has a dense gas behavior due to the very sharp decrease (or even in some cases) of its surface tension. The liquid / gas interface, then becomes difficult to locate. The evaluation of the surface tension of the liquid, a crucial point in the determination of the break regimes (based on the Weber number value) becomes therefore very delicate. The stability criteria and the empirical correlations used are based on experimental data of disintegration of a drop. The fundamental hypothesis is that a jet particle behaves like a drop and is not affected by the particles that surround it. The main problems of this approach are related to the initial discretization of the jets, near the injection hole, which is arbitrary (SMD given by the user while the visualizations highlight a continuous liquid heart) and the fact that a drop necessarily affects the disintegration of its neighbors in the dense area of the spray.

In this paper, the parameters that are used in the droplet break-up model are stored in the code to simulate the breakage mechanism during the injection period.

#### 2. Droplet break-up model

This break-up model is based on the work of Nicholls [9] who studied the breakup of a drop in a high-speed gas flow, following a shock wave, and identified mainly two fractionation regimes. Bag breakup occurs when, Weber number, Weg > 12. The central part of the droplet of diameter a, swells downstream of the flow forming a hollow bag and end, surrounded by a thick edge. The bag then explodes to give birth to many small fragments. The edge disintegrates later and there is formation of some larger fragments (Figure 1). The break time tt<sub>bb</sub> (or durability of an unstable drop) associated with this process is worth:

$$t_{bb} = C_{bb} \sqrt{\frac{\rho_l * a^3}{8\,\sigma}} \tag{1}$$



Figure 1: Bag Breakup  $(W_{eg} > 12)$  [9].

Stripping break up takes place for Weg > Reg, where Reg is the Reynolds number of the gas:

$$Re_g = \frac{\rho_g. u. a}{\mu_g} \tag{2}$$

In this model, there is no has neither bag nor edge, but liquid fragments formed on the periphery of droplet deformed and sheared. In these conditions, the droplet is peeled on its contour by the flow. A gradual decrease in the size of droplet mother and to the formation of daughters of much smaller diameter (Figure 2). Also associates with this phenomenon a break time  $t_{sb}$  defined as follows:

$$t_{sb} = C_{sb} \frac{a}{2u} \sqrt{\frac{\rho_l}{\rho_g}} \tag{3}$$

In the model, the two criteria for the formation of drops (in bags or by tearing are applied to each droplet. When one or the other is checked during a time equal to the corresponding break time, it associates a new diameter to the droplet, in order to satisfy the equality of this criterion. The mass of the droplet is conserved by increasing the number of droplets, energy by decreasing energy kinetic in order to take into account the surface energy required for training new surfaces. For O'Rourke and Amsden [10], the second criterion is open to criticism because it implies that

Tearing drops are related to the viscosity of the gas (involved in the expression of Reg); whereas this one does not appear in the expression of  $t_{sb}$  and that, the experimentally determined break times do not depend on it. On the other hand, the determination of the constants Cbb and Csb differs according to the authors. Reitz and Diwakar [1] then improved this model by assuming that the diameter has particles decreasing continuously over time for fractionation by pull-out (the most common, according to them):

$$\frac{da}{dt} = \frac{a - d_{stable}}{t_{sbg}} \tag{4}$$

Where:

$$d_{stable} = \frac{\sigma^2}{\rho_g . u^3 . \mu_g} \tag{5}$$

Where constant  $C_{\theta}$  usually set at 0.7, but depending on the geometric injector as well as the physical characteristics of the liquid.



Figure 2: Stripping breakup  $(We_g > \sqrt{Re})$ 

## 3. Three moment's schemes

Statistically, the spray moments approach proposed by Beck and Watkins [11], the transport equations were solved for three moments of the assumed distribution, defined as:

$$M_i = \int_0^\infty r^i . n(r) . dr \tag{7}$$

- 1. M<sub>0</sub>, it defined as the total number of droplets per unit volume.
- 2. M<sub>1</sub>, it defined as the sum of diameters of all the droplets.
- 3. M<sub>2</sub>, it defined as the total droplet surface area.
- 4. M<sub>3</sub>, it defined as the total droplet volume.

The general population balance by taking moments of each term in the above equation, the corresponding transport moment equations become

$$\frac{\partial}{\partial t} \int_{\Omega} XM_i \, d\Omega + \int_{S} \left[ \vec{V}_{d,i} \, \vec{n} \right] XM_i \, dS = \int_{\Omega} \Gamma_X \, grad(XM_i) \, d\Omega + \int_{\Omega} q_X M_i \, d\Omega \tag{8}$$

Thus, when X = 1 is solving for moments, X = Ui is solving for momentum and X = Ei is solving for energy. The last term in the above equation represents the source term included drag, break-up and collision processes.

#### 4. Numerical Methods

In the numerical work of injecting droplets into a static airflow, the droplets are often discretely treated in an Eulerian way. The Eulerian methods consist of solving the spray moments transport equations of point mechanics for the forces exerted by the carrier fluid and to follow the trajectory of droplets in the field of computation.

Spray momentum equations of quantity transfer of movement and atomization processes such as drag, break-up and collision are used to simulate carrying the droplets in the air flow. This approach is appropriate when the dispersed phase occupies a low volume fraction in front of the main fluid. By getting an update for the drop size distribution on the phenomenology presented in above section. The gas phase is modeled with an Eulerian framework for mass and momentum transport equations.

During their transport in a turbulent flow, the droplets encounter swirl structures whose characteristic dimensions extend from the scale integral at which turbulent kinetic energy is produced to which this same energy is dissipated. Therefore, k-q turbulence model is used.

#### 5. Results and discussion

The spray tip penetration length and the angle of spray are determined according to the liquid volume fraction and axial and radial momentum transport equations presented in paragraph 3. The macroscopic characteristics have been determined for a calculating point whose injected liquid is diesel and the injection pressure of 9.9 bar. Figure 3 shows the spray tip penetration length of the spray front depending on the injection time compared with experimental data of [12]. The percentage error in the determination of the spray penetration is the order of 10%.



#### Time after start of injection (msec)

#### Figure 3: Comparison of predicted spray penetration with the experimental data [12].

The probability density function of of droplet size distribution is obtained with diesel fuel and is shown Figure 4. The transient effect is appeared in the calculations that are taken at 0.1, 0.5 and 1.msec. It can be seen that whatever the liquid injected,

the droplet size distribution is small at the beginning and increases with time due dispersion processes.



Figure 4: Pdf distribution with droplet radius at different time.

Figure 5 shows the evolution of the droplet velocity with the droplet radius. At time=0.1, the earlier stage of injection velocity the larger droplets have the higher velocity due to their inertia. At time=0.5ms when the initial velocity of the introduced droplets is decreased most of droplets have the same velocity. Finally, at time=1.0 msec droplets suffer the effects of the atomization process, causing a sharp decrease in size.



Figure 5: Droplet velocity profile with droplet radius at different time.

Figure 6 shows the evolution of the droplet size distribution function with droplet velocity at different time. Indeed, large droplets located mainly away from the injector. Therefore, at time=0.1ms, the droplets still undergoing atomization process. At time=0.5 and 1.0 msec, it can be found that the maximum number of drops different speeds considered is very little influenced by the injected velocity.



Figure 6: Pdf distribution with droplet velocity different time.

Figure 7 shows contour plots for the Sauter mean radius at different time. The overall Sauter mean radius  $r_{32}$  can be defined here in terms of the third moment (liquid volume fraction to the second moment total surface area). From this plot and by taking into account the breakage process causes a significant decrease in the average Sauter mean radius. This reduction is the consequence of fragmentation that causes an increase in the total area drops while keeping their volume constant.



Figure 7: Contour plots of Sauter mean radius at different time.

Journal of University of Babylon for Engineering Sciences, Vol. (26), No. (7): 2018.

Figure 8 shows the contour plots of Weber number at different time. The Weber number represents the ratio of aerodynamic forces to forces surface tension. It is defined by:

$$We = \frac{\rho_g.\,d(u - U_l)}{2\sigma} \tag{9}$$

At time=0.1 msec as a function of the ratio of the intensities of shear forces and surface tension, initially spherical droplets can be only deformed or else fractionated near the injector. At time=0.5 mesc, the transition between these two evolutions allows to makes it possible to observe that due breakage process a small zone is created near the outer edge of the spray. At time=1.0 msec, the small zone moves away from the injector and graws up. In addition a large breakage can be found at the front of the spray.





Figure 8: Contour plots of Weber number at different time.

Figure 9 shows contour plots for the break time defined in equation (3) at different time. From droplet viewpoint, break time defines as the time needed for the appearance of the first waves on the surface of the droplet. Here, at all-time the contour plots matching the Weber number plots. This figure allows essentially highlighting the areas of spray development by the droplets during their travels in the field of computation. Moreover, this representation shows that the majority of breakout processes take place in the areas for which the speed of the flow is the most important. Indeed, it can be found that the higher rate is associated with this initial velocity; therefore, it easily spotted by the thickest trajectory is deflected by the flow.





Figure 9: Contour plots of break time at different time.

Figure 10 shows contour plots for the stable breakup droplet diameter, which defined in equation(5) at different time. At time=0.1 msec, it can be noticed that the  $(d_{stable})$  at lower values due high injection velocity at the beginning. Moreover, these values are tending to increase in time=0.5 and 1.0 msec. This is due the breakage process and essentially can be found at the outer edge of the spray. At the spray front can found less. Also, it observed that near the injector, the simulation can give approximately zero values for( $d_{stable}$ )



Figure 10: Contour plots of the stable breakup droplet diameter at different time.

# 6. Conclusions

The precise knowledge of the different phenomena occurring inside the combustion chamber or in the atmosphere is very important for developing diesel injectors. It is essential for the development of injector formation of spray droplets and control of the combustion inside the chamber. From the obtaining results and discussion in this research, the conclusions are summarized as follows:

- The Reitz-Diwakar [1] breakup model well describes the mechanism of breakage and fragmentation of droplets. It is also the surface and internal structure of diesel spray are numerically simulated.
- There are other models which are included other parameters should be studied such as turbulence effect.
- The break-up process is in another application have to be studied in the same manner to generalize the investigation.

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Journal of University of Babylon for Engineering Sciences, Vol. (26), No. (7): 2018.

المحاكاة الحاسوبية لأنظمة التكسير باستخدام نموذج تكسر القطيرات أحمد عبد الكاظمة التر محسن عباس عليوي علاء لائق a أحمد عبد الكاظمة الميكانيكية ، كلية الهندسة ، جامعة القادسية قسم الهندسة الميكانيكية ، كلية الهندسة ، جامعة الكوفة b norm.alhasnawi@uakufa.edu.iq

#### الخلاصة

لا توجد محاولات بحثية رقمية لمحاكاة آلية تكسر القطيرات في عملية تطوير الرذاذ. على وجه الخصوص، يشير العمل الموصوف هنا إلى دراسة وقياس تفكك نظام القطيرات وآثارها على سلوك الرذاذ. مع هذا الغرض، يتم تنفيذ نتائج معاملات النماذج، بناءً على نموذج تكسير القطيرات المقترح من قبل Reitz و هذا الغرض، يتم تنفيذ نتائج معاملات النماذج، بناءً على نموذج تكسير القطيرات المقترح من قبل Reitz وهذا الغرض، يتم تنفيذ نتائج معاملات النماذج، بناءً على نموذج تكسير المعاملات المقترح من قبل Reitz وهذا الغرض، يتم تنفيذ نتائج معاملات النماذج، بناءً على نموذج تكسير القطيرات المقترح من قبل Reitz وهذا الغرض، يتم تنفيذ نتائج معاملات النماذج، بناءً على موذج تكسير القطيرات المقترح من قبل Reitz وير، [1] Diwakar وحسابات فيض الزخم momentum flux. يتم تخزين المعاملات المستخدمة في نموذج تقسيم القطيرات في الشفرة كخصائص. ويتم حفظ هذه الخصائص في كل خلية حساب. المعاملات هي عدد ويبر، وزمن التكسير وقطر القطرة المستقر. حيث يتم تطبيق المحاكاة الرقمية كأسلوب Eulerian-Eulerian-eulerian وزمن التكسير وقطر القطرة المستقر. حيث يتم تطبيق المحاكاة الرقمية كأسلوب Leulerian-eulerian وتستخدم نظرية زخم الرذاذ للمرحلة السائلة. وأخيرا يتم تنفيذ الدراسة في نموذج للتحقق في الفوائد المحتملة وتستخدم نظرية زخم الرذاذ للمرحلة السائلة. وأخيرا يتم تنفيذ الدراسة في نموذج للتحقق في الفوائد المحتملة وتستخدم نظرية زخم الرذاذ للمرحلة السائلة. وأخيرا يتم تنفيذ الدراسة في نموذج لتحقق في الفوائد المحتملة وستخدم نظرية رخم الرذاذ للمرحلة السائلة. وأخيرا يتم تنفيذ الدراسة في نموذج لتحقق في الفوائد المحتملة وتستخدم نظرية راحم الولية تطابق جيد للنتائج العددية مع البيانات التجريبية لتغلغل الرذاذ.

الكلمات الداله: - النمذجة Droplet ، Eulerian تفكك، عدد ويبر، رذاذ.