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A stochastic droplet collision model with consideration of impact efficiency

S. Blei*, C.A. Ho*, M. Sommerfeld*

Martin.Sommerfeld@IW.Uni-Halle.de
***Institut für Verfahrenstechnik**
Fachbereich Ingenieurwissenschaften
Martin-Luther-Universität Halle-Wittenberg
D-06099 Halle (Saale), Germany
Tel.: 0049-3461-4628-79; Fax: 0049-3461-4628-78

Abstract

A stochastic droplet collision model (Sommerfeld [9]), based on the creation of a fictitious collision partner is described, taking into account impact efficiencies. The model of O'Rourke [5] is considered to predict the outcome of water-droplet collisions, being grazing or coalescing, and to predict post-collision velocities. The relevance of impact efficiencies is discussed for water droplet collisions on the basis of the inertial parameter. As a result, regions of importance are defined, in which the impact efficiency has to be taken into account. The influence of impact efficiency on coalescence rates of water droplets is discussed by comparing normalised critical displacements and collision frequencies. The assumption of a step function for modelling impact efficiencies, as valid for laminar flows, is not applicable to turbulent flows if the integral scale of turbulence is in the order of the large droplet diameter.

Introduction

Droplet collisions are a phenomenon occurring in all dispersed liquid-gas systems. By it's simple existence this phenomenon has to be taken into account in industrial processes like spray drying, atomisation in engines or Ion launders. The change of the droplet size distribution due to merging or splashing of colliding droplets may significantly influence the process performance. The occurrence of collisions assumes that the collision partners come into touch with each other. That is not a matter of course, small droplets may follow the flow field around a larger one, therefore preventing a collision and reducing the impact efficiency of the system. The impact efficiency not only depends on the diameter ratio of the approaching partners, but also on the surrounding flow-field, being laminar or turbulent. Schuch and Löffler [8] performed calculations and experiments for small solid particles and fixed droplets in a laminar flow, formulating relations for Reynolds number dependent impact efficiencies. Pinsky and Khain [7] showed the random character of hydrodynamic droplet interactions in turbulent flows and indicated the possible increase of impact efficiencies due to turbulence effects.

If collisions between droplets finally happen, one can observe different phenomena in the post-collision stage, such as permanent coalescence, bouncing or separation with production of small satellite droplets. Numerous investigators dealt with the object of defining boundaries between this collision modes. The majority of them concentrated their research on water-air systems (Brazier-Smith et al. [2]), others on organic liquids like Heptane, Propanol or glycerin (Jiang et al. [4]). The main achievement of this work was the description of boundaries of the collision scenario expressed as functions of critical Weber numbers and collision angles. Only few researchers investigated other phenomena related with droplet collisions, like mass exchange of merging or separating droplets (Potvysotsky et al. [6]). Almost no information is available about post-collision velocities of colliding droplet pairs. Such knowledge is needed for a detailed modelling these phenomena.

The present study concentrates on the modelling of droplet collisions in turbulent flows, considering impact efficiency. The relevance of the impact efficiency and it's influence on coalescence rates is discussed, concentrating on water-air systems.

Stochastic Droplet collision model

The core of the stochastic collision model is the creation of a fictitious collision partner, which is done with the help of local size and velocity distributions of the droplet phase. Hence, the fictitious droplet is a representative of the local droplet population. This way of deciding whether a collision takes place or not does not require the knowledge of locations of neighbouring droplets and the time consuming search for collision partners. Only the droplet size- and velocity distribution functions must be stored for each computational cell (Sommerfeld [9]), usually expressed by size classes or parameters of standard distribution functions. In order to describe the collision process in detail, the following physical effects have to be considered:

- The instantaneous velocity of small droplets moving in a turbulent flow are not independent. If the droplets are able to respond to the turbulent fluctuations they are moving in the same turbulent eddy upon collision. Hence, their velocity is correclated through their response to turbulence.

- With the correlated velocities a collision probability can be obtained based on kinetic theory of gases if the size of the colliding droplets is not too different.
- In case of a collision between small and large droplets, which is most likely to occur (Ho and Sommerfeld [3]), the impact probability is reduced, since the small droplet may move with the relative flow around the larger droplet, also called collector.
- Once a collision occurs it has to be decided whether this collision results in coalescence or rebound (note, that also other collision scenario are possible) and the post-collision velocities have to be determined.

For clarity of the results, the correlation of the velocities of colliding droplets (Sommerfeld [9]) was not considered in the present study.

In order to decide whether a collision between the real and fictitious droplet takes place during a time step or not, two steps are necessary: the calculation of the collision probability and the calculation of the impact probability. In order to simplify this calculation a co-ordinate transformation into a cylindrical frame of reference is carried out, in a way that fictitious droplet is set stationary. In order to find the point of impact, a collision cylinder is defined, with an axis aligned with the relative velocity vector (Fig. 1 a).

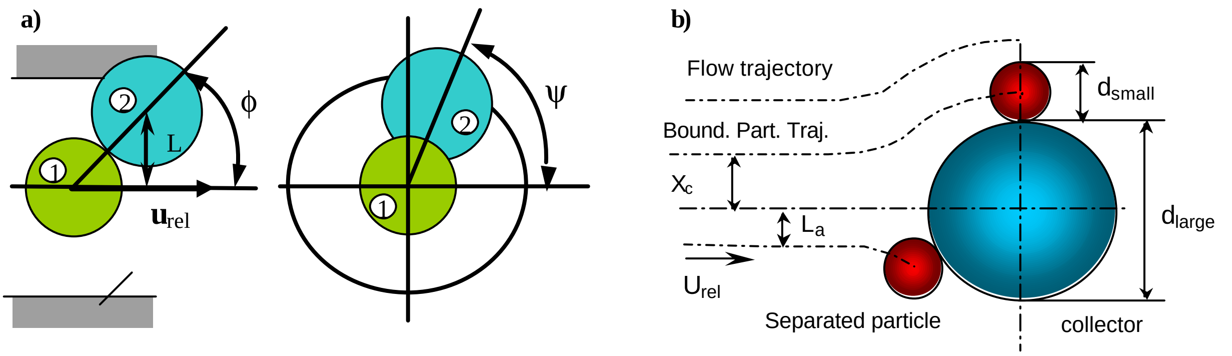

Fig. 1: Inter-droplet collision configuration (a) and the modelling of the collision efficiency (b)

The collision probability P_{coll} is calculated in this cylindrical frame of reference according to kinetic theory:

$$P_{coll} = f_{coll}\cdot\Delta t = \frac{p}{4}\cdot\left(d_{real}+d_{fict}\right)^2\cdot\left|\vec{u}_{rel}\right|\cdot n_d\cdot\Delta t \tag{1}$$

Here, n_d is the number concentration of all droplet fractions in the domain, $\vec{u}_{rel}$ the relative velocity between the real and fictitious droplet.

Now it has to be considered, that the impact efficiency for different sized droplets may be reduced, since the smaller droplet might follow the relative flow around the larger droplet (collector). The flow-pattern around the larger droplet strongly depends on the collector Reynolds number. Assuming both the real and fictitious droplet are moving within the same turbulent eddy just before the collision may happen, the hydrodynamic interaction between the droplets might be modelled in a laminar way. This implies, that the smaller droplet trajectory follows an almost straight line and that the impact efficiency is dominated by inertial effects. For this case Schuch and Löffler [8] characterised the impact efficiency by the following relation:

$$P_{impact} = \left(\frac{2\cdot X_c}{d_{large}}\right)^2 = \left(\frac{St_{small}}{St_{small}+a}\right)^b \tag{2}$$

The Stokes number of the smaller droplet, St_{small}, also called inertial parameter, is given in this case by:

$$St_{small} = \frac{r_d\cdot\left|\vec{u}_{rel}\right|\cdot d_{small}^2}{18\cdot m_f\cdot d_{large}} \tag{3}$$

The parameters a and b are coefficients, which depend on the Reynolds number of the collector. They were obtained by calculating the flow around the collector for different Reynolds numbers and determining the resulting boundary trajectory (Schuch and Löffler [8]). X_c is the radial distance of the boundary droplet trajectory from the symmetry axis of the collision cylinder. In order to account for interception the radius of the small droplet is added and one obtains the non-dimensional limiting trajectory displacement as:

$$X_c^* = \frac{2\cdot\left(X_c+0.5\cdot d_{small}\right)}{d_{large}+d_{small}} \tag{4}$$

The possible point of impact on the surface of the droplets is obtained by a random process, carried out in a frame of reference where the collector droplet is stationary. Generating two uniform random numbers *XX* and *ZZ* in the range [0,1], the location of the collision point in the lateral section of the collision cylinder is expressed with the help of the non-dimensional lateral displacement L_a and the angle f (Fig. 1):

$$L_a = \frac{2 \cdot L}{d_{real} + d_{fict}} = \sqrt[2]{XX^2 + ZZ^2} \qquad \text{with } L_a < 1 \qquad \text{and} \qquad f = \arcsin(L_a) \tag{5}$$

Additionally, the orientation of the collision plane in the cross section of the collision cylinder is randomly sampled from a uniform distribution with in the range [$0 < y < 2p$] as indicated in Fig. 1a).
In order to decide whether a collision occurs, first a random number in the interval [0,1] must become smaller than the collision probability (Eq. 1). The impact efficiency is accounted for by the requirement that the sampled impact displacement L_a must be smaller than the non-dimensional limiting trajectory displacement X_c^*.

$$RN < P_{coll} \qquad \text{and} \qquad L_a < X_c^* \tag{6}$$

The determination of the outcome of a collision between water droplets can be based on the model proposed by O'Rourke [5]. In this model only grazing collisions and coalescence are considered, other scenario are neglected. The boundary between grazing and coalescence can be described by a critical collision angle f_{crit}:

$$sin^2(f_{crit}) = min\left[2.4 \cdot \frac{f(g) \cdot 2 \cdot s_A}{r_d \cdot \vec{u}_{rel}^2 \cdot d_{large}}; 1.0\right]; \qquad g = \frac{d_{large}}{d_{small}}; \qquad f(g) = g^3 - 2.4 \cdot g^2 + 2.7 \cdot g \tag{7}$$

These equations are correspond to the fit of Amsden et al. [1], which are based on the data of Brazier-Smith et al. [2]. The droplets coalesce if the collision angle f (see Fig. 1) is smaller than f_{crit}, otherwise a grazing collision occurs. In the case of coalescence the new droplet diameter is obtained from a mass balance and the new droplet velocity after coalescence can be calculated from the impulse balance by respecting that in the considered frame of reference the fictitious droplet velocities are zero:

$$d_{real,ac} = \left(d_{real,bc}^3 + d_{fict,bc}^3\right)^{\frac{1}{3}} \qquad u_{real,ac,i} = u_{rel,bc,i} \cdot \frac{m_{real}}{m_{real} + m_{fict}} \tag{9}$$

In the case of grazing collision a momentum loss due to the transfer of translational energy to rotational energy has to be accounted for. This finally yields the new velocity components of the real droplet:

$$u_{real,ac,i} = \frac{u_{real,bc,i} \cdot m_{real} + u_{fict,bc,i} \cdot m_{fict} + m_{fict} \cdot u_{rel,bc,i} \cdot \left[\frac{(\sin f - \sin f_{crit})}{1 - \sin f_{crit}}\right]}{m_{real} + m_{fict}} \tag{10}$$

Only the velocities of the real droplet are of interest in the stochastic collision model. After carrying out all required calculations the real droplet's properties are transformed back into the global frame of reference. Since the computational particles represent a number of real particles (parcel), it is assumed that all the real particles inside the parcel collide with the same number of fictitious particles.

Relevance of impact efficiency and effect on coalescence rates

The impact efficiency is commonly defined as the ratio of two areas: the geometrical cross-section of the collector droplet, and the effective collision cross-section which is perpendicular to the axis of the collision cylinder and represents the area which is limited by the grazing tracks where the small droplet just hits the collector (see Fig. 1 and Eq. 2). Inside this cross-section the impact probability is usually defined as one, which is justified if the motion of the small droplets is not affected by turbulence. In case inertial effects govern the impact, the motion of the small droplet can be described using the Stokes number (Eq. 3), which is the ratio of the droplet response time to the time the small droplet needs to pass the collector. This implies, that the impact efficiency is increased with increasing relative velocity and the diameter of the small droplet, whereas an increase of collector diameter reduces impact efficiency. According to the result obtained by Schuch and Löffler [8] the impact efficiency needs to be considered for Stokes numbers larger then about 10 (Eq. 3). Using this condition one can estimate the importance of impact efficiency for an air-water system with the diameter ratio and the relative velocity as a parameter as shown in Fig. 2. It is obvious that the impact efficiency is only important (i.e. this value becomes smaller than one) for small diameter ratios d_{small}/d_{large} and relative velocities. High values of the relative velocity and the droplet diameter ratio yield a collision with 100% collision efficiency. For larger droplets, the impact efficiency is only important for very small diameter ratios and relative velocities, i.e. the region of interest is reduced.

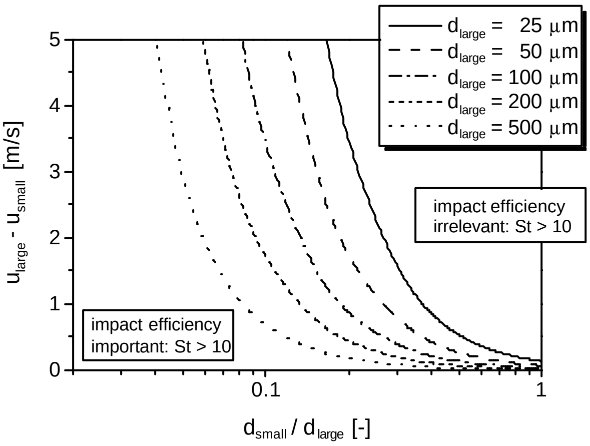

Fig. 2: Estimated regions of interest for considering impact efficiency of a water-air system

The model of Schuch and Löffler [8], as described by Eq. 2, assumes an impact efficiency of 100% inside a cross-section limited by grazing tracks of droplets just hitting the collector. This can be expressed by a step-function being equal to one inside this cross-section and zero outside. This approach was justified with the assumption of laminar flow around the larger droplet. If we consider a more realistic turbulent flow field, then recent numerical calculations indicate, that a step function is by far over-predicting impact efficiencies and does not reflect the distribution of impact efficiencies in the effective cross-section of the collision cylinder. These calculations were performed by solving the Reynolds-averaged conservation equations in connection with the k-ε turbulence model. The collector droplet was fixed and discretised by a boundary fitted mesh, whereby the flow around the collector was resolved. A cubic flow domain around the collector was considered with a defined inlet velocity and turbulence intensity. The small droplets were tracked in a Lagrangian fashion, which implies that they were treated as a point-like droplets in the flow, but considering the finite dimension for the collision with the collector. Hence, this approach does not account for the flow around the small droplet and therefore is limited to small diameter ratios. The calculations were performed for a collector Reynolds number of 10 and the integral length scale of turbulence was in the range of the collector diameter.

Calculations for different flow conditions and diameter ratios are shown in Fig. 3. Here the number of colliding droplets normalised with the number of locally injected droplets are plotted versus the lateral injection position which is 10 collector diameters upstream of the collector. The laminar calculation yields a 100% impact efficiency within an effective area having a radius corresponding to about half the collector radius (i.e. impact efficiency about 0.25) for the considered situation. In the turbulent cases, the small droplets will hit the collector even if they are releases outside this effective area and the resulting maximum lateral starting position from where the small droplets can hit the collector reaches values up to 2.5 collector radii (Fig. 3 a). Additionally, turbulent dispersion of the small droplets is associated with a drastic reduction of the impact efficiency with increasing turbulence intensity even on the centre line of the collision cylinder. With increasing diameter ratio the impact probability is enhanced since inertial effects become more dominant compared to turbulent dispersion (Fig. 3b). The radial distribution of the impact efficiency within the effective collision cross-section may be approximately described by a normal distribution function. A modelling of impact efficiency in turbulent flows, where the length scales are in the order of the collector diameter, needs further detailed investigations.

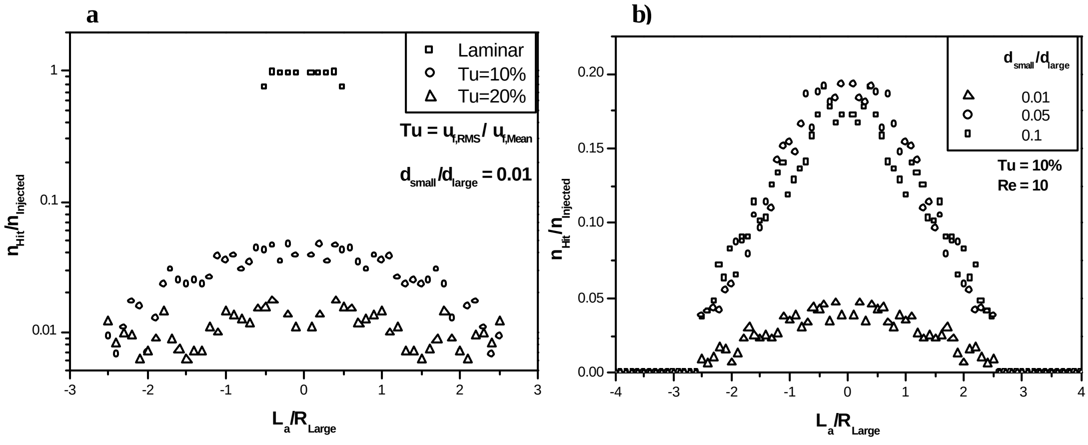

Fig. 3: Calculated profiles of impact efficiency: variation of turbulence intensity Tu (a) and diameter ratio d_{small} / d_{large} (b)

A reduced impact efficiency influences the probability of coalescence for a colliding droplet-pair. According to Brazier-Smith et al. [2], whose relations are commonly used for water-air systems, the critical lateral displacement $X_{c,BS}$ representing the boundary between bounce and coalescence of droplets depends on the Weber number and the size-ratio of the colliding droplets:

$$We = \frac{\vec{u}_{rel}^{\,2} \cdot d_{small} \cdot r_d}{2 \cdot s_A} \qquad X_{c,BS} = \frac{d_{large} + d_{small}}{2} \cdot \sqrt[2]{\frac{2{,}4}{We}} \cdot \frac{\left[1+g^2-\left(1+g^3\right)^{2/3}\right]^{1/2} \cdot \left(1+g^3\right)^{11/6}}{g^3 \cdot (1+g)} \qquad (11)$$

With help of this criterion it is possible to compare the limiting lateral displacement $X_{c,BS}$ with the limiting lateral displacement $X_{c,SL}$, given by the criterion of Schuch and Löffler [8] for laminar cases (Fig. 4). In the region where the impact efficiency is relevant (i.e. St < 10) the Brazier-Smith criterion always predicts coalescence and $X_{c,SL}$ is always significantly smaller than $X_{c,BS}$. Therefore, the impact efficiency is dominating the collision process and all collisions result in coalescence in this range. The Brazier-Smith criterion becomes relevant for larger Stokes and hence larger diameters of the impinging droplet, where the impact efficiency is not relevant.

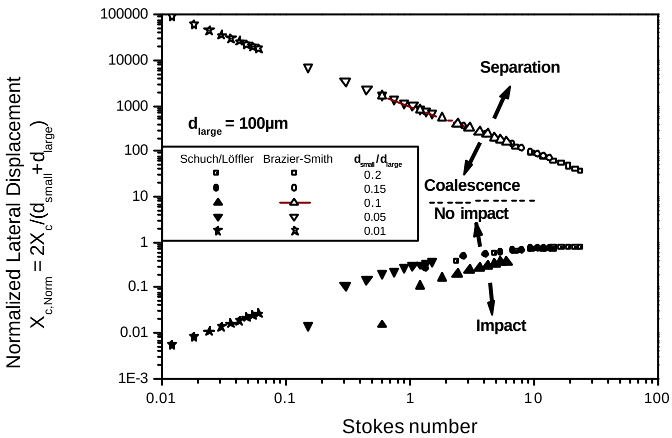

Fig. 4: Comparison of normalised limiting lateral displacements for different water-droplet pair

Numerical results

Finally, also numerical calculations based on the Lagrangian approach were conducted in order to test the performance of the stochastic collision model with consideration of the impact efficiency according to Eq. 2 using the constants a=1.24 and b=1.95, valid for a collector Reynolds number of about 10 to 20. The flow field was a homogeneous isotropic turbulence with a turbulent kinetic energy of 0.135 m^2/s^2, and an integral time and length scale of 23 ms and 7.25 mm, respectively (Sommerfeld [9]), prescribed in a cubic domain of 0.2m x 0.2m. The droplet phase was a binary mixture with a collector droplet diameter of 100 µm (fraction A) and small droplets with diameters of 5, 10, 20 and 30 µm (fraction B) settling under a gravity of 49.05 m/s^2. The volume fraction for the large droplets was $\alpha_A = 0.8\ 10^{-4}$ and for the small droplets $\alpha_B = 0.4\ 10^{-5}$, respectively.

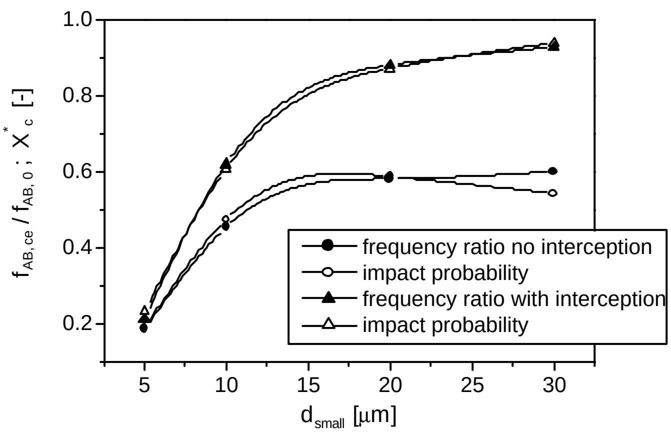

Fig.5: Numerically calculated collision frequency ratios with and without interception and comparison with the respective geometrically defined impact efficiencies

As expected, the collision frequency increases with reduction of droplets diameter, due to the increase of number density which is proportional to $1/d_{small}^3$. The collision frequencies between large (A) and small (B) droplets normalised with the value obtained without impact efficiency are shown in Fig. 5 for calculations with and without interception effect. A reduction of the small droplet size causes a drastic decrease of the collision frequency as a result of the decreasing impact efficiency for both cases. However, if the interception effect (see Eq. 4) is not accounted for, the collision frequency is much lower compared to the case with interception, since the effective collision cross-section is defined to be too low. Only for the smallest droplets ($d_{small}/d_{large}=0.05$) the difference is not important. The predicted collision frequency ratios agree very well with the ratio of the effective impact area to the geometrical area of the collision cylinder for both calculations. In the case with interception the effective impact area corresponds to Eq. 4, whereas for the condition without interception the finite size of the small droplets is neglected. These results reveal the importance of interception for larger droplet size ratios and that the impact efficiency will be unimportant for size ratios beyond about 40%.

Conclusions

A stochastic droplet collision model was described enabling the consideration of impact efficiency and coalescence or rebound of droplets. The effect of impact efficiency was discussed, pointing out that this phenomenon has a significant influence on collision frequencies and therefore on coalescence rates if the small droplet`s Stokes number is smaller than 10. Additionally, it was found that a step function, like the Schuch and Löffler model, does not correctly describe the distribution of the number-impact efficiency for turbulent flows across the injection plane located normal to the relative flow direction. The distribution of the impact efficiency depends on the turbulence intensity, the droplet-Stokes number, the diameter ratio of small and large droplets and the larger droplet's Reynolds number. Gaussian distribution functions are more appropriate to describe the impact efficiency in turbulent flows. Numerical calculations based on the Lagrangian approach revealed the proper implementation of the model and the importance of considering interception effects in modelling collision efficiency.

Nomenclature

	Latin symbols		Greek symbols		Sub-/Superscripts
a, b	Empirical parameters	γ	diameter ratio	ac	after collision
d	diameter	μ	dynamic viscosity	bc	before collision
f_{coll}	collision frequency	ξ	Gaussian Random number	BS	according Brazier-Smith et al.
i	= 1,2,3 - cartesian coordinates	ρ	density	coll	collision
L_a	lateral displacement	σ_A	surface tension	d	dispersed phase property
m	mass	σ_d	rms value of droplet velocity	f	fluid phase property
n	number	τ_p	particle response time	fict	fictitious droplet
P	probability	τ_t	Lagrangian integral time scale	SL	according Schuch / Löffler
St	Stokes-number	ϕ, ψ	angles	real	real droplet
Δt	time step			rel	relative properties
u	velocity			'	fluctuation value
X_c	radial trajectory distance				

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