Dynamic analysis of the primary breakup of an annular energetic liquid jet injecting into a confined space

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Abstract. The Large Eddy Simulation (LES) with the Volume of Fluid (VOF) method was carried out to investigate the primary breakup dynamic mechanism of an annular energetic liquid jet injecting into a confined space. The gas vortex structure and the liquid jet formation were visualized by tracking the evolution of the phase velocity and the interface location, and hence the coalescence process of the goblet-shaped liquid jet from the annular liquid jet was reproduced. Simulation results indicate that the first coalescence is caused by the Rayleigh-Taylor instability, which is generated by the interaction between the liquid jet head and the gas in the confined space. Two kinds of large-scale vortex structure expedite the secondary coalescence and the final goblet-shaped liquid jet form. Cavities are observed on the dense liquid jet column as a result of the coalescence on the upstream. Consequently, the droplet breakup occurs more frequently on the downstream liquid jet under the gas phase disturbance. The viscous shear is created by the aerodynamic interaction, and the regular fish-scale structure is presented under the Kelvin-Helmholtz instability, which promotes the bulge surface to break into droplets. The research reveals the dynamic mechanism of the annular energetic liquid jet structural destabilization observed in the previous experiments. The combination of the structural instability and the surface instability facilitate the primary breakup of the annular energetic liquid jet, which is beneficial to improve the atomization and the combustion performance.

1. Introduction
An annular energetic liquid jet injecting into a confined space is extensively used in the ordnance industry, such as the combustion systems of the gas turbine, the aerospace propulsion systems and the automotive engines [1,2]. As for the engine application, a rapid primary breakup of the energetic liquid jet has an important influence on the engine performance such as the fuel consumption rate and the exhaust gas cleanliness [3,4]. Study of the primary breakup of an annular energetic liquid jet injecting into a confined space is fundamentally important and still very challenging.

An annular energetic liquid jet primary breakup is a complex multiphase flow problem. An actual turbulent spray includes multi-scale physical processes. By the effect of the aerodynamic interaction, the liquid surface becomes unstable and ligaments are created from it. And then, droplets are created from these ligaments. This process is usually called the primary breakup. After the primary breakup, it is generally believed that large droplets may break into small droplets, known as the secondary breakup. The final droplet production is greatly dependent on the primary breakup [5]. To reveal its dynamic mechanism, experimental efforts by conducting observation on this dense and small region with high spatiotemporal resolution have been reported. By using the Laser Doppler Anemometry, Sheen et al. [6]...
examined both the confined and the unconfined annular swirling liquid jet flows. The results show that the central recirculation zone in the confined case is larger than that in the unconfined case. The flash X-ray research of Zhang et al. [7] indicates that the coalescence of the annular liquid jet injecting into a confined space will shift to the nozzle orifice by increasing the pre-pressure. Liu et al. [8] characterized the droplet sizes by using Laser Phase Doppler Analyzer. The results indicate that the mean diameter of the droplets is determined by the liquid pressure and the gas pressure. From these researches we know that the annular liquid jet have some distinctive features compared to the round liquid jet [9]. A prominent fluid dynamic characteristic of the annular liquid jet is the presence of two adjacent circular shear layers near the nozzle exit, compared to only one such shear layer in round liquid jet. And the annular liquid jet coalesce near the nozzle exit, after that the flow collapses at the downstream locations [10]. However, these researches are still insufficient to give an overall and thoroughly explanation on the primary breakup dynamics.

The researchers built different computational models based on the results of these experiments. For example, Ibrahim et al. [11] established the mathematical model of nonlinear instability and breakup of an annular liquid jet. Ahmed et al. [12] used temporal stability analysis to investigate the stability of an axially moving viscous annular liquid jet. However, these researches still cannot fully explain the coalescence mechanism of the annular liquid jet, and the primary breakup process is still unclear. The primary breakup of the annular liquid jets is an essential stage in the atomization process where new methods are still needed for further research.

Due to the lack of the primary breakup details, existing numerical spray models based on Reynolds Averaged Navier-Stokes Simulation (RANS) are with drastic simplifications, which would lead to poor predictions on the flow phenomena involving in the highly unsteady and complex vortex structures. Direct Numerical Simulation (DNS) is considered to be the most accurate method to investigate the primary breakup of a high speed liquid jet injecting into still air [13], but it needs huge amount of computation. In the last decade or so, many researches have adopted the Large Eddy Simulation (LES) approach to turbulence modelling in order to capture the unsteady effects on the interface dynamics, which can avoid the averaging in RANS and the computation in DNS. Örley et al. [14] performed LES to investigate the cavitating flow inside a 9-hole solenoid common-rail injector including liquid jet injection into gas during a full injection cycle. Wawrzak et al. [15] revealed the formation of the spiral structures located in the inner and outer mixing layers of an annular non-swirling jet by using LES. Therefore, LES can be a very powerful tool that leads to a better understanding of the primary breakup of an annular energetic liquid jet injecting into a confined space and a combination of the scientific research and the engineering application.

In this research, LES with Volume of Fluid (VOF) method was carried out to investigate the primary breakup dynamic mechanism of an annular energetic liquid jet injecting into a confined space. The gas vortex structure and the liquid jet formation were visualized by tracking the evolution of the phase velocity and the interface location, and hence the coalescence process of the goblet-shaped liquid jet from the annular liquid jet was reproduced. With sufficient grid resolution, ligaments and droplets formation can be captured in a physically sound way. Finally, a detailed analysis of the simulation results and a both qualitative and quantitative comparison between simulation predictions and experiments are given. The research reveals the dynamic mechanism of the annular energetic liquid jet structural destabilization observed in the previous experiments. The combination of the structural instability and the surface instability facilitates the primary breakup of the annular energetic liquid jet, which is beneficial to improve the atomization and the combustion performance. By the present simulation, a series of physical processes can be revealed.

2. Numerical model

2.1. Governing equations
In this calculation, the phase change between gas state and liquid state is not considered. The governing equations describing the primary breakup process of an annular energetic liquid jet injecting into a confined space consist of equations for mass, momentum and continuity for each of the phases:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]  

(1)

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{r} + \rho \mathbf{g} + \mathbf{F}_s
\]  

(2)

\[
\frac{\partial (\rho \mathbf{u}), \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}, \mathbf{u}) = 0
\]  

(3)

where \( \rho, \mu, t, \mathbf{u}, p \) and \( \mathbf{g} \) denote the density, the viscosity, the time, the velocity vector, the scalar pressure and the gravitational acceleration. \( F_s \) denotes the volumetric surfaces tension force. \( \alpha, \rho, \) and \( \mathbf{u} \), denote the volume fraction, the density and the velocity vector of phase \( i \), which are both defined in the VOF method.

2.2. Large Eddy Simulation (LES) theory

The LES is a theory between DNS and RANS, which based on a spatial filtering of the flow field to divide eddies groups into large scale and small scale [16]. The large scale eddies can be solved directly with the Navier-Stokes equation, while the influence of the small scale eddies on the large scale eddies can be dealt with an approximate model named the subgrid-scale (SGS) turbulence model. In the case of the annular energetic liquid jet injecting into the confined space, turbulent flows has a wide range of length and time scale, with the large scale eddies being generally more energetic than the small scale eddies. Therefore, it is more accurate to model only the small scale eddies with LES rather than to model all eddies with RANS. As mentioned above, this paper use the filter function \( G(x,x') \) to decompose the large scale field \( \tilde{\phi}(x) \) from the actual flow field \( \phi(x') \) in the form:

\[
\tilde{\phi}(x) = \int_{x'} \phi(x') G(x,x') dx'
\]  

(4)

where \( D \) denotes the computational fluid domain, \( x' \) is the spatial coordinates of the actual flow field, and \( x \) is the spatial coordinates of the large scale field after filtering.

For the SGS model, use the SGS stress \( \tau_i \) to denotes the SGS stress. It includes the effect of the small scales and defined by:

\[
\tau_i = 1/3 \delta_0 \tau_ii - 2\mu_{\text{SGS}} \overline{S_i}
\]  

(5)

where \( \tau_ii \) denotes the isotropic part of the SGS stresses, \( \delta_0 \) is the Kronecker delta, and \( \overline{S_i} \) is the strain rate tensor for the large scale. The SGS eddy viscosity \( \mu_{\text{SGS}} \) is modelled by the Smagorininsky-Lilly eddy viscosity [17] approach.

2.3. Volume of Fluid (VOF) method

The VOF method, first proposed by Hirt el at. [18], can model two or more immiscible fluids by solving a single set of momentum equation and tracking the volume fraction of each fluids throughout the domain. The prediction of the liquid jet breakup is a typical application. The energetic liquid is treated as the secondary phase. The liquid volume fraction \( \alpha \) works as an indicator to identify the different fluids. \( \alpha=1 \) corresponds to the case where the cell is full of liquid, \( 0<\alpha<1 \) corresponds to the case where the cell contains the interface between the liquid and gas and \( \alpha=0 \) corresponds to the case where the cell is full of gas. The density and the viscosity are interpolated by using \( \alpha \):

\[
\rho = (1-\alpha) \rho_g + \alpha \rho_i
\]  

(6)

\[
\mu = (1-\alpha) \mu_g + \alpha \mu_i
\]  

(7)

where \( \rho_g \) and \( \rho_i \) represent the density of gas and liquid, \( \mu_g \) and \( \mu_i \) represent the viscosity of gas and liquid.

The gas-liquid interface dynamic is resolved by using a Continuum Surface Force (CSF) model developed by Brackbill et al. [19], which represents the surface tension effect as a continuous volumetric
force acting within the region where the two phases coexist. The volumetric surface tension force $F_v$ is represented in a nonconservative manner as follows:

$$ F_v = \sigma \nabla \alpha $$

where $\sigma$ is the surface tension coefficient. The curvature of the interface $\kappa$ is defined by:

$$ \kappa = -\nabla \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right) $$

As a sharp resolution of the interface is crucial to calculate the surface tension force in the VOF method, one remedy to minimize the effect of the numerical diffusion is the use of so-called High Resolution Differencing Schemes, such as the Geometric Reconstruction Scheme, the Donor-Acceptor Scheme or the Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM). By comparing these three methods, Liu [20] considered that the CICSAM method has a higher accuracy. CICSAM is a high resolution differencing scheme, which is particularly suitable for the flows with high ratios of viscosities between the phases. This paper uses the same method.

3. Model validation

3.1. Computational domain and boundary conditions

A numerical simulation case was designed by reference to the experiment from Zhang et al. [7]. The computational domain and the grids that are consisted of an annular nozzle and a confined space are demonstrated in figure 1. The outer nozzle diameter is indicated by $d_1=9$mm while the inner diameter is shown by $d_2=8.6$mm, the nozzle length is $l=10$mm. Upstream of the nozzle is a tapered transition zone, which dimension refers to the experiment. The confined space is a cylindrical observation chamber with the observation chamber diameter $D=120$mm and the observation chamber length $L=120$mm. It is important to note that the pressure inlet condition is imposed on the upstream of the nozzle, the injection pressure $p_{in}=30$MPa. While the pressure outlet condition is imposed on the observation chamber downstream, the outlet pressure $p_{out}=1$MPa. The non-slip condition is prescribed for all the other walls. Since the crushing mainly occurs near the liquid jet column, a non-uniform mesh has been used to dense the mesh near it.

![Figure 1. The computational domain and the grids.](image)

At the initial moment, the chamber is full of air at a pressure of 1Mpa and the nozzle is filled with kerosene as the injected liquid at a pressure of 30Mpa. In VOF, let the gas phase be the first phase and the liquid phase be the second term. The flow properties are summarized in Table 1.

**Table 1.** The fluid properties.

| Phase | Material | Density $\rho$ (kg m$^{-3}$) | Dynamic viscosity $\mu$ (kg m$^{-1}$s$^{-1}$) | Surface tension coefficient $\sigma$ (N m$^{-1}$) |
|-------|----------|-----------------------------|----------------------------------------|-----------------------------|
| Gas   | Air      | 12.3                        | 1.89$\times$10$^{-5}$                  |                             |
| Liquid| Kerosene | 804                         | 2.76$\times$10$^{-3}$                  | 0.028                       |

Through the verification of the grids independence, it is found that the number of the grids has little influence on the liquid jet velocity and the liquid jet column crushing process, but the small droplets generated after the liquid jet column crushing can only be captured when the number of grids is large.
In this case, the number of the grids is $10^7$, so the gas-liquid interface can be effectively captured. All the residuals tolerances are set to $10^{-6}$ and the time step is $10^{-8}$s. The governing equations are solved within the OpenFOAM on a dual E5-2680V2 workstation.

3.2. Validation of simulation results

By tracking the evolution of the phase velocity and the interface location, the gas vortex structure and the annular energetic liquid jet formation are visualized in this paper. The main features of the annular liquid jet are captured in the simulation results, hence the coalescence process of the goblet-shaped liquid jet from the annular liquid jet is reproduced. At the same time, the process of the droplets shedding due to the instability of the liquid jet surface can also be captured. In Zhang’s study, the shadow photographic method was used to capture the atomization field and X-ray photography was used to capture the shape of the liquid dense region. Figure 2 shows the comparison between the simulation results and the experiment results using the shadow photographic method, and Figure 3 shows the comparison of the X-ray photography. In the simulation results, the isosurface of the instantaneous liquid volume fraction $\alpha=0.05$ is used to represent atomization field, and the colors represent the velocity. According to the comparison, the maximum velocity of the liquid jet head in the simulation results is about 164m/s, which is 4.5% different from the maximum velocity of 157m/s measured in the experiment. The spray angle in the simulation results is 15.1°, 3.4% different from that 14.6° obtained in the experiment results.

Zhang found that the annular energetic liquid jet has the tendency to continuously converge towards the centerline and finally forms a cylindrical liquid jet. There are a large number of bubbles inside the liquid jet column. The simulation results in Figure 3 show the phenomenon of coalescence in detail. It
is clear that the annular liquid jet column exhibits formation of a goblet-shaped liquid jet near the nozzle exit with the gas phase inside it. In Figure 2(b) \( t=1120\text{us} \), the annular liquid jet has a strong mixing with the ambient environment in the confined space. The simulation results are in good agreement with the experimental results, and better than the experimental results observations in the detail of structure characterization.

4. Simulation results and discussions

4.1. Liquid jet coalescence process

Figure 4 shows that the liquid jet head deforms from 40us to 250us after the start of the annular energetic liquid jet injecting into the confined space. The contour map on the left represents the liquid phase volume fraction \( \alpha \) on the axis profile, while the isosurface of the liquid volume fraction \( \alpha = 0.05 \) of the upwind surface with colors on the right represent the velocity. Because of the different densities of the liquid jet and the still air, the liquid jet head is sheared by the high density air. The Rayleigh-Taylor (RT) instability appears on the surface of the liquid jet head, which generate the RT instability waves on the upwind surface. As a result, the liquid jet head starts to roll over from the center, forming the so-called mushroom-shaped cap. At the same time, the inner diameter of the annular liquid jet shrinks sharply, and the liquid jet has the tendency to converge continuously towards the centerline near the nozzle exit. At \( t=250\text{us} \), the first coalescence of the jet occurs, as in Figure 4(d). The first coalescence is caused by the RT instability, which is generated by the interaction between the jet head and the gas in the confined space.

![Figure 4](image)

**Figure 4.** The liquid jet head deforms from 40us to 250us.

After the first coalescence, the liquid jet head converges at the centerline and forms a cylindrical liquid jet column. The instantaneous velocity vector plots at \( t=250\text{us} \) and \( t=350\text{us} \) are shown in Figure 5, the contour line for the liquid volume fraction \( \alpha = 0.5 \). It can be seen that two kinds of large-scale vortex structure developed naturally in the confined space without external perturbations: a large-scale vortex structure in the recirculation zone close to the nozzle exit and the other large-scale vortex structure between the liquid jet surface and the wall of the confined space. This formation of the recirculation zone close to the nozzle exit is a common feature of annular liquid jet flow. It is shown that because of the existence of two adjacent shear layers which are caused by the two large-scale vortex structures, the annular liquid jet flow is highly unstable and causes the secondary coalescence. After the secondary coalescence, not only the liquid jet head coalesces, but the annular liquid jet inner surface is pressed together, which gradually became goblet-shaped liquid jet. With the development of the liquid jet, the coalescence point moves toward the direction of the nozzle, the stem of the goblet-shaped become longer and longer, as Figure 5(b) \( t=350\text{us} \). The annular liquid jet converges into a cylindrical liquid jet further downstream of the computational domain and it spreads in the cross-stream direction when the convergence is taking place. The secondary coalescence and the final goblet-shaped liquid jet is expedited by the large-scale vortex structures.
4.2. Liquid jet primary breakup

With the isosurface of the liquid phase volume fraction $\alpha=0.95$ represents the liquid jet column, Figure 6 shows the fully developed annular liquid jet column at $t=1200\text{us}$. Due to the instability of liquid jet structure caused by coalescence, which makes the liquid jet column unstable and liquid shedding. It can be seen that a lot of cavities on the liquid jet column. The black box I marks the surface waves near the nozzle exit, which are impacted by the Kelvin-Helmholtz (K-H) instability. In the recirculation zone inside the liquid jet, the same instability wave can be found as also. In the process of forward propagation, the wave length and amplitude of the instability waves inside and outside the liquid jet increase continuously. Near the coalescence point, the amplitude reaches the maximum, the liquid jet column is torn into pieces. After the coalescence point, cavities are observed on the dense liquid jet column instead of the instability waves, as the black box II in Figure 6. The more close to the downstream, the more sufficient the atomization is, and the more complicated the atomization process becomes. The droplet breakup occurs more frequently on the downstream under the gas phase disturbance, as the black box III.

Figure 7 shows the liquid jet surface at $t=1200\text{us}$, the isosurface of the liquid phase volume fraction $\alpha=0.05$. With the strong primary breakup of the liquid jet surface, the annular liquid jet is widely used.
Figure 7. The liquid jet surface at t=1200us.

5. Conclusion
The LES combined with the VOF method has been implemented to investigate the primary breakup dynamic mechanism of an annular energetic liquid jet injecting into a confined space. The gas vortex structure and the liquid jet formation were visualized by tracking the evolution of the phase velocity and the interface location, and hence the coalescence process of the goblet-shaped liquid jet from the annular liquid jet was reproduced. The simulation results can effectively capture the detailed structure of the annular energetic liquid jet primary breakup, such as the surface wave development, the surface crushing and the liquid jet head crushing, etc., which are consistent with the experimental results available in literature. The simulation results indicate that the first coalescence is caused by the Rayleigh-Taylor instability, which is generated by the interaction between the liquid jet head and the gas in the confined space. The annular liquid jet flow is characterised by a recirculation zone adjacent to the nozzle exit. Two kinds of large-scale vortex structure expedite the secondary coalescence and the final goblet-shaped liquid jet. Cavities are observed on the dense liquid jet column as a result of the coalescence on the upstream. Consequently, the droplet breakup occurs more frequently on the downstream under the gas phase disturbance. The viscous shear is created by the aerodynamic interaction at the upstream, and the regular fish-scale structure is presented under the K-H instability, which promotes the bulge surface to break into droplets. The research reveals the dynamic mechanism of the liquid jet structural destabilization observed in the previous experiments. The combination of the structural instability and the surface instability facilitate the primary breakup of the annular energetic liquid jet, which is
beneficial to improve the atomization and the combustion performance. The proposed simulation methodology can be helpful for predicting the behavior of the liquid jet used in the spray combustion systems, since these applications focus on the degree of the energetic liquid jet breakup. In order to simplify the problem, cavitation inside the nozzle was ignored in this calculation. The next step is to study the turbulent cavitation inside the nozzle, which makes the calculation closer to the actual situation.

References
[1] Shen J and Li X 1996 Acta Mech. 114(1) 167-83
[2] Ryzhenkov V O, Abdurakipov S S and Mullyadzhanov R I 2019 J. Phys.: Conf. Ser. 1359 012012
[3] Som S, Ramirez A I, Longman D E, and Aggarwal S K 2011 Fuel 90(3) 1267-76
[4] Lü M, Ning Z and Yan K 2019 Nonlinear Dynam. 97(2) 1263-73
[5] Müller T, Snager A, Habislreuther P, Jakobs T, Trinis D, Kolb T and Zarzalis N 2016 Int. J. Multiphas. Flow 87 212-28
[6] Sheen H J, Chen W J and Jeng S Y 1996 AIAA J. 34(3) 572-9
[7] Zhang Y R, Jin Z M and Yu Y G 1999 Journal of Aerospace Power 1999, 14(04) 409-12
[8] Liu K, Yu Y G and Zhao N 2015 Acta Armamentarii 36(10) 1882-87
[9] Zhang Y R, Jin Z M, Li B M and Yu Y G 2000 Acta Armamentarii 21(01) 75-6
[10] Ibrahim E A and Mckinney T R 2006 P. I. Mech. Eng. C 220(220) 203-14
[11] Ibrahim A A and Mckinney T R 2006 P. I. Mech. Eng. C 220(220) 203-14
[12] Ahmed Z U, Khayat R E, Maissa P and Mathis C 2012 Fluid Dyn. Res. 44(3) 1-23
[13] Shinjo J and Umemura A 2010 Int. J. Multiphas. Flow 36(07) 513-32
[14] Örley F, Hickel S, Schmidt S J and Adams N A 2015 J. Phys.: Conf. Ser. 656 012097
[15] Wawrzak K, Boguslawski A, Tyliszczak A and Saczek M 2019 Int. J. Heat Fluid Fl. 79 1-12
[16] Leonard A 1974 Adv. Geophys. 18 237-48
[17] Smagorinsky J 1963 Mon. Weather Rev. 91 99-165
[18] Hirt C W and Nichols B D 1981 J. Comput. Phys. 39(1) 201-25
[19] Brackbill J U, Kothe D B and Zemach C 1992 J. Comput. Phys. 100(2) 335-54
[20] Liu R X, Liu X P, Zhang L and Wang Z F 2004 Applied Mathematics and Mechanics 25(03) 279-90