Numerical and Experimental Studies of Cavitation in Hydrolysis Reaction that Breaks Palm Oil into Fatty Acids and Glycerol

Harie S. Jaya, I.N.G. Wardana , Nurkholis H., Denny W

***Abstract* – The cavitation is created in complex and changeable physical phenomena, such as high speed, high pressure, multiple phases, phase transition, turbulence, and unstable features. Thus, the vapor fraction and pressure distribution have always been key problems in determining cavitation behavior and its role on the hydrolysis reaction. The aim of this study is to analyze the effect of water cavitations at various pressures on the hydrolysis reaction that breaks the oil into fatty acids and glycerol. Numerical simulations are performed to determine the flow-field characteristics of both inside and outside the nozzle of a submerged water jet. The factors that influence the cavitation intensity of pressure are simulated. The cavities were generated by injecting water via a nozzle into palm oil in the helle shaw cell, with volumes of 3ml at pressures varying between 2, 6, 10, and 16 MPa. Glycerol formed by the reaction in this study, prove that the cavitation generated energy greater than the energy of ester bond between carbon and oxygen. The turbulence kinetic energy plays important role in determining the cavitation energy.**

***Index Term*-- numerical simulation,vegetable oil, hydrolysis, hydrodynamic cavitation.**

Nomenclatures

k	kinetic energy per unit mass (J/kg,Btu/lb_m)
ε	turbulence dissipation rate (m^2/s^3,ft^2/s^3)
u	axis velocity
v	radial velocity
ρ	density
G_k	generation of turbulence kinetic energy due to mean velocity gradien
G_k	generation of turbulence kinetic energy due to bouyancy
Y_M	contribution of the fluctuating dilatation in compresible turbulence to the overall dissipation rate
α_k	inverse effective Prandtl number for k
α_ε	inverse effective Prandtl number for ε
S_k	user-defined source terms for k
S_ε	user-defined source terms for ε
$C_{1\varepsilon}$	constant
$C_{2\varepsilon}$	constant
$S_\emptyset$	source term of the $\emptyset$ equation

I. INTRODUCTION

Many research and effort has already been done for observing and visualizing cavitations jets in order to elucidate their role on hydrolysis reaction of vegetable oil so that the use of catalyst can be reduced. However, fundamental research on the relation between cavitation behavior and impulsive -pressure distribution is very rare. This fact hinders further improvement of hydrolysis process using submerged jet.

An increasing demand for the development and validation of the computational fluid dynamics (CFD) of numerical models has emerged in literature. This demand, along with the continuing efforts to obtain better experimental information under the most realistic conditions possible, has given rise to the simulation of the formation and development of cavitation in a water jet from a nozzle into oil pool under high impulsive pressure.

Surin et.al [1] conducted an experimental study of the discharge of a gas jet from a nozzle and its developmetnt in a liquid. The study is focused on the dynamics of gas jet in a liquid, the structure of the region of interaction, and the regimes of discharge from the submerged nozzle with different degrees of gas assimilation. Deshpande et al. [2] developed a solution based on the two-dimensional (2D) Navier-Stokes equations. The energy equation uses artificial compressibility and pseudo-time stepping techniques to model the thermodynamic effects of sheet cavitation in cryogenic fluids, which could be used to examine individual bubbles.

Yuan et al. [3] performed a numerical simulation of cavitation phenomena, including the growth and collapse of bubbles inside an injector nozzle, using a k-ω turbulence model. Srinivasan et al. [4] recently developed a novel modeling approach capable of simultaneously tracking cavitation events occurring within an injector nozzle with the random number generator (RNG) κ-ε turbulence model. This model includes new source terms from cavitation-induced turbulent kinetic energy production and dissipation.

Lu et al. [5] investigated the applicability of the standard κ-ε, RNG κ-ε, and standard k-w turbulent models for cavitation in a water jet field through a convergent-divergent nozzle. The result of Lu et al indicates that the RNG κ-ε turbulence model is the most suitable for the simulation of cavitation behavior. Zhang et al.[6] report that the submerged cavitation jets can induce cavitation both inside and outside a conical nozzle and a convergent-divergent nozzle when the inlet pressure is 32 MPa. Moreover, the shock wave pressure induced by the collapse of the bubble group reaches up to 300 MPa.

Therefore , the aim of this study was to analyze the effect of cavitations at various pressures on the liquid to liquids

Harie S. Jaya , Doctoral Student at Mechanical Engineering, Brawijaya University, Jl. MT. Haryono 167, Malang 65145, Indonesia and lecturer at Department of Mechanical Engineering Education, Palangka Raya University, Jl. Yos Sudarso, Tunjung Nyaho, Palangka Raya 73112, Indonesia
(harysatiyadi@gmail.com)
ING Wardana is a supervisor and Professor at Mechanical Engineering, Brawijaya University, Jl. MT. Haryono 167, Malang 65145, Indonesia
(wardana@ub.ac.id)

reaction that breaks the oil into fatty acids and glycerol. For numerical simulations, ansys fluent was used to simulate cavitation behavior inside and outside the nozzle. The cavitation behavior induced by the nozzle with different inlet pressure values was also investigated. To validate the process capability of the cavitation jet, was compared with experimental results.

II. EXPERIMENT

Crude palm oil used in this study is a mixture of about 92 to.95% oil, upto 5% free fatty acids (FFA) and about 0.5% water, water soluble and solids. Generally the oil is made up of triglyceride (94-97%), diglyceride (2-3.5%) and monoglyceride (0.3-0.5%).The experimental set up is shown schematically in figure 1. From the tank water was vertically injected through the nozzle into the open top helle shaw cell containing the palm oil with volumes of 3 ml. As water passes through a nozzle of 1mm diameter, cavities was formed at high jet speed due to the pressure drop called hydrodynamic jet cavitations. The cavitations that occurred in the helle shaw cell were recorded using a Casio ZR-200 high speed camera and the result was compared and evaluated with simulation result using ansys fluent. The experiments were conducted at ambient pressure and room temperature.

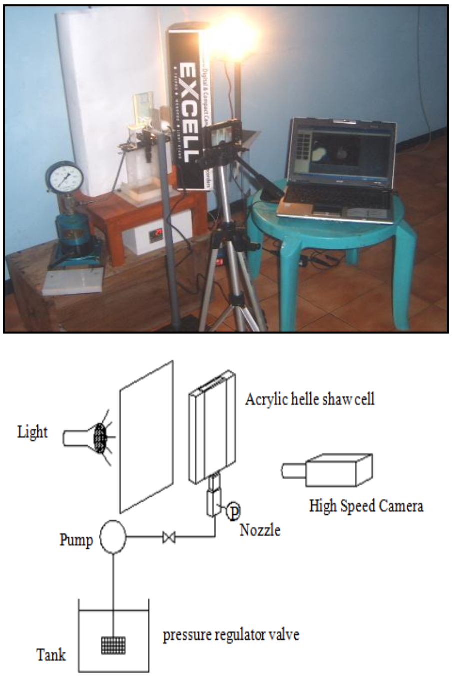

Fig.1. Experimental Set Up

III. MATHEMATIC MODEL

A. Governing Equations

The RNG based k - ε turbulence model is derived from the instantaneous Navier-Stokes equations, using a mathematical technique called “renormalization group” (RNG) methods. The analytical derivation results in a model with constants different from those in the standard k - ε model, and additional terms and functions in the transport equations for k and ε. Transport equations for the RNG k-ε model as follow :

$$\frac{\partial}{\partial_t}(\rho k)+\frac{\partial}{\partial_{x_i}}(\rho k u_i)=\frac{\partial}{\partial_{x_j}}\left(\alpha_k u_{eff}\frac{\partial k}{\partial_{x_j}}\right)+G_k+G_b-\rho\varepsilon-Y_M+S_k \quad (1)$$

$$\frac{\partial}{\partial_t}(\rho\varepsilon)+\frac{\partial}{\partial_{x_i}}(\rho\varepsilon u_i)=\frac{\partial}{\partial_{x_j}}\left(\alpha_\varepsilon u_{ef}\frac{\partial\varepsilon}{\partial_{x_j}}\right)+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+G_{3\varepsilon}G_b)-C_{2\varepsilon}\frac{\varepsilon^2}{k}-R_\varepsilon+S_\varepsilon \quad (2)$$

The 2D flow model of the incompressible fluid with the *k-ε* turbulence model under an axial symmetrical cylindrical coordinate is given by Deng et.al [7] as:

$$\frac{1}{r}\left[\frac{\partial}{\partial_x}(r\rho u\emptyset)+\frac{\partial}{\partial_r}(r\rho v\emptyset)\right]=\frac{1}{r}\left[\frac{\partial}{\partial_x}\left(r\Gamma_\emptyset\frac{\partial_\emptyset}{\partial_x}\right)+\frac{\partial}{\partial_r}\left(r\Gamma_\emptyset\frac{\partial_\emptyset}{\partial_r}\right)\right]+S_\emptyset \quad (3)$$

B. Solution Procedure

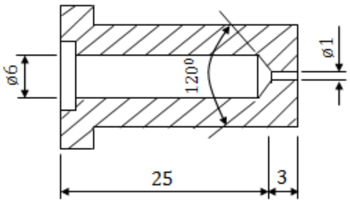

Fig. 2. Nozzle dimensions

Appropriate initial and boundary conditions are needed to solve the Navier-Stokes equations and to make the result reliable. Initial and boundary conditions can have significant influence on the results. Therefore, the initial and boundary conditions should be as realistic as possible. In this simulation, two-phase fluid is assumed to be the initial condition with three material: palm oil as primary phase, water liquid and water vapor as secondary phase. For the present computations, mixed model with three numbers of eulerian phases and the random number generator RNG *κ–ε* is adopted with a standard wall function to calculate the cavitation flow field. The boundary conditions of the wall are impermeable and no-slip for velocity. The phases interaction using mass transfer mechanism from water liguid to water vapor with schnerr-sauer cavitation model with constant vaporization pressure of 3540 Pa.

IV. NUMERICAL SIMULATION

A. Physical modeling

In this study, water with a room temperature is pressurized using a high-pressure piston pump. The pressurized water is injected via nozzles into the palm oil in helle shaw cell, thus forming the submerged cavitation jet. Large, uniform bubble clouds can then be generated. The bubbles that collapse on crude palm oil will produce a similar effect. The physical model of the working zone is simplified to simulate cavitation behavior, as shown in Fig. 3.

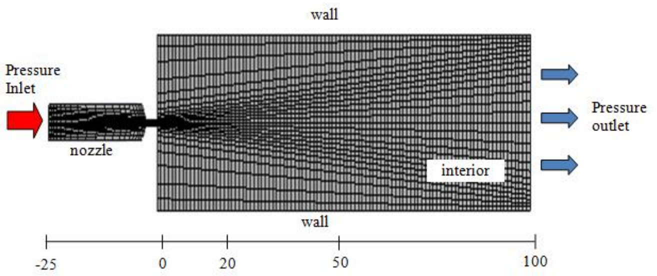

Fig. 3. meshing

The computational domain and the structured grid system are created using ansys fluent, as shown in Fig. 3. The computational domain is 100 x 30 mm. The atmospheric pressure at the outlet is 101325 Pa. The meshed flow domain includes the nozzle and the experimental cavitation cell. The grids have to be locally refined in the areas of nozzle contraction, diffusion, and exit. Governing equations are discretized with a first-order upwind. After the initial analysis, 68856 quad meshes are adequate to meet the requirement.

B. *Boundary conditions*

The model is simplified according to the process parameters and the actual environmental conditions in the liquid to palm oil experiment process. The following boundary conditions were applied: (1) The working temperature is 30°C during the process. (2) The wall is assumed to be adiabatic and convective heat transfer does not occur with the surrounding space. (3) Turbulence is specified using intensity and length scale. (4) The process is assumed to be static because the growth and collapse of the cavitation bubble traveling along the flow are not considered.

The RNG κ–ε turbulence model with standard wall functions and differential viscosity model was used to simulate the cavitation jet induced by pressure drop in the nozzles. The cavitation behavior induced by the nozzle with various inlet pressure of 2,6,10 and 16 MPa and the outlet boundary condition is outlet pressure of 101325 Pa.

V. NUMERICAL SIMULATION RESULTS

A. *Comparison of experiments and simulations*

It can be seen from figure 4 that the jet evolution from simulation result agrees reasonably well with the experimental result at 2 MPa. This suggests that the simulation method is acceptable for analyzing the cavitation phenomena of this study.

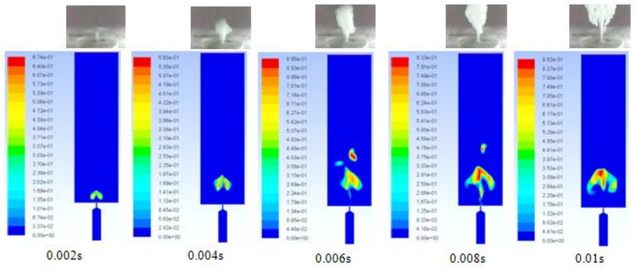

Fig. 4.Comparison of flow visualization experiments and CFD results at 2 MPa

B. *Cavitation Behavior*

The kinetic energy, 1/2 mv^2 generated from water injection into helle shaw cell gives a pressure drop at the nozzle exit. When the pressure drops below the saturated vapor pressure of water (which is equal to 4247 Pa at a temperature of 30^0C) the water liquid changes into vapor phase at a constant temperature.

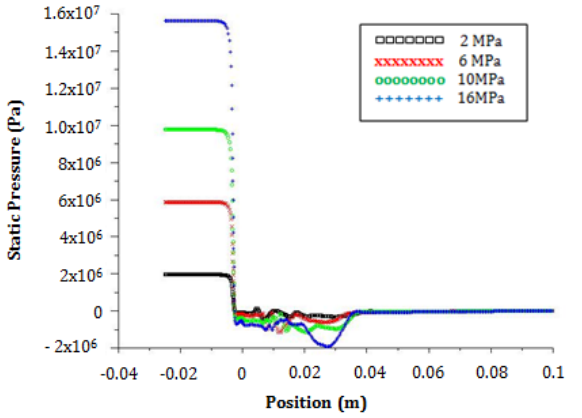

Fig. 5. Distribution of static pressure at various pressure along the axis direction

The surface tension then forms the vapor into cavitation. The characteristics of static pressure drop at the nozzle exit at various inlet pressure is shown in figure 5. It is seen that the higher the inlet pressure, makes the static pressure at the nozzle exit tends to drop lower than zero. The negative pressure fluctuation between 0 and 0.04 m indicates that cavitations are produce effectively at that region.

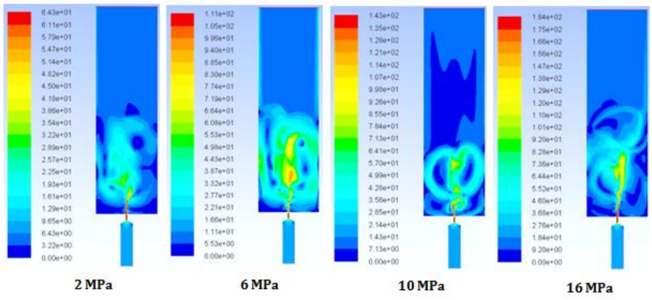

Fig. 6. Distribution of velocity of cavitation field at various inlet pressure

The distribution of the flow velocity at various inlet pressure is shown in figure 6. A potential core region in the flow field is found in the outlet zones of the nozzles. The velocity is suddenly reduced at the end of the potential core region. Moreover, an obvious change in the velocity gradient normal to the direction of the jet flow is also observed.

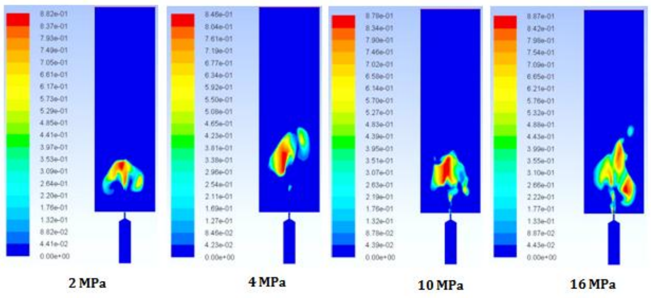

Fig. 7. Distribution of vapor phase volume at various pressure

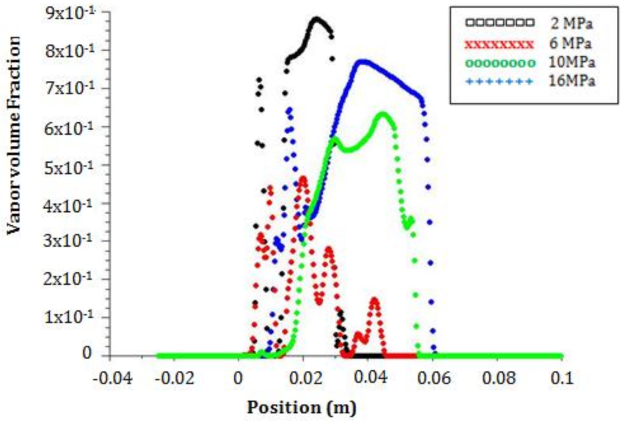

Fig. 8. Distribution of vapor volume fraction at various pressure along the axis direction

The distribution of vapor-phase volume in helle shaw cell and nozzles is shown in Fig. 7. An obvious cavitation phenomenon occurred in the helle shaw cell. It is found that the vapor fraction is fluctuated, 0.90 at 2 MPa, 0.48 at 6 MPa, 0.64 at 10 MPa and 0.80 at 16 MPa. The distribution of vapor-phase volume along the axial distance of the helle shaw cell is shown in Fig. 8. The maximum vapor fraction is found in the expansion area. In addition, the sudden increase and decrease in vapor fraction respectively represent the growth and collapse of bubbles in the nozzle.

C. *Cavitation behavior at various pressures*

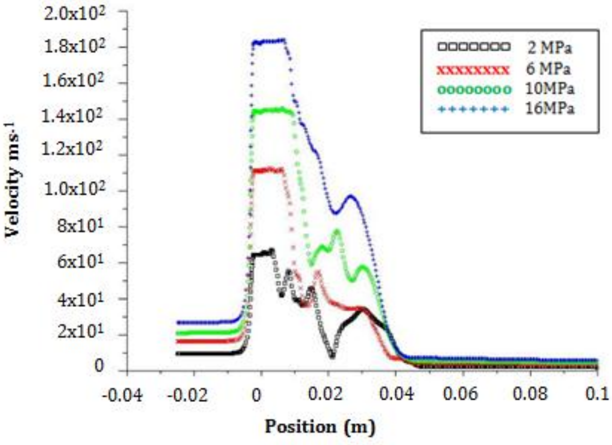

Fig. 9. Axial distribution of velocity at various pressure along the axis direction

Figure 9 shows the axial jet velocity distribution. The nozzle exit position is at 0 m. The outlet pressure is constant at 101325 Pa. The axial boundary condition is $\nu = 0$. The temperature of the working liquid is 30° C. A large flow velocity gradient is found in the nozzle. The velocity along the axis direction obviously increases with increasing inlet pressure.This indicates that increasing inlet pressure can promote the high velocity. The velocity fluctuates during deceleration which means that the turbulence energy is produced during deceleration period.

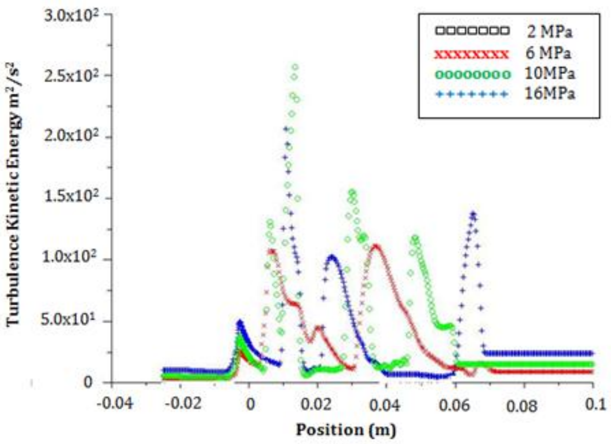

Fig. 10. Distribution of Turbulence Kinetic Energy at various pressure along the axis direction

Figure 10 shows the axial distribution of turbulence kinetic energy. The turbulence kinetic energy (TKE) is the mean kinetic energy per unit mass associated with eddies in turbulent flow. Physically, the turbulence kinetic energy is characterized by the root-mean-square (RMS) of velocity fluctuations. TKE can be produced by fluid shear, friction or buoyancy, or through external forcing at low-frequency eddy scales (integral scale). It can be seen from figure 10 that the highest TKE is produced at 0.01m. At the region the velocity decrease (deceleration) is the highest (Fig. 9). The maximum turbulence kinetik energy is 2600 m^2/s^2 at 10 MPa. This is due to the fact that at 10 MPa velocity decelerates largely at 0.01 m.

VI. DISCUSSION

A. Effect of Energy Cavitation

As discussed in [8], the minimum work required to create a sphere of vapor of radius R in the liquid is $4/3\,\pi R^3(P-P') + 4\pi R^2\sigma$ where P' is the pressure at which the vapor is at the same chemical potential as the liquid at static pressure P, and σ is the liquid–vapor surface tension. Far from the critical point, $P' - P = P_{sat}(T) - P$. The first term in equation gives the energy gained when forming a volume of the stable phase, where as the second term is the energy cost associated with the creation of an interface. Their competition results in an energy barrier, $E_b = (16\pi/3)\ (\sigma^3/(P'-P)^2)$ reached for a critical bubble of radius $R_c = 2\sigma/(P' - P)$. It is seen at figure 5 that P drops to negative between 0 m and 0.04 m. When P becomes more negative, the energy barrier or cavitation surface tension is larger. At that condition the hydrolysis reaction rate might be higher.

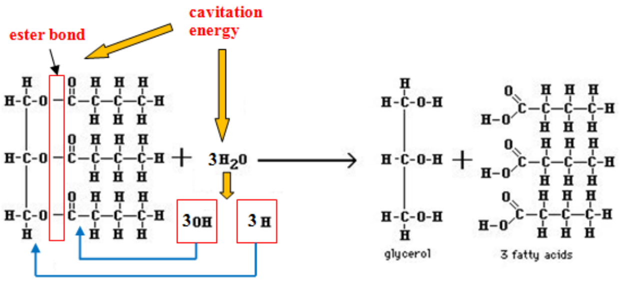

Fig. 11. The work of cavitation energy on hydrolysis

Cavitation energy is used to dissociates $3H_2O$ into 3H and 3OH and break the ester bond C - O in crude palm oil triglyceride to form glycerol and three fatty acids, as shown in figure 11. The carbon and oxygen ester bond is a single bond with an average length and bonding strength is 143 pm and 358 kJ / mol respectively. Glycerol produced from the reaction in the experimental work of this study (Fig. 12) proves that the cavitation generated energy greater than the energy bond between carbon and oxygen.

B. *Glycerol Production at the experimental work*

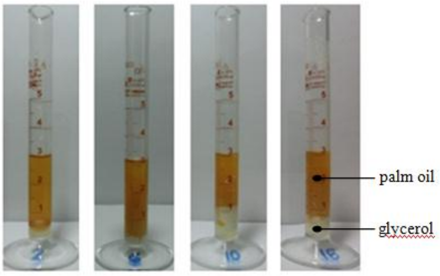

Fig. 12. Sediment formed at 2,6,10 and 16 MPa

The results of the experimental work were poured into the measuring cup to measure the glycerol production as shown in Figure 12. Yellow liquid in a measuring cup is crude palm oil (CPO) while glycerols which is transparent white color are at the bottom of the palm oil due to its density (1,261 kg/m^3) is greater than the palm oil density (0.913 kg/m^3).

The larger glycerol production was obtained at 10 Mpa though the higher surface tension of the cavitation estimated based on the equation from [18] takes place at 16 MPa due to the higher pressure drop. As presented in figure 10, the turbulence kinetic energy is the highest at 10 MPa due to the largest deceleration at 0.01 m. The highest turbulence kinetic energy corresponds to the highest glycerol production at 10 MPa. Therefore, it can be deduced from these results that the turbulence kinetic energy plays dominant role in cavitation energy.

VII. CONCLUSION

Both the experimental studies and numerical simulations in this paper were performed to facilitate further understanding of cavitation behavior in the hydrolysis reaction of palm oil. Ansys Fluent was used to simulate water cavitation behavior both inside and outside the nozzle. The conclusions are as follows:

- The RNG κ-ε turbulence model is suitable for simulating the water cavitation behavior in the flow field, including velocity, vapor fraction, turbulence kinetic energy both inside and outside the nozzle.
- Different inlet pressure values are also key factors that influence the intensity of the cavitation phenomenon when the outlet pressure remains unchanged.
- Simulation and experimental work results show that turbulent kinetic energy plays important role determining the cavitation energy that breaks the palm into glycerol and fatty acids. From this perspective, the experimental results and numerical simulation results show a good consistency.

ACKNOWLEDGEMENTS

The author is deeply grateful to Professor I.N.G. Wardana PhD (Supervisor) for encouraging and supporting this research program, and to the co-supervisor (Dr.Eng Nurkholis and Dr.Eng Denny W.) for assisting the fluid dynamic simulation.

REFERENCES

[1] Surin, V.A., Evchenko, V.N and Rubin, V.M.(1983),"Propagation of a gas jet in a liquid,"*Journal of Engineering Physics*, ,45:1091-1101.

[2] M. Deshpande, J. Feng and C.L. Merkle (1997) Numerical modeling of thermodynamic effects of cavitation, *AMSE Journal ofFluids Engineering* 119, 420–427.

[3] W. Yuan, J. Sauer and G.H. Schnerr (2000). Modeling and computation of unsteady cavitation flows in injection nozzles, in: *1st International Colloquium on Microhydrodynamics*, Paris, France

[4] V. Srinivasan, A.J. Salazar and K. Saito (2010), Modeling the disintegration of cavitating turbulent liquid jets using a novel VOF-CIMD approach, *Chemical Engineering Science* 65 2782–2796.

[5] Y.Y. Lu, X.C. Wang andY. Kang (2009), Simulation of cavitation jet flow in a convergent-divergent nozzle water jet, *Journal of China University of Petroleum* 33(6) 57–60.

[6] H.Zhang,B.Han,X.G.Yu and D.Y.Ju (2013) Numerical and experimental studies of cavitation bahavior in water-jet cavitation peening processing, *Journal Shock and Vibration* 20895-905

[7] S.S. Deng, Y.H. Shen and Z.J. Li (2008) Numerical simulation on internal flow field in nozzle with cavitations water jet, *Journal of Logistical Engineering University* 24(2), 57–60.

[8] Frédéric Caupin , Eric Herbert, (2006) Cavitation in water: a review , *Académie des sciences. Published by Elsevier Masson SAS. C. R. Physique 7 1000–1017*

Harie S. Jaya received the B.S. degree in mechanical engineering from Widya Gama University, Malang, Indonesia, in 2000 and the M.S. degree in mechanical engineering from Institut Sepuluh November, Surabaya, Indonesia, in 2010. I am currently pursuing the Doctoral degree in mechanical engineering at Brawijaya University, Maleng, Indonesia. From 2006 until now he was a lecterur in Mechanical Engineering Education at Palangka Raya University, Palangka Raya, Kalimantan Tengah, Indonesia.

Prof. Ir. ING Wardana M.Eng.,PhD received the B.S. degree in mechanical engineering from Brawijaya University, Malang, Indonesia, in 1983 and the M.S. degree in Keio University Yokohama Japan, in 1988. Ph.D. degree in mechanical engineering from Keio University Yokohama Japan, in 1994. From 1983 until now , he has been a Professor at Mechanical Engineering Department, Brawijaya University. In 2006-2007, he was

Extraordinary Professor in Faculty of Science & Technology, Keio University, Yokohama, Japan. And 2011 until now join PhD Supervision with Prof. Aizawa form Shibaura Institute of Technology Japan.
. He is the author of more than 100 articles and hold a pengkabut cawan berputar paten . His research interests include advance Technology for Bio-fuel, Biomechanics, Biochemistry and Biomedical Engineering, hydrogen Technology.

Dr. Eng. Nurkholis Hamidi ST.,M.Eng received the B.S. degree in mechanical engineering from Brawijaya University, Malang, Indonesia, and the M.S. degree and Doctor in Kyushu Institut of Technology eio University Yokohama Japan, in mechanical engineering.
From 1999 until now , he has been a lecturer at Mechanical Engineering Department, Brawijaya University. His research interests include freezing technology,advance Technology for Bio-fuel, Biomechanics and Biochemistry.

Dr.Eng. Denny Widhiyanuriawa ST.,M.T received the B.S. degree in mechanical engineering from Brawijaya University, Malang, Indonesia, and the M.S. degree from Gadjah Mada University, Yogyakarta, Indonesia and Doctor in Pukyong National University, Busan, South Korea in mechanical engineering. From 200 until now , he has been a lecturer at Mechanical Engineering Department, Brawijaya University. His research interests include mechanical technology,advance Technology for Bio-fuel, Biomechanics and Biochemistry