Simplified model for predicting the onset of multicomponent droplet microexplosion

Xinyi Huang

Microexplosion is an important phenomenon which will happen during the process of heating, and is very important for combustion progress. A simplified model for predicting the onset of microexplosion can help design combustors properly.

Literature review

Microexplosion is the rapid disintegration of a multicomponent droplet caused by the evaporation of a lower boiling point component [1]. It can happen to emulsified droplets, where water is much easier to evaporate than the fuels. This process is widely observed in all kinds of experiments. Gravity does not decide the occurrence of microexplosion, and microexplosion has been observed during both the Leidenfrost effect [4] and the microgravity environment [9]. Both experiments show that there should be phase separation before the droplet explodes. The insolubility of water and fuel makes this process much easier. Microexplosion can also happen to soluble fuels, where appearance of gas bubble due to nucleation [10] enables the breakup of the droplet. However, such reports are few and microexplosion of this kind is described by Wang et al. [10] as "distillationlike". It shall attribute to the great boiling point difference among the fuel components.

Microexplosion has shown its great significance through enhancing the efficiency of combustion and reducing the production of NO_x. The secondary atomization of the droplet is also strengthened and this means longer penetration and better evaporation [8] in fuel sprays. In the meantime, water evaporation of emulsified droplets reduces local temperature, thus helps soot reduction. The control of microexplosion becomes an important problem.

The experiments have inspired some efforts on predicting the onset of microexplosion and the size distribution of secondary droplets. Among these, Law's superheat criterion [3] and Chia-fon Lee's perturbation criterion [2] are the most detailed and solid models, especially when the focus is on the onset of microexplosion. Law's superheat criterion is based on the nucleation process inside the water sub-droplets of emulsified fuels. The assumptions involve the existence of homogeneous water component. Thus, it totally ignores the physical process of gas bubble formation. Also, the only criterion using droplet temperature leads to the limitation of model prediction. Instead, Chia-fon Lee's model intrinsically includes the existence of gas bubble and the liquid phase. Dynamically, the bubble growth and its instability eventually leads to its explosion. The variation of ambient temperature and pressure directly changes the heat and mass transfer. Similar analysis enables the prediction of the onset time and condition of droplets.

Model building

Since the whole model is based on the work of Chia-fon Lee's group, we would like to make it clear how it works. Using the equations of momentum, temperature and diffusion, assuming the droplet and all its properties and process are all homogeneous, the equations can be simplified into 3, with boundary conditions. Still, many properties should be decided by the temperature, which coupled all equations strongly.

Big idea - Dynamic model

To get a simplified model of multicomponent droplet microexplosion for reducing the calculation cost, further assumptions are needed based on Chia-fon Lee's model. Since the calculation is based on the dynamic process of gas bubble, we try to use only the dynamic description of the bubble, and temperature profile will be approximated to obtain properties. Similarly assuming the homogeneousness of the droplet, imitating the deduction of Rayleigh-Plesset equation, using boundary conditions specially set for the droplet, we can get modified Rayleigh equation concerning the radius of gas bubble and the radius of the droplet. Assuming the invariance of liquid volume or given an approximated volume change, the variable can be reduced to one, resulting in an ODE problem.

$$\rho_\ell\left[R_{\mathrm{i}}\frac{\mathrm{d}^2R_{\mathrm{i}}}{\mathrm{d}t^2}+1.5\left(\frac{\mathrm{d}R_{\mathrm{i}}}{\mathrm{d}t}\right)^2\right]=P_{\mathrm{gi}}-P_\ell-\frac{2\sigma}{R_{\mathrm{i}}}-\frac{4\mu}{R_{\mathrm{i}}}\frac{\mathrm{d}R_{\mathrm{i}}}{\mathrm{d}t}$$

Thus, through linear stability analysis, we can get the perturbation equation and solve the cubic equation, which will decide how perturbation is growing through time. Criterion of judging the onset of microexplosion can be got

$$(\Delta-\Delta^2-\psi_{\mathrm{o}}\Delta)\Omega^2+(-1+\Delta^4+\psi_{\mathrm{o}})We_{\mathrm{o}}^{1/2}\Omega+2\Delta^2+2\Delta^{-2}-3\psi_{\mathrm{i}}\frac{We_{\mathrm{i}}}{Ma_{\mathrm{i}}^2}\frac{\Omega}{\Omega+3We_{\mathrm{i}}^{1/2}}\Delta^2=0$$

$$\Omega=\sqrt{\frac{\rho_\ell\overline{R_{\mathrm{i}}}^3}{\sigma}}\omega,\quad We_{\mathrm{o}}=\frac{\rho_\ell\overline{V_{\mathrm{o}}^2}\overline{R_{\mathrm{i}}}}{\sigma},\quad We_{\mathrm{i}}=\frac{\rho_\ell\overline{V_{\mathrm{i}}^2}\overline{R_{\mathrm{i}}}}{\sigma},\ Ma_{\mathrm{i}}=\frac{\overline{V_{\mathrm{i}}}}{c},\quad \Delta=\frac{\overline{R_{\mathrm{o}}}}{\overline{R_{\mathrm{i}}}},\quad \psi_{\mathrm{o}}=\frac{\rho_{\mathrm{go}}}{\rho_\ell},\quad \psi_{\mathrm{i}}=\frac{\rho_{\mathrm{gi}}}{\rho_\ell}.$$

Model of bubble growth - Mikic

The model of bubble growth has been thoroughly examined before by a lot of research groups. Mathematicians [6] have studied some oscillating analytical solutions of the bubble, which is based on that there is no diffusion and that gas inside the bubble will not change its mass. At the same time, using Clausius-Clapeyron relation, which assumes that the gas is saturated, Mikic [5] developed a model for approximating its growth, which is especially helpful when the diffusion reaches any limitation.

$$R^{+} = \tfrac{2}{3}[(t^{+}+1)^{3/2} - (t^{+})^{3/2} - 1]$$

$$R^{+} = \frac{R}{B^2/A} \quad t^{+} = \frac{t}{B^2/A^2} \qquad A = \left(\frac{2\Delta T h_{\mathrm{fg}}\rho_{\mathrm{v}}}{3T_{\mathrm{sat}}\rho_{\mathrm{l}}}\right)^{1/2} \quad B = \left(\frac{12}{\pi} Ja^2 \alpha_{\mathrm{l}}\right)^{1/2}$$

For droplet growth, there should be more possible models which carefully incorporate the diffusion properties and the mixing of components. This model has omitted the boundary conditions of the outer layer, which is easy to be added into the model since we can always get Rayleigh-Plesset equation with slight changes due to the boundary conditions. Then we will have more specific equations similar to Mikic's solution for this case. Another important part which might need consideration is the evaporation of the inner layer, which is really important for temperature profile, but also might have some influence on pressure. Also, there is still no good enough way for how properties of mixing fuels behave. That should be easier to solve, since that is chemistry things.

Model for temperature profile

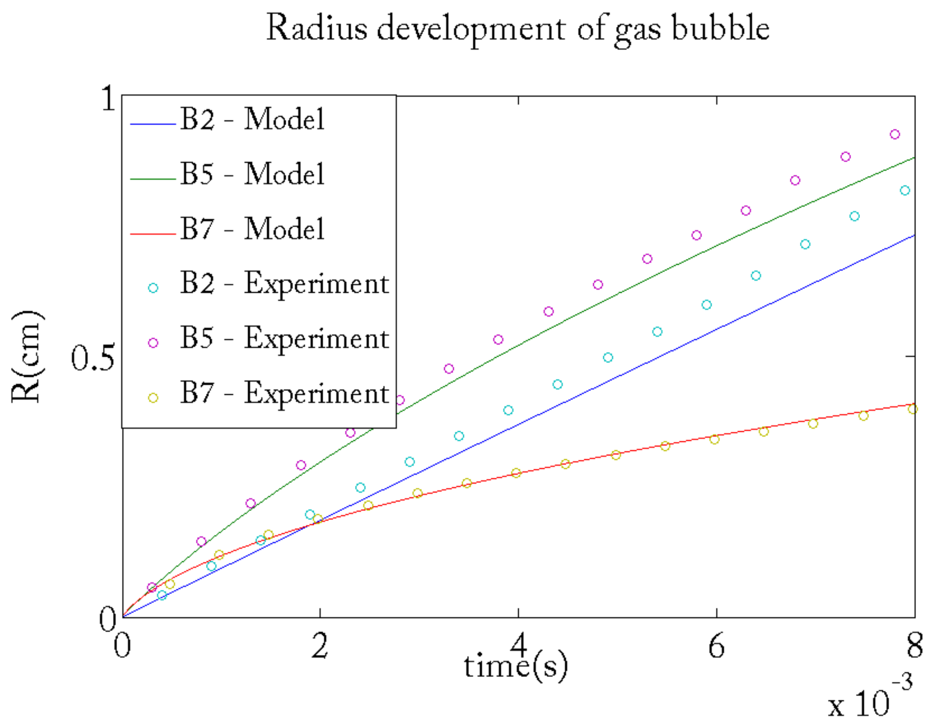
There is no proper idea of how to develop an analytical temperature profile for all conditions. Basically, the progress is 1-dimensional. Using some approximation, there might be a proper evaluation for how gas bubble properties change. If the bubble components are not greatly varying throughout the process, representative temperature and properties are allowed, which is an important and proper assumption throughout the modeling, since microexplosion happens rapidly.

Numerical method

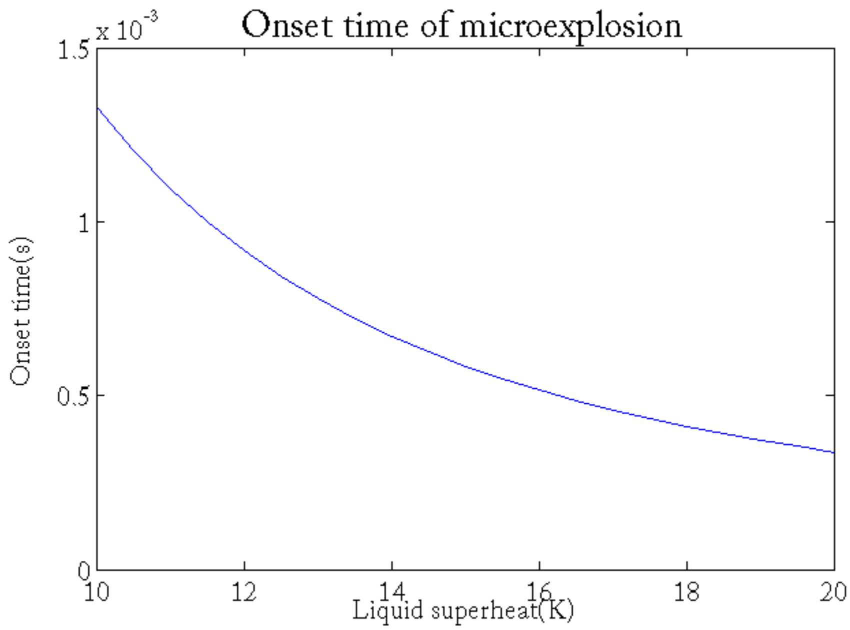
Using Matlab's ode solver, the bubble growth is possible. For Mikic's case, the growth can be directly expressed analytically. Its possible problems have been listed above, so a modified model for the growth of bubble is better. Up till now, there is no sudden growth of the bubble, since it means the sudden thinning of liquid layer. A temperature profile might be got through the solving of a heat transfer equation.

Recent result

The correctness of Mikic's equation has been verified through comparison with Lien's experiment [7]. The comparison is attached below.



According to Mikic's model, we got a preliminary prediction for different liquid superheat, which has other conditions the same as B5. Since there is no further experiment for similar conditions, it is best to do further experiments.



Acknowledgement

Great thanks to Pavan Govindaraju and Prof. Matthias Ihme in Stanford University for their instructions and help.

Reference

1. Zeng, Y., & Chia-fon, F. L. (2007). Modeling droplet breakup processes under micro-explosion conditions. *Proceedings of the Combustion Institute*, 31(2), 2185-2193.
2. Zeng, Y. (2000). Modeling of multicomponent fuel vaporization in internal combustion engines *(Doctoral dissertation, University of Illinois at Urbana-Champaign).*
3. Law, C. K. (1977). A model for the combustion of oil/water emulsion droplets.*Combustion Science and Technology*, 17(1-2), 29-38.
4. Kadota, T., Tanaka, H., Segawa, D., Nakaya, S., & Yamasaki, H. (2007). Microexplosion of an emulsion droplet during Leidenfrost burning. *Proceedings of the Combustion institute*, 31(2), 2125-2131.
5. Mikic, B. B., Rohsenow, W. M., & Griffith, P. (1970). On bubble growth rates.*International Journal of Heat and Mass Transfer*, 13(4), 657-666.
6. Mehrem, A. M. Estudio teo rico de la dina mica de microburbujas bajo la accio n de un campo ultraso nico.

7. Lien, Y. C. (1969). Bubble growth rates at reduced pressure *(Doctoral dissertation, Massachusetts Institute of Technology)*.
8. Shinjo, J., Xia, J., Ganippa, L. C., & Megaritis, A. (2014). Physics of puffing and microexplosion of emulsion fuel droplets. *Physics of Fluids*, 26(10), 103302.
9. Segawa, D., Yamasaki, H., Kadota, T., Tanaka, H., Enomoto, H., & Tsue, M. (2000). Water-coalescence in an oil-in-water emulsion droplet burning under microgravity. *Proceedings of the Combustion Institute*, 28(1), 985-990.
10. Wang, C. H., Liu, X. Q., & Law, C. K. (1984). Combustion and microexplosion of freely falling multicomponent droplets. *Combustion and Flame*, 56(2), 175-197.