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CFD Efficient Models of Droplet Heating and Vaporization

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Abstract: There exist a large number of models of droplet heating and vaporization rates with different complexities and computational costs. This paper reviews briefly those which are currently or have a good potential to be used for efficient CFD (computational fluid dynamics) simulation, e.g. commercial CFD packages such as Fluent. All the models discussed in this paper are simple and CFD efficient, i.e., incorporation of them would not add substantial computational cost. However, many assumptions (e.g. infinite thermal conductivity in the droplet) are made for these models, and the models may have limited accuracy if the assumptions made are not satisfied.

Models of determination of droplet heating and vaporization rates are critical for spray problem modeling in various applications, such as spray combustion, spray cooling, droplet-based coating and painting, and pharmaceutical particle precipitation etc. After implementing the droplet heating and vaporization models and other relevant models (e.g, thermodynamic and transport properties [1-4]), CFD (computational fluid dynamics) is a very powerful tool to predict features and performance of many processes. For example, it can predict energy efficiency in internal engines, and morphology of biomedical spray-dried polymer particles.

There are six types of droplet-vaporization models from Sirignano's categorization [5]. In order of increasing complexity, they are (1) constant-droplet temperature model (which yields the famous d^2 law whereby the square of the droplet diameter decreases linearly with time), (2) infinite-liquid-conductivity model (uniform but time-varying droplet temperature), (3) spherically symmetric transient droplet-heating (or conduction-limit) model, (4) effective-conductivity model, (5) vortex model of droplet heating, and (6) Navier-Stokes solution. Such categorization is very useful for a quick assessment of computational cost of various models, as discussed in a recent review paper by Sazhin [6]. Only the first two types are efficient enough and have been used in CFD commercial packages so far. The first type is inaccurate in most of cases because transient heating of the droplet is usually non-negligible. So, only the second type of models is discussed in this review.

1. Droplet heating

1.1. Ranz and Marshall model

The following correlation of Ranz and Marshall [7] has been widely used in CFD packages such as Fluent [8].

$$Nu = \frac{hd_p}{k_\infty} = 2.0 + \beta_c Re^{\frac{1}{2}} Pr^{\frac{1}{3}} \qquad (1)$$

Nu is the Nusselt number, which is a non-dimensional measure of the heat transfer coefficient. Re and Pr are the Reynolds number, and Prandtl number, respectively. h is the heat transfer coefficient, d_p is the droplet diameter, and k_∞ is the thermal conductivity of the free stream. The coefficient of β_c is usually taken as 0.6, for example, in [8, 9]. Many other papers used the value of 0.552,for example, in [5, 10].

The $Re^{\frac{1}{2}} Pr^{\frac{1}{3}}$ dependence in Ranz and Marshall model was obtained from qualitative analysis of problems at large Re, but in the laminar boundary layer region. This model has the common drawback of type two models - they do not consider the real droplet effect of liquid-phase heat or mass transport and internal

circulation [5]. So, these models are more accurate for slowly vaporization droplets, for which the droplet lifetime is long compared with a characteristic time for liquid-phase transport and thus the real droplet effect is not important. Note that the droplet heating model in Eq. 1 is based on non-vaporizing cases, as the classical stationary heated-sphere (no vaporization) result (Nu = 2) is extracted when Re = 0.

1.2. Spalding number correction

Chiang and Sirignano [11] has correlated their numerical results, relating the Nusselt number to the instantaneous Reynolds number and Spalding transfer number B.

$$Nu = 1.275(1 + B_H)^{-0.678} Re_m^{0.438} Pr_m^{0.619} \quad (2)$$

where Re_m and Pr_m are based on average gas-film values (except for the use of free-stream density in Re_m), and are varied from 30 to 200, and 0.7 to 1.0, respectively. B_H is the Spalding number of heat transfer and ranges from 0.4 to 13. It is defined as follows:

$$B_H = \frac{h_e - h_S}{L_{eff}} \quad (3)$$

where h_e and h_S are the enthalpy at the edge of boundary layer and at the droplet surface, respectively. L_{eff} is the effective latent heat [5].

ANSYS Fluent [8] uses a modified version of Eq. (1) when the vaporization rate is fast and the convection of the vapor is substantial. The modified equation is:

$$Nu = \frac{hd_p}{k_\infty} = \frac{ln(1 + B_M)}{B_M}\left(2.0 + \beta_c Re^{\frac{1}{2}} Pr^{\frac{1}{3}}\right) \quad (4)$$

where B_M is the Spalding number of mass transfer given by

$$B_M = \frac{Y_{v,S} - Y_{v,\infty}}{1 - Y_{v,S}} \quad (5)$$

$Y_{v,S}$ and $Y_{v,\infty}$ are the mass fraction of vapor at the droplet surface and in the free stream, respectively.

The two models with Spalding number correction are more accurate in vaporizing cases. The Chiang and Sirignano model [11] is recommended in the specific ranges as mentioned above. The model in [8] can be used for general vaporizing cases.

1.3. Re correction

The above models might be more accurate if distinguishing the flow conditions determined by Reynolds number. Clift et al. [12] and Abramzon and Sirignano [10] have considered the following form with Re correction:

$$Nu = 1.0 + (1 + Re\,Pr)^{\frac{1}{3}} f_c(Re) \quad (6)$$

$f_c(Re)$ is 1 when Re is less than 1, and is $Re^{0.077}$ when Re is in the range of 1~400. This model with Re correction should not be used for Re out of the explored range of 1~400.

1.4. Asymptotic models

Several papers (e.g. [13, 14]) proposed asymptotic models from analytical estimation for low Pe (Peclet number) limit and high Pe limit.

At low Pe limit:

$$Nu = 2\left[1 + \frac{1}{4}Pe + \frac{1}{8}Pe^2 \ln(Pe) + 0.01702Pe^2 + \frac{1}{32}Pe^3 \ln(Pe) + O(Pe^3)\right] \quad (7)$$

where the Peclet number Pe is defined as the product of Reynolds number Re and Prandtl number Pr.

At high Pe limit:

$$Nu = 0.991Pe^{\frac{1}{3}}\left[1 + \frac{1}{16}Re + \frac{3}{160}Re^2\ln(Re) + O(Re^2)\right] \quad (8)$$

The asymptotic models are rarely used, and are only recommended when the asymptotic conditions are well satisfied.

1.5. Viscosity ratio dependence

Some papers have considered the effect of viscosity ratio of the liquid phase and vapor phase, for example, Feng and Michaelides [15] proposed the following equations.

At $Re < 1$ and $10 < Pe < 1000$:

$$Nu(\lambda_v, Pe, Re) = \left[\frac{0.651}{1+0.95\lambda_v}Pe^{1/2} + \frac{0.991\lambda_v}{1+\lambda_v}Pe^{1/3}\right][1 + \alpha_v(Re)] + \left[\frac{1.65(1-\alpha_v(Re))}{1+0.95\lambda_v} + \frac{\lambda_v}{1+\lambda_v}\right] \quad (9)$$

where λ_v is the kinetic viscosity ratio of the liquid phase and vapor phase, and $\alpha_v(Re)$ is given by,

$$\alpha_v(Re) = \frac{0.61Re}{Re + 21} + 0.032 \quad (10)$$

At $1 < Re < 500$ and $10 < Pe < 1000$:

$$Nu(\lambda_v, Pe, Re) = \frac{2 - \lambda_v}{2}Nu(0, Pe, Re) + \frac{4\lambda_v}{6 + \lambda_v}Nu(2, Pe, Re) \quad (11)$$

for $\lambda_v < 2$, and

$$Nu(\lambda_v, Pe, Re) = \frac{4}{2 + \lambda_v}Nu(2, Pe, Re) + \frac{\lambda_v - 2}{\lambda_v + 2}Nu(\infty, Pe, Re) \quad (12)$$

for $\lambda_v > 2$.

Refer to Sazhin [6] for the detailed equations for $Nu(0, Pe, Re)$, $Nu(2, Pe, Re)$ and $Nu(\infty, Pe, Re)$.

The effect of liquid-to-vapor viscosity ratio is important and needs to be considered when the viscosity of vapor phase is not much smaller than that of liquid phase.

2. Droplet vaporization

2.1. Ranz and Marshall model

As mentioned above, Ranz and Marshall model [7] has been widely used in CFD packages such as Fluent [8]. According to Ranz and Marshall model, the dimensionless number determining the droplet vaporization rate, i.e. Sherwood number Sh, is given by:

$$Sh = \frac{h_m d_p}{D_{v,m}} = 2.0 + \beta_c Re^{\frac{1}{2}}Sc^{\frac{1}{3}} \quad (13)$$

where h_m is the mass transfer coefficient, $D_{v,m}$ is the diffusion coefficient of vapor in the mixture, and Sc is the Schmidt number. This equation simply replaces Nusselt number (Nu) in Eq. (1) with Sherwood number (Sh), and replaces the Prandtl number (Pr) with the Schmidt number (Sc). Other equations in the last section for Nusselt number may be also transformed in a similar way to the equations for the estimation of Sherwood number [6]. Similar to Nu number estimation, the Ranz and Marshall model in Eq. (13) is not accurate for fast vaporizing cases.

2.2. Spalding number correction

Nafziger [16] proposed the following empirical equation with effect of Spalding number B_M.

$$Sh = (1 + B_M)^{-0.7}\left[2 + 0.87Re_f^{\frac{1}{2}}Sc_f^{\frac{1}{3}}\right] \quad (14)$$

The subscript "f" indicates film properties which are based on an average at the droplet surface

and in the free stream [5]. The Spalding number B_M is given by Eq. (5).

Sazhin [6] proposed the following model from hydrodynamic analysis.

$$Sh = \frac{\ln(1+B_M)}{B_M} Sh_0 \quad (15)$$

where Sh_0 can be estimated from Eq. (13).

Section 1.2 has discussed the Chiang and Sirignano model [11] for the Nusselt number. The corresponding correlation for Sherwood number is as follows:

$$Sh = 1.224(1+B_M)^{-0.568} Re_m^{0.385} Sc_m^{0.492} \quad (16)$$

where Sc_m is based on average gas-film values, and is varied from 0.4 to 2.2. B_M (given by Eq. (5)) ranges from 0.2 to 6.5.

ANSYS Fluent [8] uses a modified form of Eq. (13) when the vaporization rate is fast and the convection of the vapor is substantial. The modified equation for Sh given as:

$$Sh = \frac{\rho_\infty ln(1+B_M)}{M_{W,v}(C_{v,S} - C_{v,\infty})} \left[2.0 + \beta_c Re^{\frac{1}{2}} Sc^{\frac{1}{3}}\right] \quad (17)$$

where $M_{W,v}$ is the molecular weight of the vapor, ρ_∞ is the free stream density, and $C_{v,S}$ and $C_{v,\infty}$ are the vapor molar concentration at the droplet surface and in the free stream, respectively.

The models with Spalding number correction are more accurate for vaporizing cases. Among these models, the Chiang and Sirignano model [11] also considers the effect of film properties and is recommended in the specific ranges as mentioned above. The model in [8] can be used for general vaporizing cases.

2.3. Consideration of droplet interactions

For multi-droplet cases, the interactions amongst droplets would decrease the droplet vaporization rate if the spacing amongst droplets is not large enough (e.g. <8d_p) [17-24]. Imaoka and Sirignano [17, 18] proposed a correction factor to take account of the interaction effect. Spherical symmetry was assumed. The correction factor η_A for a droplet array of N droplets is given as:

$$\eta_A = 1 - \frac{1}{1 + 0.725671\xi^{0.971716}}$$

$$\xi = \frac{\left[\frac{4\pi V_A N}{3V_l}\right]^{1/3}}{[N^{1/3}-1]N^{0.72}} \quad (18)$$

where V_A, V_l, and N are the droplet array volume, total liquid volume, and droplet number, respectively.

The model with consideration of droplet interactions is recommended when the spacing amongst droplets is not large enough (e.g. <8d_p). The effect of droplet interactions is more important when there is no forced convection or the forced convection is not strong.

This paper reviews the models of droplet heating and vaporization that assume uniform temperature distribution inside of the droplets. These models represent a reasonable compromise of the computational accuracy and efficiency; so, they are either commonly used or have a good potential to be used in commercial CFD packages. The diffusion and convection effects have been well considered by tuning the dependence on Re, Pe, B_M (or B_H), Pr and Sc. Effect of droplet interaction has been studied for spherically symmetric cases. However, the models for the more general cases with forced convection are yet to be developed. The models need also to be improved to take account of turbulence in high Re cases, chemical kinetics in chemically reacting cases, and high-temperature-high-pressure effect at near-critical conditions.

Reference

1. Wu, G., *Predictive Capability of Equations of State for Investigating Effect of Isomeric Structures of Branched Cyclic Hydrocarbons on Densities at Elevated Temperatures and Pressures.* PostDoc Journal, 2013. **1**(9): p. 26-28.
2. Dabiri, S., et al., *Mixing of single-component hydrocarbon droplets and water at supercritical or near-critical conditions.* The Journal of Supercritical Fluids, 2012. **67**(0): p. 29-40.
3. Wu, G., et al., *Fractionation of multi-component hydrocarbon droplets in water at supercritical or near-critical conditions.* The Journal of Supercritical Fluids, 2012. **72**(0): p. 150-160.
4. Wu, G., et al., *Mixing of Hydrocarbon Droplets and Water at Supercritical or Near-Critical Conditions*, in *10th International Symposium on Supercritical Fluids*. 2012: San Francisco, CA, USA.
5. Sirignano, W.A., *Fluid dynamics and transport of droplets and sprays*. 2nd Edition ed. 2010: Cambridge University Press.
6. Sazhin, S.S., *Advanced models of fuel droplet heating and evaporation.* Progress in energy and combustion science, 2006. **32**(2): p. 162-214.
7. Ranz, W. and W. Marshall, *Evaporation from drops.* Chem. Eng. Prog, 1952. **48**(3): p. 141-146.
8. *ANSYS FLUENT Theory Guide (Release 14.5)*. 2012.
9. Bird, R.B., W.E. Stewart, and E.N. Lightfoot, *Transport phenomena*. 2007: Wiley. com.
10. Abramzon, B. and W. Sirignano, *Droplet vaporization model for spray combustion calculations.* International journal of heat and mass transfer, 1989. **32**(9): p. 1605-1618.
11. Chiang, C. and W. Sirignano, *Interacting, convecting, vaporizing fuel droplets with variable properties.* International journal of heat and mass transfer, 1993. **36**(4): p. 875-886.
12. Clift, R., J. Grace, and M. Weber, *Bubbles.* Drops and Particles (Academic, New York, 1978), 1978: p. 1870.
13. Michaelides, E.E., *Hydrodynamic force and heat/mass transfer from particles, bubbles, and drops: The Freeman Scholar Lecture*. Journal of fluids engineering, 2003. **125**(2): p. 209-238.
14. Acrivos, A. and T.D. Taylor, *Heat and mass transfer from single spheres in Stokes flow.* Physics of Fluids, 1962. **5**: p. 387.
15. Feng, Z.-G. and E.E. Michaelides, *Heat and mass transfer coefficients of viscous spheres.* International journal of heat and mass transfer, 2001. **44**(23): p. 4445-4454.
16. Nafziger, R. and U.o.W.D.o.M. Engineering, *Convective Droplet Transport Phenomena in High - Temperature Air Streams*. 1988.
17. Imaoka, R.T. and W.A. Sirignano, *Vaporization and combustion in three-dimensional droplet arrays.* Proceedings of the Combustion Institute, 2005. **30**(2): p. 1981-1989.
18. Imaoka, R.T. and W.A. Sirignano, *Transient vaporization and burning in dense droplet arrays.* International journal of heat and mass transfer, 2005. **48**(21): p. 4354-4366.
19. Sirignano, W.A. and G. Wu, *Multicomponent-liquid–fuel vaporization with complex configuration.* International Journal of Heat and Mass Transfer, 2008. **51**(19): p. 4759-4774.
20. Wu, G. and W.A. Sirignano, *Transient burning of a convective fuel droplet.* Combustion and flame, 2010. **157**(5): p. 970-981.
21. Wu, G. and W.A. Sirignano, *Transient convective burning of a periodic fuel-droplet array.* Proceedings of the Combustion Institute, 2011. **33**(2): p. 2109-2116.
22. Wu, G. and W.A. Sirignano, *Transient convective burning of interactive fuel droplets in single-layer arrays.* Combustion Theory and Modelling, 2011. **15**(2): p. 227-243.
23. Wu, G. and W.A. Sirignano, *Transient convective burning of interactive fuel droplets in double-layer arrays.*

Combustion and Flame, 2011. **158**(12): p. 2395-2407.

24. Wu, G., W.A. Sirignano, and F.A. Williams, *Simulation of transient convective burning of an n-octane droplet using a four-step reduced mechanism.* Combustion and Flame, 2011. **158**(6): p. 1171-1180.