NOVA

University of Newcastle Research Online

nova.newcastle.edu.au

Mitra, Subhasish; Sathe, Mayur; Doroodchi, Elham; Utikar, Ranjit; Shah, Milin; Pareek, Vishnu; Joshi, Jyeshtharaj; Evans, Geoffrey, "Droplet impact dynamics on a spherical particle". Originally published in Chemical Engineering Science Vol. 100, p. 105-119 (2013)

Available from: <http://dx.doi.org/10.1016/j.ces.2013.01.037>

Accessed from: <http://hdl.handle.net/1959.13/1037054>

Droplet impact dynamics on a spherical particle

Subhasish Mitra^a, Mayur J. Sathe^a, Elham Doroodchi^a, Ranjeet Utikar^b,
Milin K. Shah^b, Vishnu Pareek^b, Jyeshtharaj B. Joshi^c, Geoffrey M. Evans^{a*}

^aDiscipline of Chemical Engineering, School of Engineering, University of Newcastle,
NSW 2308, Australia

^bDepartment of Chemical Engineering, Curtin University, Perth, WA 6102, Australia

^cInstitute of Chemical Technology, Mumbai 400019, India

*Corresponding author. Tel: +61-2- 40339068; fax: +61-02-0339095;

E-mail address: Geoffrey.Evans@newcastle.edu.au

- Experiments and CFD of droplet impact on a spherical particle were carried out
- Droplet spread measured at different Weber numbers and surface temperatures
- Droplet spread better predicted by dynamic contact angle than static angle
- Heat transfer coefficients during impact reduced towards film boiling regime
- Vapor region around evaporating droplets were captured by Schlieren imaging

t = 3 ms

t = 6 ms

t = 9 ms

t = 12 ms

t = 18 ms

CFD simulations

Leidenfrost effect levitates droplet in film boiling regime leading to non wetting surface contact

Abstract

In this work, subcooled droplet impact on a highly thermally conductive spherical surface was investigated both theoretically and experimentally. Specifically, the effect of Weber number on spreading of droplets of three different liquids namely water, isopropyl alcohol and acetone was studied. The droplet shape evolution and surface wetting upon droplet impact at surface temperatures ranging between 20°C and 250°C were investigated using a high speed camera. Maximum droplet spread was measured and compared with available correlations. Generally wetting contact was observed at surface temperatures below or close to saturation temperature whilst a non-wetting contact was exhibited at surface temperatures significantly greater than the saturation temperature. The drop in surface temperature was found to be significantly lower in this non-wetting contact regime which led to significant reduction in heat transfer coefficient. Despite a very small temperature drop in the film boiling regime indicating small fraction of vaporization, Schlieren imaging of acetone droplets showed qualitative vapour field around the rebounding droplets. The droplet spreading patterns in cold condition and film boiling regime were simulated using the 3D CFD models which were found to be in good agreement with the experimental observations.

Keywords: Drop, Evaporation, Heat transfer, Hydrodynamics, CFD modeling, VOF method

1. Introduction

The impact of liquid droplets on solid surfaces is a subject of practical interest in many industrial applications. These application areas can be broadly classified into two distinct categories – cold and hot. The first category includes applications like cold spray coating, painting and printing processes while the second one includes plasma spray coating, spray cooling in casting processes of metallurgical industries, vaporization process in internal combustion engines, cooling of turbine blades, core cooling of nuclear reactors, and feed vaporization in fluidized bed. The wetted surface area and associated heat transfer rate governed by the droplet spreading characteristics are the key focus of all these applications. In process industries, multiphase flow processes involving contact of liquid over solid surface are predominant in many areas like adsorption, leaching and heterogeneous catalytic reactions. In trickle bed reactor, adequate wetting of catalyst particle is required by the flowing liquid to ensure catalyst efficiency and therefore the process performance. Feed evaporation plays a critical role in the fluid coking process to upgrade bitumen by means of thermal cracking (Gray, 2002) and in fluidized bed catalytic reactor (Buchanan et al., 1994; Mirgain et al., 2000; Gao et al., 2001; Nayak et al., 2005). In FCC, feedstock is introduced at the bottom of the riser through atomizing nozzles. Atomized droplets contact the hot catalyst particles, vaporize, and are converted to smaller molecules instantly. Depending on the nature on contact, the droplets may splash, rebound or remain on the catalyst particle surface after the impact (Mundo et al., 1995; Mao et al., 1997; Ge and Fan, 2005). To facilitate cracking reactions in vapour phase, it is essential to establish proper contact of liquid droplets over catalyst surface so that the droplets evaporate instantly. Fast vaporization results in higher yields.

Despite all these industrial applications, understanding of droplet impingement on solid surface is not complete yet. Being a challenging problem to both physicists and engineers,

significant research has been carried out in last few decades to understand droplet impact dynamics on the solid surface. Upon impact, droplet's vertical momentum causes radial flow. The impact kinetic energy and surface energy of the droplet are converted to surface energy of the splat and viscous dissipation energy (Bechtel et al. 1981, Kim and Chun, 2001). Depending on surface tension, the droplet undergoes an oscillatory motion with gradually decaying amplitude till it reaches a sessile state. The oscillation process consists of the initial spreading of the droplet until it reaches its maximum spread diameter and subsequent oscillatory motions of recoiling and weak re-spreading. The spreading pattern of the droplet depends both on liquid and surface characteristics, in particular it depends on fluid surface tension and viscosity and the roughness, inclination and hydrophobicity of the surface. Three dimensionless numbers are often used to characterize droplet spread dynamics – Weber number (We): $\rho u^2 d / \sigma$, Reynolds number (Re): $\rho u d / \mu$, and Ohnesorge number (Oh): $\mu / (\rho d \sigma)^{1/2}$. Droplet recoiling behaviour is primarily determined by Weber number, Ohnesorge number, and the equilibrium contact angle. Maximum spread diameter depends on the Weber number which constitutes an initial condition for the recoiling phenomenon. Capillary force arising from the difference between the equilibrium state and the excessively spread shape then drives this recoiling process while flow is continuously resisted by inertia and viscosity. This resisting force can be scaled by Ohnesorge number. When Ohnesorge number is small, resisting forces is contributed by both inertia and viscosity while at large Ohnesorge number, viscosity plays the significant role (Kim and Chun, 2001). When impact kinetic energy overcomes the viscous resistance, a droplet may splash upon impact on the solid surface. Scheller and Bousfield (1995) studied droplet splashing over a wide range of viscosity (1 – 300 mPa.s). Based on their experimental data, they proposed a correlation for maximum spread as a function of Reynolds number and Ohnesorge number which agreed well with the available models. Rebounding is another interesting aspect droplet impingement on solid

surface which can take place on both cold and hot surface. Under cold condition, significant rebound occurs when a low-viscous liquid, such as water, impinges on a super-hydrophobic surface like wax (Clanet et al., 2004). Because of very low viscous dissipation on a super-hydrophobic surface, the restitution coefficient of the shock is quite high (0.9) which makes this type of collision almost elastic and attributes to rebound. Under hot condition, during droplet impingement on the solid surface, a thin vapour film forms at the contact surface when solid surface temperature is kept sufficiently higher than the saturation temperature of the droplet. The vapour flows in radial direction in the film and pressure drop thus incurred eventually overcomes the weight of droplet resulting into rebounding of droplet off the surface (Ge and Fan, 2005, 2006).

The droplet shape evolution depends greatly on contact angle which changes over the entire period of deformation until the droplet comes to a sessile state. Unlike static contact angle this dynamic contact angle does not depend on material properties and is affected by the macroscopic hydrodynamics in high capillary number regime. Inclusion of dynamic contact angle in the numerical models therefore remains as a challenging problem. Droplet shape evolution depends to a large extent on the contact angle of the liquid interface at the solid surface which changes over the impact and recoil period. Interestingly, this contact angle does not remain constant over the period of deformation and thus understanding dynamic contact angle (Shikhmurzaev, 1997; Sikalo et al., 2005; Vadilo et al., 2009) of the droplet upon impingement on the solid surface has been a matter of active research, for many years. The dynamic contact angle often is correlated to the three phase contact line velocity. McHale et al. (1994) used Frenkel's method to obtain a relation between the edge velocity and the dynamic contact angle for the spreading of small spherical droplets of viscous and non-volatile fluids. The change in surface free energy was equated to the viscous dissipation caused by Poiseuille flow, first in a wedge and then in a cone inscribed within the spherical

cap. An equation relating the edge velocity to the dynamic contact angle for both complete and partial wetting was obtained. In the small angle limit, this formula corresponded to a generalized Tanner's law (Tanner, 1979, 1986) and, in the case of the cone model, also predicted the variation of the edge velocity over a wide angular range. Good agreement of the edge velocity angular dependence with literature data for complete spreading was found. Dusan (1979) presented a good treatise on dynamic contact line of liquid on solid surface. A singularity problem often arises due to the assumption that the liquid layer in contact with solid surface is stationary. Three different approaches are widely recognized in literature to model dynamic wetting phenomenon – hydrodynamic, molecular kinetic and combined molecular-hydrodynamic. The hydrodynamic model (Cox, 1986; Voinov, 1976) considers the dynamic wetting of the surface in terms of bulk viscous dissipation ignoring the effect of the solid surface. In molecular kinetic approach (Blake and Haynes, 1969; Hayes and Ralston, 1994; Pismen and Rubinstein, 2001), the dynamic wetting is interpreted as a rate process of simultaneous molecule adsorption and desorption on the solid surface. The third one, molecular-hydrodynamic approach (Petrov and Petrov, 1992) takes into account effect of these two phenomena to describe the dynamic wetting process.

Pasandideh-Fard et al. (1996); Bussmann et al. (1999); Fukai et al. (1993, 1995, 2000); Šikalo et al. (2002, 2005) discussed many aspects of droplet surface interaction including modelling aspects of dynamic contact angle in their work. A number of different numerical modelling approaches namely deforming finite element method (Fukai et al., 1993), SOLA-VOF (Pasandideh-Fard et al., 1996), Eulerian fixed-grid algorithm based on the RIPPLE code utilizing a volume tracking approach (Bussman et al., 1999) and Volume of Fluid method (Šikalo et al., 2005, Lunkad et al., 2007) are reported. The most critical aspect of these numerical modellings was formulation of contact line motion. Experimentally measured dynamic contact angles were used in most of these works (Fukai et al., 1995;

Pasandideh-Fard et al., 1996; Bussman et al., 1999). In a later work, Sikalo et al., (2005) incorporated an empirical dynamic contact angle model as a function of contact line velocity in their VOF based axisymmetric simulations. A firm dependence of dynamic contact angle on contact line velocity could not be achieved because of limitation of the numerical model which calculated velocity field away from contact line while the dynamic contact angle model was valid only in the vicinity of contact line at low Capillary number. The predicted droplet spreading characteristics was reported to be in good agreement with their experimental data on water impacting on glass and wax surface. Although, formulation of dynamic contact angle in the numerical modelling is a critical component, the effect is seemingly less pronounced when flow is not in capillary regime (Fukai et al., 1995; Sikalo et al., 2005).

When the surface is hot, the spreading pattern is essentially influenced by the heat transfer characteristics at the surface. Although all three modes of heat transfer may be applicable, usually heat transfer by conduction is often considered significant. Depending on the surface temperature, droplet contact with the hot surface can be distinctly classified into two categories – wetting and non-wetting (Shi et al., 1993). In the wetting contact case, the liquid droplet after impingement keeps continuous or semi-continuous direct contact with the surface and enters into nucleate boiling or transition boiling at the end of the initial spreading phase. Due to rapid change in liquid temperature in contact with solid surface, boiling occurs close to interface. In this wetting regime, the surface temperature drop is significant which leads to a high cooling rate. In the case of non-wetting contact, contrary to the wetting contact, the surface temperature remains significantly above the saturation temperature of the liquid. Rapid growth of heterogeneous and homogeneous nucleation occur at the interface resulting in coalescence of numerous bubbles which forms a thin vapour film at the end of the initial heat conduction period during the spreading phase. The vapour film acts as an

insulating barrier between the droplet and heated surface and inhibits heat transfer process significantly which in turn increases vaporization time. This phenomenon is known as Leidenfrost effect and depending of impact Weber number, droplet in this boiling regime undergoes interesting impingement dynamics. Wachters and Westerling (1966) are often noted for conducting pioneering investigation in this area. They carried out an impingement experiment with water droplet of approximately 2 mm diameter on a polished gold surface heated to 400°C. Many more experiments thereafter were conducted in the similar line of approach to study droplet impingement dynamics in and beyond Leidenfrost regime at different Weber number employing droplets of different fluids e.g. acetic acid, benzene, carbon tetrachloride, diesel, ethanol, n-heptane, n-octane etc., on both flat and inclined different metal surfaces e.g. aluminium, copper, nickel, silver stainless steel, inconel alloy etc. (Gottfried et al., 1966; Akao et al., 1980; Chandra and Avedisian, 1991,1992; Hatta et al., 1995,1997; Bernardin and Mudawar, 1999; Karl and Frohn, 2000; Kang and Lee, 2000; Chen et al., 2007a,b; Fujimoto et al., 2010). Experimentally, droplet impingement dynamics were studied using high speed camera (Akao et al., 1980), flash photography (Chandra and Avedisian, 1991,1992), video camera (Crafton et al., 2004) high speed digital camera (Chen et al., 2007a, 2007b, Fujimoto et al., 2010). In general, at $We < 30$, surface tension was found to dominate the impact process and the droplet recoils and rebounds from the surface without disintegration. A similar spreading and recoiling process was observed at $30 < We < 80$, where the droplet disintegrated into smaller droplets during the rebounding process. At $We > 80$, the impact kinetic energy dominated surface tension leading to splashing and disintegration of the droplet into a number of smaller droplets during the early stage of the impact. Collision dynamics in most of these studies mainly focussed on influence of surface temperature (Chandra and Avedisian, 1991; Fujimoto et al., 2010) and impingement angle (Hatta et al., 1997; Karl and Frohn, 2000; Kang and Lee, 2000; Chen et al., 2007a) on droplet

shape deformation and disintegration. Maximum droplet spread was of interest to many of these studies which were correlated to Reynolds number and Weber number (Akao et al., 1980, Chandra and Avedisian, 1991). The heat flux on the particle surface was found to reach a higher level during the spreading process, and then sharply decreased during the recoiling process (Ge and Fan, 2007). Both subcooled and saturated droplet impact on the hot surface were studied. A weak relation between surface energy and Leidenfrost point was reported while surface conditions and liquid subcooling were found to have negligible effect (Bernardin and Mudawar, 1999). More recently, boiling phenomena during droplet impingement on hot solid surface was explained by Fujimoto et al. (2010) in terms of interfacial temperature and limit of superheat. Interfacial temperature was found to be more appropriate than surface temperature. Deformation behaviour of droplet was reported to be affected by Reynolds number, contact angle and motion of boiling vapour bubbles at lower temperature.

Numerical modelling study for droplet impingement dynamics in the film boiling regime mostly employed the Volume of Fluid method (VOF) (Karl et al., 1996; Harvie and Fletcher, 2001) and the Level Set (LS) with Arbitrary Eulerian Lagrangian (ALE) method (Ge and Fan, 2005, 2006, 2007, Yu et al., 2007). Two different approaches are observed in these numerical studies – with and without vapour film model. The simpler approach neglected the vapour flow model and but included effect of vapour layer by means of a free slip condition at the contact surface and a contact angle of 180° implying a non-wetting contact with the solid surface (Karl et al., 1996). The more complex approach included the vapour flow model essentially necessitating a multiscale modelling approach due to order of magnitude difference between the vapour film thickness ($\sim \mu\text{m}$) and the droplet diameter ($\sim \text{mm}$) (Harvie and Fletcher, 2001; Ge and Fan, 2005, 2006, 2007; Yu et al., 2007). In this approach, vapour layer underneath the droplet was separately modelled to simulate the

pressure and velocity distribution along the vapour layer. Heat transfer both inside each phase and at the solid-vapour/liquid-vapour interface was considered. The vapour flow dynamics and the heat flux across the vapour layer were solved with consideration of the kinetic discontinuity at the liquid-vapour and solid-vapour boundaries in the slip-flow regime.

The review of the literature highlights the significant research that has been carried out into quantifying and modelling the behaviour of droplets impacting onto hot and cold surfaces. The observed phenomena are the result of complex interaction involving momentum, heat and mass transfer. Not surprisingly, there is still only limited understanding of industrial processes where this interaction takes place. For example, in petroleum processing a fluidized catalytic cracking (FCC) unit is used to convert heavier petroleum fractions into valuable lighter hydrocarbons with an evaporating jet of atomized feed droplets to provide effective contact with hot catalyst particles. Since cracking reactions occur essentially in the vapour phase, efficient evaporation of oil droplets plays a critical role in controlling the reactor yield. The vaporisation process can take place either as the droplet passes through the hot gas space or contacts the hot catalyst particles. Whilst the evaporation process of a droplet suspended in a gas is well understood, much less is known about the collision and vaporisation of the droplets striking a hot solid particle surface. For this reason the current study is focussed on quantifying, both experimentally and by computational modelling, the behaviour of an impacting droplet onto a hot spherical particle. In particular, the aims are to: (1) Experimentally examine the influence of Weber number on distilled water, isopropyl alcohol and acetone droplet deformation; (2) Measure droplet spreading and heat transfer coefficient during impact as a function of impact velocity on the surface of a highly thermally conductive particle at different surface temperatures in both nucleate and film boiling regimes, and compare with the available correlations in literature; (3) Quantify the effect of static and dynamic contact angle on the spreading ratio; (4) Apply Schlieren

imaging technique to visualize vapour region around the acetone droplets during impact; and finally (5) Computationally model the process and compare with the experimental measurements.

2. Experimental methodology

In this work, the experiment for studying collision between an impinging droplet and a stationary solid particle was conducted. An experimental setup with a temperature controlled test piece and an adjustable height droplet delivery system was used to examine the effect of Weber number on the droplet deformation and evaporation at temperatures ranging between 20 to 250°C. The schematic diagram of the experimental setup is shown in Fig. 1. The main components of the experimental apparatus were the heating billet, brass particle, syringe pump, high speed camera, and light source. A 12 mm × 20 mm size hollow aluminium block was used as a heating billet with a 200 watt cylindrical cartridge heater placed inside the block. The billet was fully insulated on all sides except the upper surface. A 10 mm diameter brass particle was placed on top of the heating billet. Two 1 mm probe diameter T type thermocouples were inserted into the brass particle. One of these thermocouples was connected to the PID controller while the other one was connected to a data acquisition system. A variac was used along with the controller to regulate the voltage of the heater to prevent over-heating. Both thermocouples were located in the same radial plane having a gap of 5 mm in between. The polished brass particles used in the experiments had surface roughness of 0.12 μm. A CMOS type high speed digital camera (Dantec IDT) was used to capture the images of droplet impact on the particle. Since the image resolution varies inversely to the capturing frame rate, therefore, the frame rate and shutter speed were optimized to obtain the best possible image. The typical frame rate and shutter speeds used in the experiments were 1000-1400 frames/sec and 50-500 μsec. The camera was placed

parallel to the impact surface at a zero degree angle to the setup. This arrangement allowed the best view of the liquid-solid interaction at the interface. A 10 ml syringe fitted with a 21G X 1½" hypodermic needle was placed in a syringe pump and used as the droplet delivery system. The stroke length of the syringe pump was adjusted to allow a single droplet to fall onto the impacting surface. Although both the height and gauge of the needle could be varied to change the Weber number of the impinging droplet, only the height of the needle was considered in the present work as the controlling variable. A 50 watt, 230V halogen bulb was used as the light source. Three different imaging methodologies were carried out to study the droplet surface interaction. The illumination of the light was made uniform in the images by placing white paper diffusers behind the impacting object when droplet interaction dynamics on the surface was of interest. The shadowgraphy technique was applied by placing a plastic diffuser screen between the test setup and the light source when high contrast images were required for measuring maximum spread of the droplets on the surface. Finally, Schlieren imaging was carried out in order to visualize the vapour trail around the impinging acetone droplets on the hot surface. In this technique, the gradient of refractive index can be measured optically and same can be recorded using a camera. Due to order of magnitude difference in the refractive index of air and acetone vapour, a light ray while passing through these media will significantly bend at locations of nonzero gradient of refractive index and would result in change in image intensity in these locations (Kelly-Zion et al., 2009). In Schlieren imaging, the test setup (Fig. 1) was kept close to a large focal length ($f = 6D$) 200 mm diameter (D) concave mirror mounted in an aluminium frame equipped with vibration resisting pads. A microscope lamp source (12 V DC) mounted on an optical table at the focal length of the mirror. The focal point was ascertained by carefully positioning the light source until a clear view of the bulb filament was obtained on a white background. A knife-edge was positioned on a precision screw-operated traverse at this focal point. The intensity of the image was

made uniform by fine forward or backward movement of the knife edge. The high speed camera with 100 mm focal length lens (Nikon-Nikkor) was positioned close to the razor edge. Importantly, the centre-point of the camera lens needs to be coincided with the incident light ray. A portion of the undisturbed light upstream of the camera lens is blocked by the knife edge position. Any gradient in the refractive index upstream of the lens causes light ray to deflect either away from or towards the knife edge thus allowing more or less light ray passing the knife edge. This change in light intensity creates corresponding brightening and darkening regions in the images. Only gradients normal to the edge of the blade can be measured by this technique. The Schlieren system is very sensitive to change of medium density. Hence, to prevent any draft disturbing the headspace above the fluidized bed, all four sides of the experimental setup excluding the front and bottom were covered. The experiments were performed in the enclosed system under controlled room temperature.

Before each experiment, the brass particle was thoroughly cleaned with soft liquid soap followed by isopropyl alcohol and acetone rinsing to remove any dirt or greasy substances from the surface. The cleaning procedure was repeated after each set of experiments was completed. A steady state surface temperature was ensured during the experiments before the data were collected. The system took several minutes to reach steady state condition depending on the temperature set point. The Weber numbers in the experiments were varied by changing the height of the needle relative to the heated surface ranging from 10 mm to 100 mm.

To generate the voltage and temperature relationship, the thermocouples were calibrated. Three thermocouples were immersed in a glass beaker filled with distilled water. The beaker was placed on a hot plate with a set point of 250°C. All the thermocouples were connected to the data acquisition system. The data acquisition system captured signals from the thermocouples in both temperature and millivolt format. Temperature readings were taken

at interval of 100 ms until the water started boiling at 100°C. All thermocouples readings were consistent within $\pm 0.1^\circ\text{C}$. Having ensured consistency in measurement of all the thermocouples, data acquisition mode for one thermocouple was changed to millivolt while the other one was kept in temperature mode. The data acquisition in millivolt format was preferred to temperature since the sampling time of the system was 5 to 10 times faster. This was particularly beneficial to measure temperature change of the surface when system dynamics were fast and occurred in milliseconds range. The same procedure was continued for 15 minutes until the water boiled and both temperature and millivolt output were recorded. A linear calibration curve was therefore obtained which was used to measure particle surface temperature drop.

3. Computational model

A Volume of Fluid (VOF) approach (Hirt and Nichols, 1981) was adopted in finite volume method based commercial solver ANSYS Fluent (version: 14) as a modelling platform. 3D models in Cartesian coordinates comprising of continuity, momentum and energy equations were solved as follows,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (1)$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot [\mu (\nabla \vec{v} + (\nabla \vec{v})^T)] + \rho \vec{g} + \vec{F}_s \quad (2)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\vec{v} (\rho E + P)) = \nabla \cdot (k \nabla T) + S_h \quad (3)$$

In VOF method, a single energy equation is solved for the mixture phase considering both continuous and discrete phase share the same temperature. Energy of the mixture phase can be expressed as

$$E = \frac{\sum_{q=1}^n \alpha_q \rho_q E_q}{\sum_{q=1}^n \alpha_q \rho_q} \quad (4)$$

Similarly, the mixture density and viscosity are also calculated using the volume fraction of each phase. These can be written as,

$$\rho_{mix} = \rho_l \alpha_l + \rho_g (1 - \alpha_l) \quad (5)$$

$$\mu_{mix} = \mu_l \alpha_l + \mu_g (1 - \alpha_l). \quad (6)$$

Volume fraction of each dispersed phase is solved by the following advection equation,

$$\frac{\partial \rho_l \alpha_l}{\partial t} + \vec{v} \cdot \nabla \rho_l \alpha_l = 0 \quad (7)$$

while the volume fraction of the continuous phase can be calculated from the following mass conservation equation,

$$\sum_{i=1}^n \alpha_q = 1. \quad (8)$$

The momentum equation, in addition to pressure, gravity and viscous stress, contains a surface force which can be written according to continuum surface force model of Brackbill et al. (1992),

$$F_s = \sigma \frac{\rho \kappa \nabla \alpha_l}{0.5(\rho_l + \rho_g)}. \quad (9)$$

The curvature of the interface used in Eq.9 can be expressed in terms of surface normal as follows,

$$\kappa = - \frac{1}{|n|} \left[\left(\frac{n}{|n|} \cdot \nabla \right) |n| - (\nabla \cdot n) \right]. \quad (10)$$

This surface normal however in VOF approach is expressed as gradient of phase volume fraction at the interface and can be written as

$$n = \nabla \alpha_l. \quad (11)$$

Wall adhesion is significant for fluids with non zero contact angle on the surface. This effect can be incorporated in the model expressing unit normal at the wall boundary in terms of unit vectors $\hat{n}_w$ for fluid and $\hat{t}_w$ for wall and the contact angle as follows,

$$\hat{n} = \hat{n}_w \cos(\theta_w) + \hat{t}_w \sin(\theta_w) \quad (12)$$

The computational domain for 3D simulations is presented in Fig. 2. Domain dimensions of the mesh were decided based on the experimental observations of maximum spread diameter of the impinging droplet. A domain size of 12 mm $\times$ 9 mm $\times$ 12 mm was used for 3D

simulations. ICEM CFD meshing tool was used to build the 3D grid because of its capability to generate a hexahedral mesh which in turn allowed resolving the interface more effectively. Minimum orthogonal quality was 0.509 and maximum aspect ratio was 13.42. Total 321538 hexahedral cells were used in the mesh which was found to calculate the droplet volume with less than 1% deviation. Cells were denser near the spherical surface and gradually coarser towards the boundaries for better resolving of the interface near the solid surface. Total 10592 cells were patched to model the droplet in 3D mesh. For 3D simulation of isopropyl alcohol droplet, 4412 cells were patched. Two different cases were simulated - the impact of water and isopropyl alcohol droplet at 20°C, and the impact of isopropyl alcohol and water droplet at 250°C. No slip boundary condition was applied at the particle wall in the cold simulation cases while a free slip condition was applied on the surface in the film boiling regime cases. A contact angle was applied as a wall boundary condition. Pressure inlet boundary condition was applied on all the surrounding faces. For simulating isopropyl alcohol droplet impact, a static contact angle of 0° was used. In case of water, both static contact angle (90°) and an experimentally measured dynamic contact angle profile was used. The vapour layer in the film boiling regime has not been modelled in the current study (see Results and discussion section for detail explanation). Instead, the simplified approach proposed by Karl et al. (1996) was used to simulate film boiling regime cases. A free slip condition was applied on the wall along with a constant contact angle of 180° to model nonwetting behaviour of the vapour layer. Second order upwind scheme was used for discretization of momentum and energy equation. Volume fraction was discretized using Geo-Reconstruct scheme. Pressure was discretized using Presto scheme while pressure-velocity coupling was obtained by SIMPLE scheme. A residual of 10^{-4} was set for convergence of continuity, momentum and volume fraction equations while a residual of 10^{-6} was used for energy equation. All simulations were performed using a time step of 10^{-6} with

20-30 iterations per time step. A first order implicit time stepping method was used in all the simulations.

4. Results and discussions

The effect of Weber number on the dynamics of the droplet impact on a spherical brass particle with controlled surface temperatures of 20°C and 250°C was investigated experimentally and numerically. Three different fluids – water, isopropyl alcohol and acetone were used and droplet impact dynamics were studied in the Weber number range of 8-84, 14-136 and 13-130 respectively. Fig. 4 shows the droplet spreading characteristics of a 15.6 μ L water droplet with corresponding diameter of 3.1 mm on the particle with a surface temperature of 20°C. This experiment was performed at a Weber number of 8. Fig. 4a shows a series of high speed images of the water droplet undergoing shape deformation upon impingement. During the impact phase, the free surface of the droplet deforms continuously due to conversion of impact kinetic energy into surface energy and viscous dissipation. The impact kinetic energy stretches the droplet to the maximum spread diameter which occurs in between 4.3 ms to 7.1 ms. The droplet takes shape of a doughnut at this phase. The peak of droplet visible at 4.3 ms takes a dip at 7.1 ms initiating the recoil phase. The oscillation of droplet primarily occurs due to opposite contributions from inertial and surface force. Considering these two forces, the oscillation period can be estimated from below expression proposed by Schiaffino and Sonin (1997),

$$t_{osc} = \sqrt{\frac{D^3 \rho_l}{\sigma}}. \quad (13)$$

Using above expression, oscillation time was found be 20.6 ms which was 30% higher than the experimentally observed oscillation period of first spreading and recoiling phase. Fig. 4b shows the CFD simulation of the droplet deformation using a static contact angle as the wall boundary condition. Using static contact angle, the simulations cannot fully capture the actual

dynamics of the system. In spreading phase (Fig. 4a: 0-7.1 ms); droplet deforms and spreads rapidly in the radial direction due to sudden rise in pressure at the point of impact (Mao et al., 1997). The impact kinetic energy drives the free surface of droplet resulting into viscous dissipation and increased surface energy. Increase in velocity of three phase contact line results in advancing contact angle greater than sessile state contact angle of 90° . At a later stage, gradual loss of kinetic energy and increased surface force decelerates the droplet spread. At the maximum spread, the further increase in velocity ceases and then surface force retracts the free surface initiating the recoiling phase. Due to reduction in velocity, receding contact angle in this phase (Fig. 4a: 7.1-12.9 ms) decreases below sessile state contact angle of 90° . CFD modeling using a constant contact angle delays in capturing this recoiling phase. This is evident from the Fig. 4b where recoiling phase in the simulation (7.1 ms onwards in the experimental images) using constant contact angle is significantly delayed. This, therefore, clearly explains, why CFD simulations with static contact angle always indicate higher droplet spread ratio when compared to the experimentally measured one. This drawback of delayed prediction of recoiling phase was overcome by incorporating a dynamic contact angle (Fig. 4c). Clearly the dynamics of the system was captured more effectively when a dynamic contact angle boundary condition was used in the simulation.

Fig. 5 shows a comparison between the maximum spread diameters of the water droplet obtained from the experiment (Fig. 4a) and the CFD model predictions using static (Fig. 4b) and dynamic contact angle (Fig. 4c) boundary conditions. The model with static contact angle boundary conditions predicts the maximum spread at a later time than that of the model with the dynamic contact angle boundary condition. This delay is considered to be due to a sluggish movement of the interface as explained earlier. The CFD model predictions improved significantly when the experimentally measured dynamic contact angle profile was imposed hence providing a better agreement with the experimental data. The deviations

occurred using dynamic contact angle model can be attributed to the following possibilities.

(1) An experimentally measured contact angle was imposed as boundary condition. Measuring contact angle was difficult since experimentally it is very difficult to deposit the droplet axi-symmetrically especially at higher Weber numbers. To deal with this, both advancing and receding contact angles were measured on either side of the image (Fig. 3) and an average contact angle profile was used. Implementation of contact line motion in simulation possibly therefore has some mismatch with the actual contact line motion in the experimental images attributing to the deviation in the spread of droplet diameter. (2) Although the brass particles used in the experiments had polished surface with surface roughness of $0.12\ \mu\text{m}$ and surface was thoroughly cleaned before the experiment, the surface might have deteriorated a bit over the duration of experiment giving some extra roughness thus additional friction which prohibits the spread of the droplet. This change in surface roughness has not been accounted in the CFD simulations. Therefore, CFD simulation prediction can be larger compared to the experimental value. (3) As explained in (1), due to difficulty in depositing the droplet exact axi-symmetrically on the top of the particle, the droplet spread diameters calculated from images are little different than those calculated from CFD simulations where the droplet spread was calculated based on axi-symmetric position of the droplet on the particle surface.

The effect of Weber number on the dynamic contact angle of 3.1 mm water droplet spreading on the particle at a surface temperature of 20°C is shown in Fig. 6. During the first spreading and recoiling phase, droplet reached the maximum spread diameter at a faster rate. This was followed by a weak recoiling phase maintaining a lower contact angle with the surface over the remaining period of deformation. The contact angle at the equilibrium state therefore reduced from 40° to below 20° as the Weber number increased from 8 to 84 indicating greater spread at higher Weber numbers.

The spreading behaviour of a 2.1 mm in diameter isopropyl alcohol droplet was also studied at 20°C surface temperature. Fig. 7a shows the spreading behaviour of the isopropyl alcohol droplet obtained experimentally. Contrary to water, isopropyl alcohol droplet does not show oscillating type surface deformation pattern. This can be attributed to its lower surface tension (i.e. less than 1/3rd of the water surface tension) which leads to a weaker surface force preventing a retract from the particle surface. That in turn leads to a continual spread of the isopropyl alcohol droplet resulting in a complete wetting of the surface even at low Weber numbers. Also, the isopropyl alcohol viscosity is almost twice as much as the water viscosity and hence all the impact kinetic energy is expected to convert to viscous dissipation. Fig. 7b presents the CFD simulations of isopropyl alcohol spreading behaviour which is in good agreement with the experimental observations.

Generally, the droplet impingement on a heated surface involves both heat and mass transfer phenomena coupled with the fluid flow dynamics. To gain a better insight into these phenomena the evaporation of a softly deposited water droplet (height of fall < 10mm) on the surface of the particle was studied at a surface temperature of 100°C. Average evaporation time of the water droplet was obtained from the surface temperature drop recorded by the data acquisition system. The droplet was deposited when the surface attained the steady state temperature according to the set point and varies within +/- 0.5°C. Fig. 8 shows the change in particle surface temperature during the droplet impingement process. First, a sharp fall in the surface temperature was observed as the droplet undergoes evaporation. The time associated with the fall in the surface temperature is the droplet evaporation time. The surface temperature then regained its initial temperature following the droplet evaporation. The average evaporation time for the water droplet at the surface temperature of 100°C was measured to be 30.27s. Theoretically, the evaporation time of a water droplet can be

estimated by classical D^2 law (Faeth, 1977; Sirigano, 1999) which is stated as follows,

$$\frac{dD^2}{dt} = -K \quad (14)$$

where K is given by,

$$K = \frac{8\rho D_{AB}}{\rho_l} \ln\left(\frac{1-y_{A,\infty}}{1-y_{A,sat}}\right). \quad (15)$$

Mole fraction (y) of water at saturation temperature and ambient temperature can be obtained from the following expression,

$$y_{water} = \left(\frac{M_{water}}{M_{air}}\right) \left(\frac{P_{sat}}{P_{atm}}\right) \quad (16)$$

where saturation pressure (P_{sat}) for water at different temperature can be obtained from Antoine's equation,

$$\log_{10} p_{sat} = A - \frac{B}{T-C} \quad (17)$$

where Antoine's coefficients for water are $A = 8.07131$, $B = 1730.63$ and $C = 233.426$.

Diffusivity (D_v) of water can be obtained from correlation proposed by Hall and Pruppacher (1976) as follows,

$$D_v = 2.11 \times 10^{-5} \left(\frac{T}{T_0}\right)^{1.94} \left(\frac{P_0}{P}\right) \quad (18)$$

Eq. 14 can be integrated in the time limit of 0 to t and droplet diameter of D_0 to 0 to obtain evaporation time using the physical properties given in Table 1. Using this expression, evaporation time of the droplet was found to be 25.8 s which was comparable with the experimental result.

Similar to cold surface study at 20°C (Fig. 4), impact dynamics of water droplet were studied at four different surface temperatures - 125°, 150°, 175° and 250°C (Fig. 9) in the Weber number range of 8-84. Fig. 9a presents water droplet impingement behaviour on the particle at the surface temperature of 125°C. At a low Weber number (We-8) (Fig. 9a), initially (1.4 ms – 11.4 ms), the droplet displayed similar shape evolution to that of the cold case at surface temperature of 20°C (Fig. 4a) with very little nucleate boiling being observed

in this phase. In later stage of the oscillation phase in the time interval of 5.7-25.7 ms (images after 11.4 ms not shown), the water droplet was sufficiently heated up and began vibrating due to formation of small vapour bubbles at the contact area. This was followed by the droplet sliding off the surface due to an increase in the vibration frequency of small vapour bubbles. An increase in the Weber number at the same time interval increased the droplet spread and hence the contact area with the surface which ultimately improved the heat transfer efficiency. At Weber number of 42, droplet spread was more and some tiny secondary droplets were observed around the droplet due to increased boiling (t : 11.4 ms). A major mass of the droplet was repeatedly observed to leave the surface afterwards due to increases boiling without being evaporated. At higher Weber number (We -84), the water droplet rapidly reached the maximum spreading phase (t : 4.3 ms) creating a thin liquid film over the surface while the most of the liquid mass accumulated at the periphery. This thin liquid film evaporated soon leading to disintegration of the droplet into smaller satellite droplets. Due to higher impact kinetic energy, these smaller droplets left the surface without much evaporation. The droplet impact dynamics at the surface temperature of 150°C are presented in Fig. 9b. Due to the increased surface temperature, the rapid boiling with interface tearing was found to be the predominant phenomenon. Boiling occurred during the first spreading phase. Due to higher temperature differences between the droplet and the surface, vapour bubble generation was fast at the contact area which tore off the free surface and ejected tiny subcooled secondary liquid droplets. The droplet was found to slide off the surface due to increased vibration. Rupture of interface was more prominent at higher Weber numbers (We -42 to 84) due to an increase in heat transfer area. At surface temperature of 175°C , droplet exhibited similar characteristics however boiling was more intense due to an increased temperature gradient between the droplet and the surface. Similar surface

deformation was observed at Weber numbers 8-42. At Weber number 84, the water droplet disintegrated into multiple satellite droplets after reaching the maximum spreading phase.

Droplet spread factor is an important parameter which determines surface wettability and depends on impact Weber number. The maximum water droplet spread diameter at the surface temperature of 125°, 150°, 175° and 250°C in the Weber number range of 8-84 are presented in Fig. 10. It can be seen that the spread diameter in all these cases increases with an increase in Weber number. The observed trend can be attributed to increase in the droplet surface deformation which is driven by an increase in the impact kinetic energy. The experimental data for maximum spread diameter of the water droplet were also compared with the existing correlations of Akao et al. (1980) and Chandra et al. (1991). These two correlations are given below.

$$\beta_{max} = 0.613We^{0.39} \quad (19)$$

$$\frac{3We}{2Re}\beta_{max}^4 + (1 - \cos\theta)\beta_{max}^2 - \left(\frac{We}{3} + 4\right) = 0 \quad (20)$$

In general, prediction of Akao et al.'s (1980) correlation was in a better with the experimental data at all temperatures compared to Chandra et al.'s (1991) correlation. Deviations were lower for Akao et al.'s (1980) correlation (deviations: 5-17% (20°C), 9-26% (125°C), 3-26% (150°C), 6-25% (175°C) and 11-24% (250°C)) compared to Chandra et al.'s (1991) correlation (deviations: 30-80% (20°C), 45-74% (125°C), 18-33% (150°C), 35-61% (175°C) and 54-108% (250°C)) which was found to over-predict at all temperatures. The reason, Akao et al.'s (1980) correlation predicts better because it is empirical in nature and correlated over wide range of data up to 400°C while Chandra et al.'s (1991) correlation is based on purely theoretical consideration of energy conservation. The correlation is derived equating kinetic and surface energy of the droplet before impact to surface energy and viscous dissipation

after impact. Also the viscous dissipation term in the equation includes an assumed velocity profile. All these aspects can be attributed to larger deviations found in the prediction by Chandra et al.'s (1991) correlation.

Fig. 11 presents fall in particle surface temperature during droplet impact at different Weber numbers. At surface temperature of 125°C, temperature drop varied in the range of 7.5-8.9°C. Temperature drop is observed to increase somewhat at higher Weber numbers due to increase in wetted surface area. At higher Weber numbers close to 84 (Fig. 9a) however, the droplet upon impingement disintegrated into smaller droplets and left the surface without much evaporation which led to relatively smaller drop in surface temperature. At surface temperature of 150°C, temperature drop following the droplet impact on the particle over the entire range of Weber numbers was found to be relatively lower (4.5-7.5°C). This can be attributed to the lower residence time of the droplet on particle surface due to increased rate in vapour generation (Fig. 9b) in the contact area which forces the droplet to slide off the surface. Increasing Weber number also increases wetted contact area hence boiling. When surface temperature is further increased to 175°C, more vapour bubbles form at the contact area and subsequent explosions of these vapour bubbles cause intense vibrations and generate many subcooled tiny satellite droplets around (Fig. 9c). This phenomenon leads to shorter contact time period between the droplet and the hot surface which results in much smaller changes in surface temperature. This boiling regime can be considered as a transition boiling regime where presence of the vapour film at the contact area reduces the heat transfer significantly. This argument is supported by the small surface temperature drop in the range of 0.95-1.8°C which was also found to be almost independent of the droplet impact Weber numbers.

Quantifying heat transfer coefficient during droplet particle impact is critical in many applications. Based on the measured temperature difference (ΔT) of the particle and wetted

contact area (A_w) and assuming negligible heat loss to surrounding, following energy balance equation can be written,

$$m_p C_p \frac{dT}{dt} = h A_w (T_s - T_d) \quad (21)$$

where m_p is the particle mass, C_p is particle heat capacity, h is the heat transfer coefficient and T_s and T_d are particle surface and droplet temperatures respectively. The wetted contact area (A_w) is calculated from the images considering spherical cap geometry of the spreading liquid film. Fig. 12 presents the heat transfer coefficients calculated from Eq.21 for three different surface temperatures in the Weber number range of 8-84. Heat transfer coefficients are found to decrease with Weber numbers at increasing surface temperatures. As explained earlier, with increase in surface temperature, boiling regime shifts from nucleate boiling to towards film boiling which due to generation of more vapour bubbles at the contact area significantly reduces surface temperature drop hence the heat transfer coefficient.

When surface temperature remains much higher than the saturation temperature of the droplet, a stable vapour film is formed at the contact area between the droplet and the particle surface. The vapour acts as an insulating film which significantly reduces the heat transfer process. In the absence of the direct contact between the liquid and the solid surface, nucleation and hence boiling is prevented. Droplet in this state evaporates slowly (Biance et al., 2003). This is the well known Leidenfrost phenomenon which is the characteristic of the film boiling regime. To gain a better insight into this phenomenon, the water droplet impact at surface temperature of 250°C was investigated both experimentally and computationally. Fig. 13a presents the high speed images of the water droplet behaviour upon impingement on the particle at the surface temperature of 250°C. The Weber number in this case was 8. The droplet upon impact underwent free surface deformation similar to the cold case however during the recoiling phase, the droplet continued to elongate axially until it lost contact with the surface. Due to a very high temperature difference between the droplet and the particle

surface, the rate of the vapour generation at the contact area is significantly high which leads to high pressure drop in the vapour film formed beneath the droplet by the end of the first spreading phase. Due to the presence of a stable vapour film, the particle surface becomes strongly hydrophobic and the droplet floats on the vapour cushion resulting into a contact angle $\sim 180^\circ$. At the lower Weber number regime (lower normal component of the droplet impact velocity), during the recoiling phase, the pressure drop in the vapour film deforms the droplet surface resulting in increase in surface energy. Eventually this excess surface energy overcomes weight of the entire droplet and the droplet rebounds off the surface. Fig. 13b compares the CFD simulations of the droplet spreading pattern with the experimental observations. Clearly, there is a good agreement between the model predictions and the experimental data. It should be noted that for the purpose of simplification in the present CFD simulations, a separate vapour model (Harvie and Fletcher, 2001; Ge and Fan, 2005, 2006) was not considered. Generally, the vapour layer thickness is much smaller than the droplet radius. Based on the operating conditions, the vapour layer thickness can be estimated using the expression developed by Biance et al. (2003):

$$e \sim \left(\frac{D}{2}\right)^{4/3} \left[\frac{(T_s - T_d) \rho_l g \mu_{vap} k_{vap}}{\sigma^2 L \rho_v} \right]^{1/3} \quad (22)$$

Considering surface temperature of 250°C and droplet temperature 20°C and using physical properties given in Table-1, water vapour film thickness (e) was estimated to be ~ 10 microns. In order to resolve the vapour layer with VOF simulation, grid element size of at least 2 microns (considering at least 5 cells) is required near the droplet-particle interface, leading to significant increase in computation time. Instead, a simpler approach was adopted in the current work. Considering that in the film boiling regime a stable vapour film always exists at the droplet and the surface contact area, and that the droplet floats on the vapour cushion underneath, a free slip condition was imposed on the wall boundary instead of the

no-slip condition. The presence of the vapour film at the contact area prevents wetting of the surface hence a contact angle of 180° was also applied on the wall as a boundary condition to implement a non-wetting state. This approach was also used by Karl et al. (1996) in their VOF simulations of droplet impingement on hot wall in Leidenfrost regime. Chandra and Avedisian (1991) also reported an increase in the contact angle with a rise in the surface temperature approaching 180° at a very high wall temperature. The CFD model was also tested for higher Weber number. Fig. 14a compares disintegration characteristics of water droplet at the Weber number of 84. Because of the high impact kinetic energy associated with high Weber numbers, the droplet spreads on the surface like a thin film accumulating most of the mass near the periphery and splashes as soon as the film evaporates. The CFD model (Fig. 14b) also predicts the disintegration of the droplet providing good agreements with the experimental observations. The surface temperature drop in the film boiling regime could not be measured due to limitation of thermocouple time constant. However as shown in the case of 175°C , the change in surface temperature is expected to be very low because of the vapour film resistance which leads to a pure non-wetting contact. Fig. 15 presents, deformation behaviour of a 2.1 mm isopropyl alcohol droplet upon impingement ($We=15$) on the surface at the same operating conditions. The isopropyl alcohol droplet deformed similar ($t: 0-9$ ms) to the water droplet however due to lower surface tension, exhibited greater shape change similar to a bowling pin during the rebound phase ($t: 15-21$ ms). Unlike water, the isopropyl alcohol and acetone droplet's shape deformed while in air with periodic axial contraction and expansion due to opposing effect of kinetic energy and surface energy with gradually decay in the amplitude of oscillation till it fell back on the ground again (not shown in the images). These deformations of isopropyl alcohol droplet were also captured by the CFD model providing good agreement with experimental visualizations. While water droplets were found to disintegrate at Weber number > 50 , isopropyl alcohol and acetone droplets disintegrated at

Weber number close to 80. The increase in the surface temperature leads to early droplet disintegration during the spreading phase due to quick evaporation of the liquid film. Hence in the film boiling regime the contact time between the droplet and the surface was observed to reduce significantly with an increase in the Weber number. This observation is presented in Fig. 16. However, the change in contact time was relatively smaller at the higher Weber numbers. Isopropyl alcohol and acetone droplets were found to have more contact time compared to water in the similar range of Weber numbers. This can be explained by lesser surface tension of isopropyl alcohol and acetone which lead to sluggish recoiling of droplet. Residence time of a droplet on the particle surface in the film boiling regime can be estimated by the first order vibration time (Wachters et al., 1966) which is expressed as follows,

$$\tau = \pi \left(\frac{\rho_l D^3}{16\sigma} \right)^{1/2}. \quad (23)$$

Using physical properties given in Table 1, residence times of 16 ms, 13 ms and 14 ms were obtained for water, acetone and isopropyl alcohol droplets respectively. The natural vibration time was found comparable for water in the Weber number < 30 . However, at Weber number > 30 , residence time was found to be less than half of the estimated time to the limit of Weber number used in the experiment. Estimated natural vibration time for acetone and isopropyl alcohol droplet was found to deviate largely at higher limit of Weber number. The droplet contact time for the film boiling regime is lower than nucleate boiling regime. This difference leads to lesser evaporation, and the corresponding surface temperature drop is smaller. Schlieren imaging technique was used to identify vapour region around the droplets. Fig. 17 presents series of images of a 2.1 mm acetone droplet impacting (We-39) on the particle at the surface temperature of 150°C. Acetone was chosen because of higher refractive index of its vapour (1.001090) than air (1.000292) which made it possible to detect the vapour zone. The gradient in refractive indices normal to knife edge created corresponding brightening and darkening regions in the images. The grey pixel values in these regions were different than

the background pixel values. A distinct boundary of acetone vapour region from air therefore could be marked. A simple linear calibration method was followed. The background pixel values were subtracted from all the images and 100% mass fraction of acetone vapour was assigned on droplet interface and solid surface after impingement and 0% mass fraction of acetone vapour was assigned to the background. The masked images (Fig. 17a) clearly identify the boundary of the droplet and the surface while Fig. 17b shows the vapour region around the droplet. Due to high vapour pressure of acetone, even at room temperature, significant vaporization is observed in the vicinity of droplet. However, the evaporation rate increases many times when droplet impinges on the hot particle surface indicating higher mass fraction of vapour near the droplet surface and gradually lower mass fraction in the bulk. Due to Leidenfrost effect, the droplet rebounds off the surface leaving off clearly visible vapour trail behind. Fig. 18 shows impingement of acetone at higher Weber number ($We=78$) on the surface heated at 250°C . Vapour regime is visible (Fig 18b) around the droplet trajectory however the background contribution due higher refractive index of air could not be completely eliminated in this case. The refractive index of the medium changes with temperature and background contribution thus becomes significant at higher surface temperature. The droplet disintegrates into smaller droplets upon impingement and all the droplets rebound leaving the visible vapour trail behind. Schlieren imaging thus identifies vapour region around the evaporating droplet which can further be used to quantify both concentration and temperature by suitable image processing techniques.

6. Conclusions

The impact of water, isopropyl alcohol and acetone micro-litre droplet on a heated spherical brass particle in the temperature range of $20\text{-}250^{\circ}\text{C}$ were studied both experimentally and numerically. Inclusion of dynamic contact angle in the CFD model was found to be in better

agreement in cold case simulation of droplet shape evolution with experimental observations by correctly predicting the recoiling phase compared to static contact angle model. Droplet shape deformation and associated heat transfer phenomena during impact on the particle surface was investigated over a range of Weber number. Maximum spreads of the water droplet were compared with correlations of Akao et al. (1980) and Chandra et al. (1991). Akao et al.'s (1980) correlation was found to agree well with the experimental data compared to the Chandra et al.'s (1991) model. Depending on the surface temperature, wetting and non-wetting contact were observed. Wetting contact was observed when surface temperature was in the range of room temperature to nucleate boiling regime. Surface temperature change was found to be significant in this temperature range. In the film boiling regime however surface wetting was prevented by a thin vapour film at the contact area which led to a smaller temperature drop at the surface. Heat transfer coefficient during impact of droplet on the particle surface decreased with increase in Weber number however the change became relatively smaller towards higher Weber numbers and higher surface temperatures. Due to smaller temperature drop, heat transfer coefficient was found to reduce several times towards the film boiling regime. Contact time of droplet was observed to decrease with increasing Weber number. Two cases were simulated – droplet impacting at room temperature and film boiling regime. In lieu of a vapour flow model, a free slip condition at the contact area and a contact angle of 180° were applied to simulate film boiling phenomena. Droplet rebound and disintegration phenomena at lower and higher Weber numbers respectively were captured by the CFD simulations which agreed well with the high speed images from the experiments. Although a very small fraction of liquid is evaporated in the film boiling regime, a distinct vapour concentration profile around the rebounding acetone droplets was captured by Schlieren imaging technique which can be used for quantifying both concentration and temperature by using suitable image processing algorithm.

Acknowledgement:

The authors gratefully acknowledge the financial support from Australian Research Council (ARC) and British Petroleum (BP), Kwinana, Western Australia for this work.

Notation:

C_p	heat capacity
D	droplet diameter
D_v	diffusivity
e	vapour layer thickness
E	energy
F_s	surface tension force
g	gravitational constant
k	thermal conductivity
L	latent heat of evaporation
m_p	mass of particle
M	molecular weight
Oh	Ohnesorge number
P	pressure
R	initial radius of the droplet
T	temperature
Re	Reynolds number
u	droplet velocity
v	fluid velocity
S_h	energy source term

t	time
We	Weber number
y	mole fraction of vapour component

Greek letters

α	volume fraction
β	maximum spread ratio ($D/D_{\max}$)
ρ	density
μ	viscosity
σ	surface tension
κ	surface curvature
θ	contact angle
τ	vibration time

Subscript

0	initial state
∞	bulk state
d	droplet
g	gas
l	liquid
max	maximum
osc	oscillation
q	q^{th} phase
sat	saturation
s	surface
v	vapour

References

- Akao et al., 1980. Deformation behaviours of a liquid droplet impinging on to hot metal surface. *Transactions of Iron and Steel Institute of Japan*, 20, 737-743.
- Bechtel, S.E., Bogy, D.B., Talke, F.E., 1981. Impact of a liquid drop against a flat surface. *IBM Journal of Research and Development* 25 (6), 963-971.
- Bernardin, J.D., Mudawar, I., 1999. The Leidenfrost point: experimental study and assessment of existing models. *Transaction of the ASME, Journal of Heat Transfer* 121, 894-903.
- Biance, A-L., Clanet. C., Quere, D., 2003. Leidenfrost drops. *Physics of Fluids* 15 (6), 1632-1637.
- Blake, T. D, Haynes, J.M. 1969. Kinetics of Liquid/Liquid Displacement, *Journal of Colloid and Interface Science*, 30 (3), 421-423.
- Brackbill, J.U., Kothe, D.B., Zemach, C., 1992. A continuum method for modelling surface tension. *Journal of Computational Physics* 100, 335–354.
- Buchanan, S.J., 1994. Analysis of heating and vaporization of feed droplets in fluidized catalytic cracking risers. *Ind. Eng. Chem. Res.* 33, 3104-3111.
- Bussmann, M., Mostaghimi, J., Chandra, S., 1999. On a three dimensional volume tracking of droplet impact. *Physics of Fluids* 11 (6), 1406-1417.
- Chandra, S., Avedisian, C.T., 1991. On the collision of droplet with solid surface. *Proceedings of Royal Society London A* (432), 13-41.
- Chandra, S., Avedisian, C.T., 1992. Observation of droplet impingement on a ceramic porous surface. *International Journal of Heat and Mass Transfer* 35 (10), 2377-2388.
- Chen, R-H., Chiu, S-L., Lin, T-H., 2007a. Resident time of a compound drop impinging on hot surface. *Experimental Thermal and Fluid Science* 32, 587-595.

- Chen, R-H., Chiu, S-L., Lin, T-H., 2007b. On the collision behaviour of a diesel drop impinging on hot surface. *Applied Thermal Engineering* 27, 2079-2085.
- Clanet, C. et al., 2004. Maximal deformation of an impacting drop. *Journal of Fluid Mechanics* 517, 199-208.
- Cox, R. G., 1986. The dynamics of the spreading of liquids on a solid surface. Part 1. Viscous flow. *Journal of Fluid Mechanics* 168, 169-194.
- Crafton, E.F., Black, W.Z., 2004. Heat transfer and evaporation rates of small liquid droplets on heated horizontal surfaces. *International Journal of Heat and Mass Transfer* 47, 1187-1200.
- Faeth, G. M., 1977. *Progress of Energy Combustion Science* 3, 191.
- Fujimoto, H. et al., 2010. Hydrodynamics and boiling phenomena of water droplets impinging on hot solid. *International Journal of Multiphase Flow* 36, 620-642.
- Fukai, J. et al., 1993. Modelling of the deformation of a liquid droplet impinging upon a flat surface. *Phys. Fluids A* 5 (11), 2588-2599.
- Fukai, J. et al., 1995. Wetting effects on the spreading of a liquid droplet colliding with a flat surface : experiment and modelling. *Physics of Fluids* 7 (2), 236-247.
- Gao, J. et al., 2001. Simulations of gas-liquid-solid 3-phase flow and reaction in FCC riser reactors. *AIChE Journal*, 47 (3), 677-692.
- Ge, Y., Fan, L-S., 2005. Three dimensional simulation of impingement of a liquid droplet on a flat surface in the Leidenfrost regime. *Physics of Fluids* 17 (027104), 1-20.
- Ge, Y., Fan, L-S., 2006. 3-D modelling of dynamics and heat transfer characteristics of subcooled droplet impact on a surface with film boiling. *International Journal of Heat and Mass Transfer* 49, 4231-4249.
- Ge, Y., Fan, L-S., 2007. Droplet-particle collision dynamics with film boiling evaporation. *Journal of Fluid Mechanics* 573, 311-337.

- Gottfried, B.S., Lee, C.J., Bell, K.J., 1966. The phenomenon : film boiling of liquid droplets on a flat plate. *International Journal of Heat and Mass Transfer* 9, 1167-1187.
- Gray, M.R., Le, T., McCaffrey, W.C., Berruti, F., Soundararajan, S., Chan, E., Huq, I., Thorne, C., 2001. Coupling of mass transfer and reaction in coking of thin films of an Athabasca vacuum residue. *Ind. Eng. Chem. Res.* 40, 3317–3324.
- Hall, W. D., Pruppacher, H. R., 1976. The survival of ice particles falling from cirrus clouds in subsaturated air. *Journal of Atmospheric Science* 33, 1995–2006.
- Harvie, D.J.E., Fletcher, D.F., 2001. A hydrodynamic and thermodynamic simulation of droplet impacts on hot surfaces, part-I: theoretical model. *International Journal of Heat and Mass Transfer* 44, 2633-2642.
- Harvie, D.J.E., Fletcher, D.F., 2001. A hydrodynamic and thermodynamic simulation of droplet impacts on hot surfaces, part-II: validation and applications. *International Journal of Heat and Mass Transfer* 44, 2643-2659.
- Hatta, N. Et al.,1995. Collision dynamics of a water droplet impinging on a rigid surface above Leidenfrost temperature. *Iron and Steel Institute of Japan* 35, 50-55.
- Hatta, N. Et al.,1997. Experimental study of deformation mechanism of a water droplet impinging on hot metallic surfaces above Leidenfrost temperature. *Transaction of ASME Journal of Fluids Engineering* 119, 692-699.
- Hayes, R. A., Ralston, J., 1994. The molecular-kinetic theory of wetting, *Langmuir* 10, 340-342.
- Hirt, C.W., Nichols, B.D., 1981. Volume of fluid (VOF) method for the dynamics of free boundaries. *Journal of Computational Physics* 39, 201–225.
- Kang, B. S., Lee, D.H., 2000. On the dynamic behaviour of a liquid droplet impacting upon an inclined heated surface. *Experiments in Fluids* 29, 380-387.

- Karl, A. et al., 1996. Deformation of liquid droplets during collisions with hot walls: experimental and numerical results. *Particle and Particle System Characterization* 13, 186.
- Karl, A., Frohn, A., 2000. Experimental investigation of interaction process between drops and hot walls. *Physics of Fluids* 12, 785-796.
- Kelly-Zion, P. L. et al., 2009. Evaporation rates of pure hydrocarbon liquids under the influences of natural convection and diffusion. *International Journal of Heat and Mass Transfer* 52, 3305-3313.
- Kim, H.Y., Chun, J.H., 2001. The recoiling of liquid droplets upon collision with solid surfaces. *Physics of Fluids* 13 (3), 643-659.
- Lunkad, S.F., Buwa, V.V., Nigam, K.D.P, 2007. Numerical simulation of drop impact and spreading on horizontal and inclined surfaces. *Chemical Engineering Science* 62, 7214-7224.
- Mao, T., Kuhn, C.S., Tran,H., 1997. Spread and rebound of liquid droplets upon impact on flat surfaces. *AIChE Journal* 43 (9), 2169-2179.
- McHale, G., Rowan, S.M., Newton, M.I., 1994. Frenkel's method and spreading of small spherical droplets. *Journal of Physics, D: Applied Physics*, 2619-2623.
- Mirgain, C. et al., 2000. Modelling of feed vaporization in fluid catalytic cracking. *Ind. Eng. Chem. Res.* 39, 4392-4399.
- Mundo, C., Sommerfield, M., Tropea, C., 1995. Droplet-wall collisions: experimental studies of the deformation and breakup process. *International Journal of Multiphase Flow* 21 (2), 151-173.
- Nayak, V. S. et al., 2005. Modelling of vaporization and cracking of liquid oil injected in a gas–solid riser. *Chem. Eng. Sci.* 60, 6049-6066.
- Pasandideh-Fard, M. et al., 1996. Capillary effects during droplet impact on a solid surface. *Physics of Fluids* 8 (3), 650-659.

- Petrov, P. G. and Petrov J. G., 1992. A Combined Molecular-Hydrodynamic Approach to Wetting Kinetics, *Langmuir* 8, 1762-1767.
- Pismen, L.M., Rubinstein, B.Y., 2001. Kinetic slip conditions, van der Waals forces, and dynamic contact angle. *Langmuir* 17, 5265-5270.
- Scheller, B.L., Bousfield, D.W., 1995. Newtonian drop impact with a solid surface. *AIChE Journal* 41 (6), 1357-1367.
- Schiaffino, S., Sonin, A.A., 1997. Molten droplet deposition and solidification at lower Weber numbers. *Physics of Fluids* 9, 3172-3187.
- Shi, M.H., Bai, T.C., Yu, J., 1993. Dynamic behaviour and heat transfer of a liquid droplet impinging on a solid surface. *Experimental Thermal and Fluid Science* 6, 202-207.
- Shikhmurzaev, Y.D., 1997. Spreading of drops on solid surfaces in quasi-static regime. *Physics of Fluids* 9 (2), 266-275.
- Sikalo, S. et al., 2002. Analysis of impact of droplets on horizontal surface. *Experimental Thermal and Fluid Science* 25, 503-510.
- Sikalo, S. et al., 2005. Dynamic contact angle of spreading droplets: experiment and simulations. *Physics of Fluids* 17 (062103), 1-13.
- Sirignano, W.A., 1999, *Fluid Dynamics and Transport of Droplets and Sprays*. Cambridge University Press, Cambridge.
- Tanner, L. H., 1979, The spreading of silicone oil drops on horizontal surfaces. *Journal of Physics D: Applied Physics* 12, 1473-1484.
- Tanner, L. H., 1986, An edge angle and velocity relation for silicone oil films for the full angular range. *Journal of Physics D: Applied Physics* 19, 751-760.
- V. Dusan E.B., 1979. On the spreading of liquids on solid surfaces: static and dynamic contact lines. *Annual Review of Fluid Mechanics* 11, 371-400.

- Vadillo, D.C. et al., 2009. Dynamic contact angle effects onto the maximum drop impact spreading on solid surfaces. *Physics of Fluids* 21 (122002), 1-8.
- Voinov, O. V., 1976. Hydrodynamics of Wetting, *Journal of Fluid Dynamics* 11, 714-721.
- Wachters, L.H.J., Bonne, H., Nouhuis van, H.J., 1966. The heat transfer from a hot horizontal plate to sessile water drops in the spheroidal state. *Chemical Engineering Science* 21, 923-936.
- Yu, Z., Ge, Y., Fan, L-S., 2007. Multi-scale simulation of oblique collisions of a droplet on a surface in the leidenfrost regime. *Chemical Engineering Science* 62, 3462-3472.

List of Figures

Fig. 1. Schematic diagram of the experimental set up – a) light source b) diffusing screen c) syringe pump d) hypodermic needle e) heating billet f) brass particle g) thermocouple -1 h) thermocouple -2 i) variac j) controller k) data acquisition system l) camera m) computer n) parabolic mirror o) knife edge.

Fig. 2. a) 3D Computational domain used for simulation b) sectional view of the hexahedral mesh indicating boundary conditions.

Fig. 3. Measurement of contact angle and maximum spread diameter from images.

Fig. 4. Comparison of water droplet (3.1 mm) spreading characteristics at 20°C (We-8) a) experimental images (1400 fps) and b) CFD simulations using static contact angle c) CFD simulations using dynamic contact angle.

Fig. 5. Comparison of maximum spread diameter of water droplet at We-8 obtained from experiments and CFD simulations.

Fig. 6. Comparison of dynamic contact angles of a water droplet (3.1 mm) on particle surface (20°C) during first spreading and recoiling phase at Weber number 8, 42 and 84.

Fig. 7. Comparison of an isopropyl alcohol droplet (2.1 mm) spreading characteristics at 20°C (We -15) a) experimental images (1400 fps) and b) CFD simulation.

Fig. 8. Fall in particle surface temperature when a water droplet (3.1 mm) is softly deposited on the particle surface heated at 100°C.

Fig. 9. Shadowgraphy images (1400 fps) of a water droplet (3.1 mm) spreading characteristics at two different time intervals (1.4ms and 11.4 ms) on the particle surface heated at a) 125°C at b) 150°C and c) 175°C at We-8, 42 and 84.

Fig. 10. Comparison of a water droplet (3.1 mm) spreading characteristics at 20°C, 125°C, 150°C, 175°C and 250°C with correlations of Akao et al. (1980) and Chandra et al. (1991).

Fig. 11. Fall in particle surface temperature heated at 125°C, 150°C and 175°C due to impact of a water droplet (3.1 mm) at different Weber numbers.

Fig. 12. Heat transfer coefficients during impact of a water droplet (3.1 mm) on the particle surface heated at 125°C, 150°C and 175°C at different Weber numbers.

Fig. 13. Comparison of water droplet (3.1 mm) levitation characteristics (We-8) at particle surface temperature of 250°C a) high speed images (1000 fps) and b) CFD model predictions.

Fig. 14. Comparison of water droplet (3.1 mm) disintegration characteristics (We-84) at particle surface temperature of 250°C a) high speed images (1000 fps) and b) CFD model predictions.

Fig. 15. Comparison of experimental images (1000 fps) and CFD simulations of an isopropyl alcohol droplet (2.1 mm) levitation characteristics at 250°C (We-14).

Fig. 16. Contact time of isopropyl alcohol (2.1 mm), acetone (2.1 mm) and water (3.1 mm) droplet on particle surface at 250°C.

Fig. 17. Schlieren imaging of an acetone droplet (2.1 mm) impacting (We: 39) on heated particle surface at 150°C. (a) Masked images indicate droplet and surface profile (b) calibrated images indicate mass fractions of vapour around droplet trajectory.

Fig. 18. Schlieren imaging of an acetone droplet (2.1 mm) impacting (We: 78) on heated particle surface at 250°C. (a) Masked images indicate droplet and surface profile (b) calibrated images indicate mass fractions of vapour around droplet trajectory.

Fig. 1

Pressure inlet

Pressure inlet

Pressure inlet

Wall

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

Fig. 8

(a)

(b)

(c)

Fig. 9

Fig. 10

Fig. 11

Fig. 12

(a)

(b)

$t = 3 \text{ ms}$

$t = 6 \text{ ms}$

$t = 9 \text{ ms}$

$t = 12 \text{ ms}$

$t = 18 \text{ ms}$

Fig. 13

$t = 0 \text{ ms}$

$t = 2 \text{ ms}$

$t = 4 \text{ ms}$

$t = 6 \text{ ms}$

$t = 8 \text{ ms}$

(a)

(b)

Fig. 14

Fig. 15

Fig. 16

Fig. 17

Fig. 18

List of Tables

Table 1: Physical properties of fluids at 1 atm pressure. Liquid properties are specified at 20°C and Vapour properties are specified at 250°C. (Physical properties are obtained from ASPEN HYSYS (ver V7.3) using UNIQUAC property package for isopropyl alcohol and acetone and ASME Steam property package for water.)

Table 1

Physical properties	Water vapour	Water	Isopropanol	Acetone
Density (kg/m ³)	0.421	998.2	780.8	785
Viscosity (Pa.s)	1.82×10^{-5}	0.001	0.0022	0.0032
Surface tension (N/m)	-	0.0735	0.0236	0.0249
Heat capacity (kJ/kg/K)	1.99	4.2	3.099	1.989
Thermal conductivity (w/m/K)	0.0386	0.6	0.1405	0.1596
Latent heat of evaporation (kJ/kg)	-	2257	663.3	501.9
Boiling point (°C)	-	100	82	56