EFFECT OF SURFACE HYDROPHOBICITY ON HEAT TRANSFER DURING DROPWISE CONDENSATION: A NUMERICAL STUDY

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ABSTRACT

Formation of individual droplets at specified nucleation sites, with the area in-between these droplets essentially remaining dry/inactive, is one of the popularly acceptable mechanism of dropwise condensation on a hydrophobic surface. Accordingly, heat transfer is postulated to occur only through these individual droplets. While there are a series of thermal resistances in the path of condensing vapor releasing its latent heat to the cold substrate, the most dominant is the diffusional resistance of the liquid droplet; this necessitates accurate 3D modeling of this dominant resistance. The diffusional resistance is a strong function of the droplet size and its shape, the latter guided by degree of hydrophobicity of the liquid-substrate combination. Once this detailed information of the effect of hydrophobicity on heat transfer through individual droplets is discerned, an ensemble of various generations of these droplets can then be handled, to simulate the entire engineering process of quasi-steady state dropwise condensation.

In the context of estimation of the diffusion resistance, 3-D Energy Equation on unstructured tetrahedral grid representing the individual droplets on a hydrophobic surface has been solved. Simulation parameters include the Bond Number, apparent contact angles (degree of hydrophobicity), liquid Prandtl numbers and degree of subcooling, has been considered to study the effect of these parameters on the heat transfer through individual drops. The database so generated is used to correlate the conduction resistance of droplets with the independent parameters by regression. These correlations are then incorporated into a previously developed model of complete dropwise condensation process of the authors (Sikarwar et al., 2011), to get the local/average heat transfer coefficient during quasi-steady state dropwise condensation process on large flat surfaces. Here, we also investigate the effect of nucleation site density, varied from $10^4/cm^2$ to $10^7/cm^2$. After achieving quasi-steady state dropwise condensation, the heat transfer rate through the drops as well as number of available nucleation sites underneath the substrate, for given initial site density and sub-cooling, increases as hydrophobicity increases. At any instance, more nucleation sites remain active on substrates having higher hydrophobicity; this too increases heat transfer. In addition, a higher site density decreases the minimum radius of drop required for coalescence with the neighboring droplets. This early coalescence allows early drop fall-off, hence exposing virgin areas for fresh nucleation for the next droplet generation. Heat transfer coefficient also increases in this process. Overall, we show that increasing hydrophobicity has a positive effect on heat transfer enhancement.

INTRODUCTION

The process of condensate condensing in form of discreet drops at isolated nucleation sites on/underneath a hydrophobic substrate is called as dropwise condensation. The resulting heat transfer coefficient can be up to one order of magnitude higher than other modes of condensation (Rose 2002). The formation of drops can be promoted by treating the surface in such as way that it becomes hydrophobic due to the creation of low surface energy layer. The bulk effect of this affects the equilibrium apparent contact angle of the liquid droplet on the substrate (Rykaczewski et al. 2011). The formation of drops on preferred nucleation sites, while the area between the droplets being largely inactive with respect to heat transfer is the more acceptable mechanism of heat transfer in dropwise mode of vapor condensation (Carey 1992). Accordingly, dropwise condensation is necessarily quasi-cyclic process, with a chain of intermediate processes such as initial nucleation, growth of drops by direct condensation, coalescence, drop instability and movement followed by fresh nucleation (Sikarwar et al. 2012a). The transient process of drop formation, coalescence, growth and drainage underneath a horizontal/inclined hydrophobic substrate, obtained from simulation as well as experiments is depicted in Figure 1 (Sikarwar et al. 2011). During dropwise condensation, initial growth of droplets is by direct condensation; the later stage of growth is governed by drop coalescence dynamics. There are a series of thermal resistances, Figure 2(a), in the path of condensing vapor releasing its latent heat to the cold substrate; the most dominant is the diffusional resistance of the liquid droplet (Carey 1992; Bansal et al. 2009). Therefore, eventually droplet growth is limited by their diffusional thermal resistance. Hence, accurate modeling of this dominant resistance is necessary to predict the

precise rate of condensation. The diffusional resistance is a strong function of the droplet size and its shape, the latter guided by degree of hydrophobicity of the liquid-substrate combination (Dietz et al. 2010).
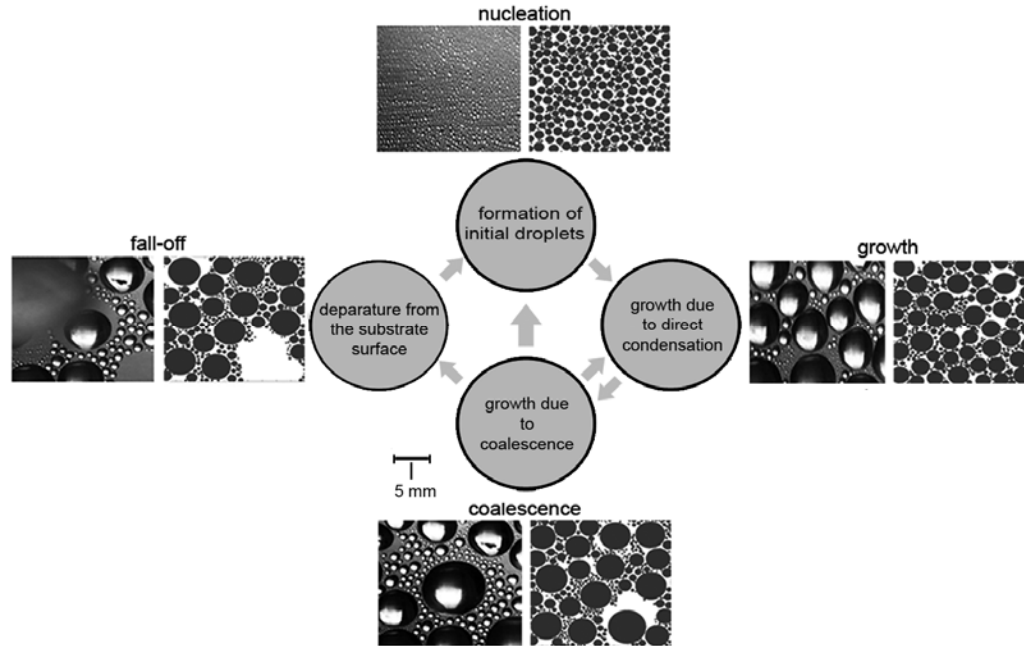

Figure 1 Cycle of individual processes at various time instants in condensation of vapor underneath a horizontal substrate (Sikarwar et al. 2011); inter-relationship shown among the distinct processes are: (i) nucleation and growth of drops at each nucleation site by direct vapor condensation; (ii) joint growth by direct condensation and coalescence; (iii) growth of large drops mainly by coalescence and smaller drops by direct condensation; and (iv) drop instability and condensate removal from the substrate. Fresh nucleation (step i) is initiated at the newly exposed sites.
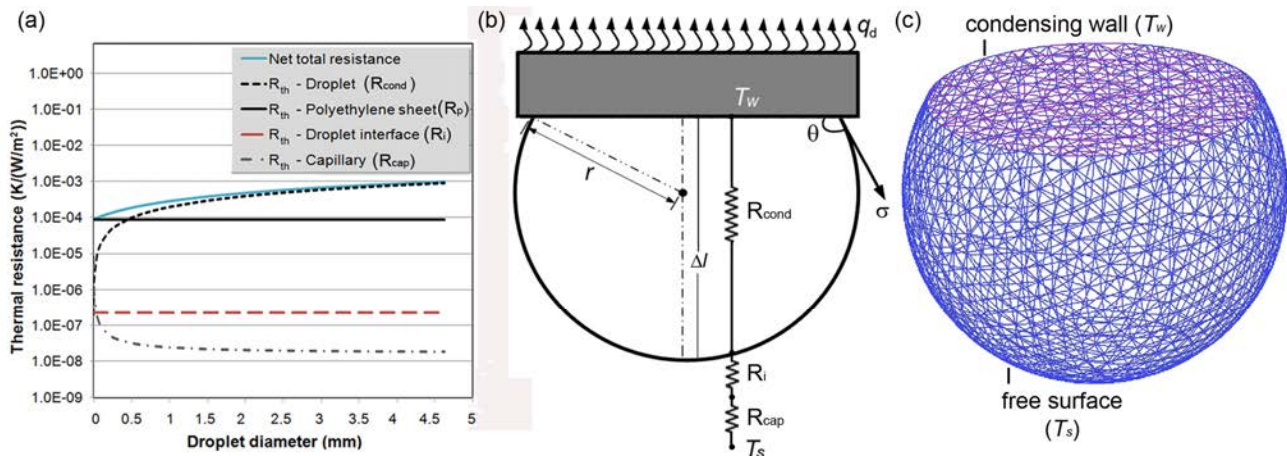

Figure 2 (a) Thermal resistances variation with respect to size of droplet observed in an experiment of dropwise condensation underneath a hydrophobic substrate (Bansal et al. 2009). (b) Schematic view of a drop of contact angle θ and radius r underneath a substrate with thermal resistances in the droplet growth equation, shown. T_s, is the vapor saturation temperature and T_w is the wall temperature (c) Computation domain of drop with tetrahedron mesh on its surface for numerical computation of heat flow through diffusion in drop.

Many research groups (Graham and Griffith1967, Carey, 1992, Sikarwar et al. 2011, Kim and Kim 2011) have attempted the modeling of the diffusional droplet resistance, albeit with some approximation. Graham and Griffith (1973) modeled conduction resistance of liquid drops by applying an indirect approach by using the temperature drop through the droplet from the wall to the liquid-vapour interface. Sikarwar et al. (2011) reported that such an indirect approach leads to unacceptable estimation of the thermal resistance, especially for hydrophobic surfaces. Modifications were suggested to handle drops having contact angle more than 90°. Kim and Kim (2011) also reported that the diffusional resistance of condensate is strong function of contact angle. To estimate this resistance on super-hydrophobic surfaces, they introduced an approximate technique based on the spherical geometry of the drop and the ensuing neighbouring internal isotherms inside the drop. While it is now established that

the conduction resistance of the drop is the most critical heat transfer limiting entity of the series of resistances, a comprehensive analytical model for its estimation is not available. Most models present some approximation.

In the present manuscript, the diffusional resistance of drop is determined by solving the 3-D Energy Equation on unstructured tetrahedral grid representing the individual droplets on a hydrophobic surface. A range of droplet characteristic dimensions (Bond Number), contact angles (degree of hydrophobicity), liquid Prandtl numbers and degree of subcooling, has been considered to study the effect of these parameters on the heat transfer through individual drops. The database so generated is used to correlate the diffusional resistance of droplets with the independent parameters by regression. These correlations are then incorporated into a previously developed drop population model of the authors (Sikarwar et al. 2011, 2012a), to get the local/average heat transfer during quasi-steady state pendant mode of drop in dropwise condensation process. Once this detailed information of the effect of hydrophobicity on heat transfer through individual droplets is discerned, an ensemble of various generations of these droplets can then be handled, to simulate the entire process on an engineering scale. Here, we have also investigated the effect of apparent contact angle (degree of hydrophobicity) and nucleation site density, varied from $10^4/cm^2$ to $10^7/cm^2$, on heat transfer during dropwise condensation.

It is observed that after quasi-steady state dropwise condensation is achieved, the heat transfer rate through the drops as well as the density of small drops on the substrate, for given initial site density and degree of sub-cooling, increases as the hydrophobicity of the condensing substrate increases. At any instance, more nucleation sites remain active on substrates with higher hydrophobicity; this in turn, further increases the net heat transfer. In addition, a higher initial site density decreases the minimum radius of drop required for coalescence with the neighbouring droplets. This early coalescence allows early drop slide-off, hence exposing virgin areas for fresh nucleation for the next droplet generation. Heat transfer coefficient also increases in this process. Overall, we show that increasing hydrophobicity has a positive effect on heat transfer.

MODELLING OF DIFFUSIONAL RESISTANCE

The schematic diagram of heat transfer through the single drop (for contact angle $\theta = 120^\circ$; volume 100µl) and its corresponding computational domain generated with triangular faced unstructured tetrahedron grid is shown in Figure 2 (b) (c). Similarly, the computational domains for other droplets in the contact angle range of 70° to 160° and size range of 1 to 140 µl are taken for various fluids (Pr = 0.001 to 10) in the simulations reported here. The governing equation and appropriate boundary condition are as:

$$\rho C_p \frac{\partial T}{\partial t} = k \cdot \nabla^2 T \tag{1}$$

The boundary conditions are as:

$$T_{free} = T_1 \tag{2}$$

$$T_w = T_2 \tag{3}$$

Hence, the effective temperature drop associated with diffusional resistance is $\Delta T_{cond} = (T_1 - T_2)$. The details of the finite volume parallel computing solver had been described by the authors elsewhere (Sikarwar et al. 2012b). The diffusion term is discretized using a 2nd order central-difference scheme. Geometry invariant features of the tetrahedral element are used so that the calculation of gradients at cell faces is simplified using nodal quantities of a particular variable. The discretized system of algebraic equations is solved by the Stabilized Bi-Conjugate Gradient method (biCGStab) with a diagonal pre-conditioner. Iterations within the code are run till a convergence in terms of the absolute residual of order $\sim 10^{-7}$ is reached. In this way, the temperature field inside droplets and temperature gradient near the wall are determined. Then wall heat transfer through the condensing wall of droplet is calculated.

$$\left(q_d\right)_{cond} = \left[\frac{1}{S} \sum_{i=1}^{S} -k \left(\frac{\partial T}{\partial n}\right)_{i,w}\right] A_{sl} \tag{4}$$

Therefore the conduction resistance per unit liquid vapour interface (K-m^2/W) is as:

$$R_{cond} = \left(\frac{\Delta T_{cond} A_{lv}}{\left(q_d\right)_{cond}}\right) \tag{5}$$

Comprehensive three-dimensional numerical simulations have been performed for various fluids, droplet shapes and contact angles. The heat transfer rate of individual drop is correlated in later section. This correlation is used in the present manuscript to determine the growth rate of drop at each nucleation site during the dropwise condensation. In this way, an ensemble of drops of various sizes and generations growing on a large substrate can be handled.

SINGLE DROP HEAT TRANSFER MODEL

During dropwise condensation model assumed here, heat gets transferred through individual drops only. Therefore, determining the amount of heat transferred through a single drop is necessary in predicating the overall heat transfer by dropwise condensation. The first step towards developing a model of heat transfer through a single drop is to recognize all contributing thermal resistances between the saturated vapour and the cold condensing surface.

For the present model, the thermal resistances are composed of the vapour-liquid interface resistance, the resistance due to the conduction through the drop itself, and the resistance due to the curvature of the drop. The other resistance reported in literature (e.g. Rose 2002) are neglected in the present modelling. The primary novelty of the present modeling approach is the

way the conduction resistance has been estimated, as suggested by Eq. 5. All the other nuances of the comprehensive dropwise condensation model are described by the authors elsewhere (Sikarwar et al. 2011).

Therefore, the heat transfer rate through a drop of radius r is expressed as:

$$q_d = \frac{2\pi r^2 \, \Delta T \left[1 - (r_{min}/r)\right](1 - \cos\theta)}{\left(h_{int}^{-1} + R_{cond}\right)} \qquad (6)$$

Equation 6 demonstrates that the heat transfer rate q_d varies with the drop size and the contact angle.

$$q_d = \rho(\pi/3)h_{lv}r^2\left(2 - 3\cos\theta + \cos^3\theta\right)(dr/dt) \qquad (7)$$

Hence, the growth rate of drop is as:

$$\frac{dr}{dt} = \frac{6\left[1 - (r_{min}/r)\right](1 - \cos\theta)\Delta T}{\rho\left(2 - 3\cos\theta + \cos^3\theta\right)h_{lv}\left(h_{int}^{-1} + R_{cond}\right)} \qquad (8)$$

MODELLING OF COMPLETE DROPWISE CONDENSATION

Atomistic modelling of drop formation in heterogeneous dropwise condensation has been carried out by Sikarwar et al. (2012a). The authors reported that the minimum drop radius does not provide controllability of macro-scale dropwise condensation at large timescales when dynamic steady-state is achieved. Therefore, drops formed at the initial nucleation site are assigned a minimum possible stable radius from thermodynamic considerations. The basic methodology includes random assignment of initial nucleation sites on which droplets of radius $= r_{min}$ start growing following the derived growth rate model. Subsequently, a coalescence model is incorporated which continuously checks for conditions of droplet mergers with neighbouring drop. Criticality of size is checked with respect to slide-off or fall-off, as per the case. This re-exposes fresh nucleation sites where a new generation of droplets again start growing from their initial radius $= r_{min}$. Depending on the surface wettability condition and inclination of the substrate, the growth model, coalescence model and criticality model needs to be chosen and activated.

A pendant drop underneath a flat horizontal substrate is shown in Figure 2b. The drop is considered as a portion of a sphere of radius r making a contact angle θ. From the geometry, the drop volume V, area of liquid-vapour interface A_{lv}, and area of solid-liquid interface A_{sl}, are given by:

$$V = \left(\frac{\pi r^3}{3}\right)\left(2 - 3\cos\theta + \cos^3\theta\right) \qquad (9)$$

$$A_{lv} = 2\pi r^2 \left(1 - \cos\theta\right) \qquad (10)$$

$$A_{sl} = 2\pi r^2 \left(1 - \cos^2\theta\right) \qquad (11)$$

For a specified wall sub-cooling, the smallest stable droplet size possible can be found from thermodynamic considerations as (Carey 1992):

$$r_{min} = \frac{2\sigma \cdot v_l \cdot T_w}{h_{lv}[T_s - T_w]} \qquad (12)$$

Although the arguments leading to this equation do not include the substrate surface energy, Leach et al. (2006) and Walpot et al. (2006) have shown that such effects are of higher order and can be neglected for engineering calculations on the micro-scale. As droplets grow in size, the meso/macro scale droplet dynamics cannot neglect the bulk contact angle ensuing from the surface energy of the substrate. The maximum drop diameter is calculated from balancing the surface tension with the weight of the drop and is derived as:

$$r_{max} = \sqrt{\left(\frac{6\sin^2\theta}{2 - 3\cos\theta + \cos^3\theta}\right) \cdot \left(\frac{\sigma}{g \cdot (\rho_l - \rho_v)}\right)} \qquad (13)$$

DROPLET POPULATION AND GROWTH TRACKING ALGORITHM

A quick outline of the numerical scheme is summarized as: (i) Initialize all variables and input the properties of condensates. Randomly distribute the nucleation sites on the substrate. (ii) Determine the thermodynamically possible minimum radius of droplets r_{min} and set droplets of r_{min} at all nucleation sites. (iii) Calculate the intermediate distance between nucleation sites and area of active and in-active of the substrate. (iv) Solve the growth equation by fourth order Runge-Kutta method and find out the new radius at each nucleation sites (v) Check for coalescences; if coalescence criterion is met, put a drop of equivalent volume on the mass averaged center of the respective coalescing droplets. (vi) Check the nucleation sites covered by drop and make them hidden sites and, in parallel, check the nucleation sites re-exposed due coalescences; put droplets of thermodynamic r_{min} on these re-exposed nucleation sites. (vii) Check the critical radius of drop fall-off (r_{max}) and identify all hidden sites underneath this droplet and make them active by supplying r_{min} again. (viii) Repeat (iii)-(vii) again till stopping criterion is met, i.e., the maximum time considered for condensation.

RESULTS AND DISCUSSION

Local wall heat flux distribution at the base of the water droplets with various contact angles and various volume (1µl and 10 µl), estimated by the single droplet transport model, are shown in Figure 3. Obtained results show that the wall heat flux is higher in the immediate vicinity of three-phase contact line and it decreases towards the centre of drop base. Similar qualitative distribution is also obtained for other drop sizes. Figure 3a shows wall heat flux transfer through two drops of different sizes (1µl) and (10µl) respectively, both with different contact angles. A large heat flux on the liquid-solid contact is estimated for the smaller drop, Figure 3(a). The wall heat flux, for a drop having a fixed volume, increase as its contact angle is increased. This is explained by the fact that for a fixed drop volume, a higher contact angle increases the net interfacial area. In addition, condensation surface covered by large number of small sized drops provides a better condensation performance than the same surface covered by a population of large drops. This is consistent with the results found in many previous studies (for example, a recent study by), which report that more condensation heat transfer occurs through small drops (Carey 1992, Leach 2006, Walpot 2006). The mathematical estimation of heat transfer due the diffusion in condensate drop, as given in literature (Kim and Kim 2012, Sikarwar et al. 2011, Graham and Griffith 1973), is compared with that calculated from Eq. 4, as depicted in Figure 4. A more convenient and generic form to represent the entire collection of 3D-numerical data of heat transfer through a single drop (for drops of various sizes, shape and Prandtl numbers), the diffusion heat transfer can be casted as:

$$\left(q_d\right)_{cond} \propto (kA_{sl})\left(\frac{\Delta T_{cond}}{\Delta l}\right) = C(kA_{sl})\left(\frac{\Delta T_{cond}}{r(1-\cos\theta)}\right) \tag{14}$$
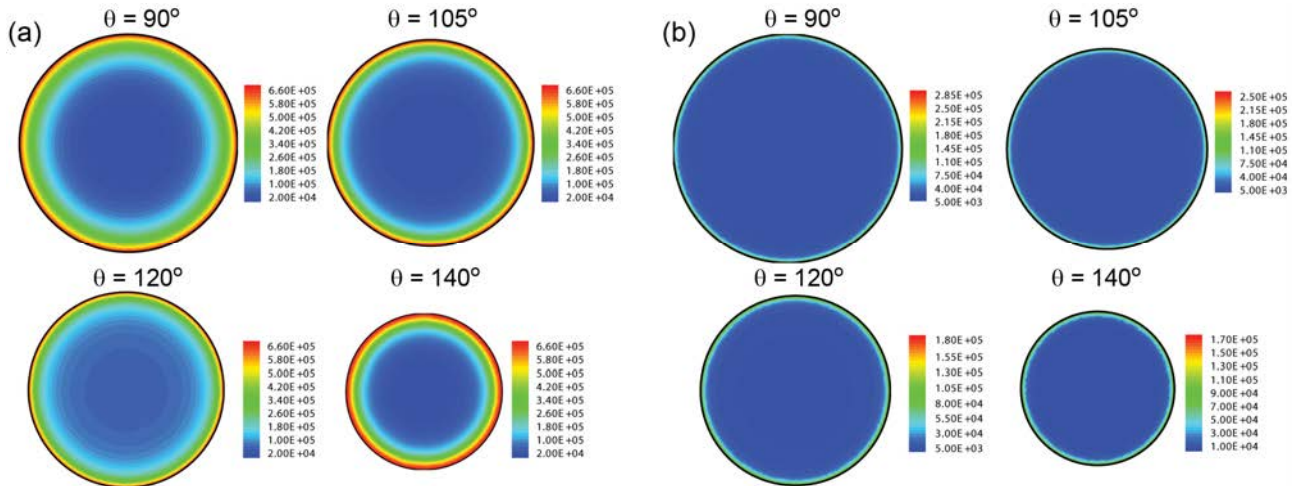

Figure 3 Variation of heat flux at various size and shape of water drop at temperature 303 K and temperature drop, $(\Delta T_{cond}) = 1$ K. (a) 1µl and (b) 10µl.
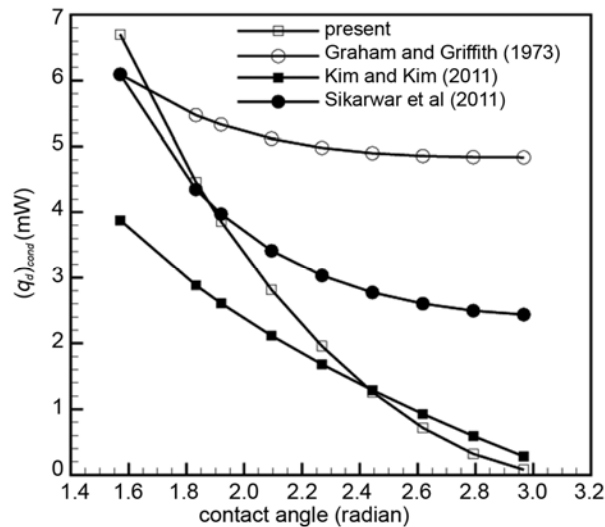

Figure 4 Heat transfer (in mill-Watt) through of drop of volume of 1µl due to diffusion at various shapes (contact angle) at temperature 303 K and temperature drop, $(\Delta T_{cond}) = 1$ K.

In the present range of simulation, the value of the constant comes out to be equal to 2.14. The length scale is taken to be the droplet height, Δl. It is clear that as compared to an imaginary cuboid which fully encompasses the droplet, the nature of the truncated spheroidal geometry of the drop reduces the diffusional resistance of heat through it. While the overall trend of the present estimation of diffusional heat transfer is same as reported in the literature, it is an improved estimate as complete three-dimensial geometry has been considered with no approximation. For small contact angle drops the present results are closer to those provided by Graham and Griffith (1973) while for large contact angles, the approximate estimate given by Kim and Kim (2011) are satisfactory.

Table 1: Results of simulation of dropwise condensation of water vapor at 303 K and degree of sub-cooling 2K

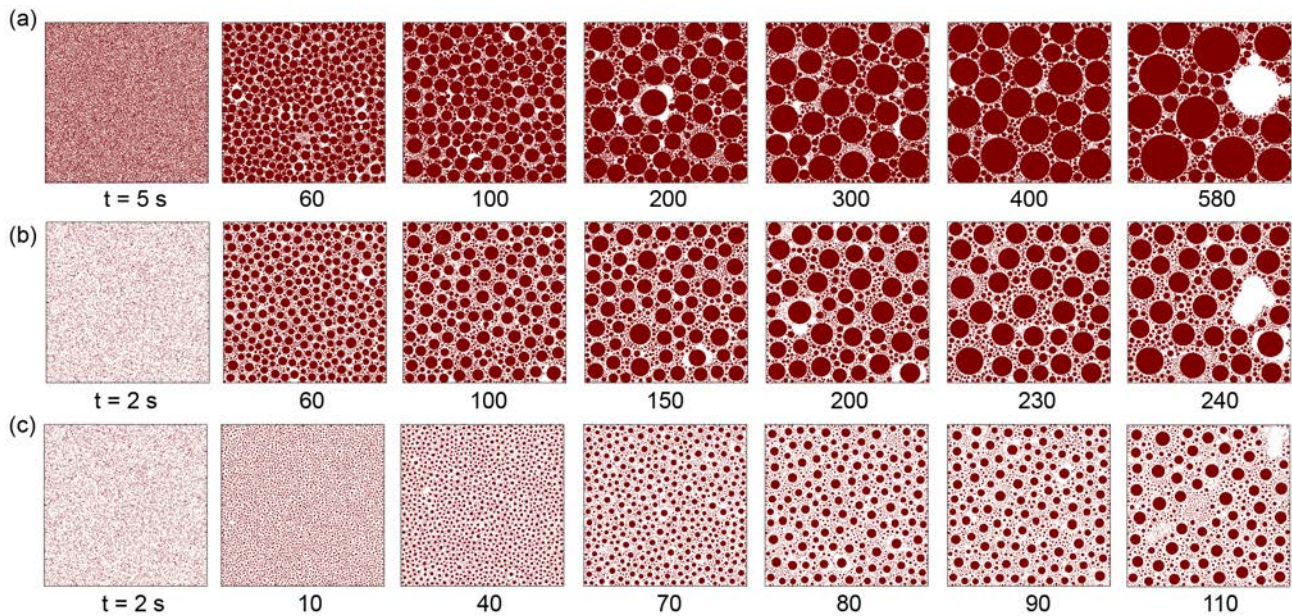| Contact angle	Radius		Initial nucleation sites	Available nucleation sites	First fall-off	frequency	Heat transfer coefficient
degree	r_{min} (mm)	r_{max} (mm)	Per cm^2	30mm×30mm	(s)	(per s)	(KW/m^2 –K)
90	9.1×10^{-6}	4.64	10^6	~1100	580	155	210
			10^7	~1115	412	87	222
120	9.1×10^{-6}	3.08	10^6	~1955	240	98	315
			10^7	~1958	178	68	418
140	9.1×10^{-6}	2.14	10^6	~3656	109	29	452
			10^7	~3674	88	20	502

Figure 5 (a) Spatio-temporal drop distribution during dropwise condensation of water vapor at 303 K with sub-cooling of ΔT = 2 K from initial time step to first fall-off for (a) contact angle 90°, (b) contact angle 120° and (c) contact angle 140°.

Figure 5 depicts the spatio-temporal drop distribution in dropwise condensation of water vapour at 300 K and degree of sub-cooling = 2K, underneath various hydrophobic substrates, form initial nucleation (taken here = 10^6/cm^2) to the instance of first drop fall-off. It is clear that the size of the drop at fall-off and the time required for fall-off, both decrease as the hydrophobicity of the substrate increases. Accordingly, the substrates having higher hydrophobicity result in the condensate having smaller drop size distributions, which results in lowering the overall diffusional resistance offered by the condensing drops; In addition increased hydrophobicity generates high number of available nucleation sites, at any given time, as shown in figure 4. The frequency of drop fall-off, size of the minimum drop, size of the maximum drop, for substrate having various degree of hydrophobicity, during water vapour condensation are given in Table 1.

The area of coverage by drops at various hydrophobic substrates is shown in Figure 6a. The hydrophobicity of substrates decrease the area of coverage by drop, hence the higher hydrophobic substrates have higher available nucleation sites density at any given time of condensation, Figure 6b. Hence, the size and population of maximum drops have a significant impact on dropwise condensation, due to the limitations posed by the diffusional resistance. The effect of substrate hydrophobicity on heat transfer during the dropwise condensation is shown in Figure 6c. The apparent contact angles clearly affect the heat transfer rate. For a given initial nucleation site density, the heat transfer can be increased by having a contact angle higher than the 90°. As given in Table 1, the substrate hydrophobicity decreases the critical size (of fall-off), hence resulting in a higher population of small drops. Therefore, one concludes that a substrate having a high hydrophobicity with the condensate fluid is desirable in dropwise condensation. The available sites at any instance of time which are available for nucleation are shown in Figure 6b. Initially it decreases according to a power law but after reaching the dynamic steady state it varies randomly due to drops

coalescence and fall-off. At any given time the available nucleation sites are higher for high contact angle fluids. The effect of initial nucleation sites density on the heat transfer is shown in Figure 6d. A high density of nucleation sites creates large overall heat transfer in dropwise condensation. From the view point of the current model, a high density of nucleation sites leads to decreases in the size of drop before coalescence commences. This early coalescences allows virgin spaces for new initial drops, causing a high population of small drops. One can conclude that surface providing more initial nucleation sites is desirable for dropwise condensation.
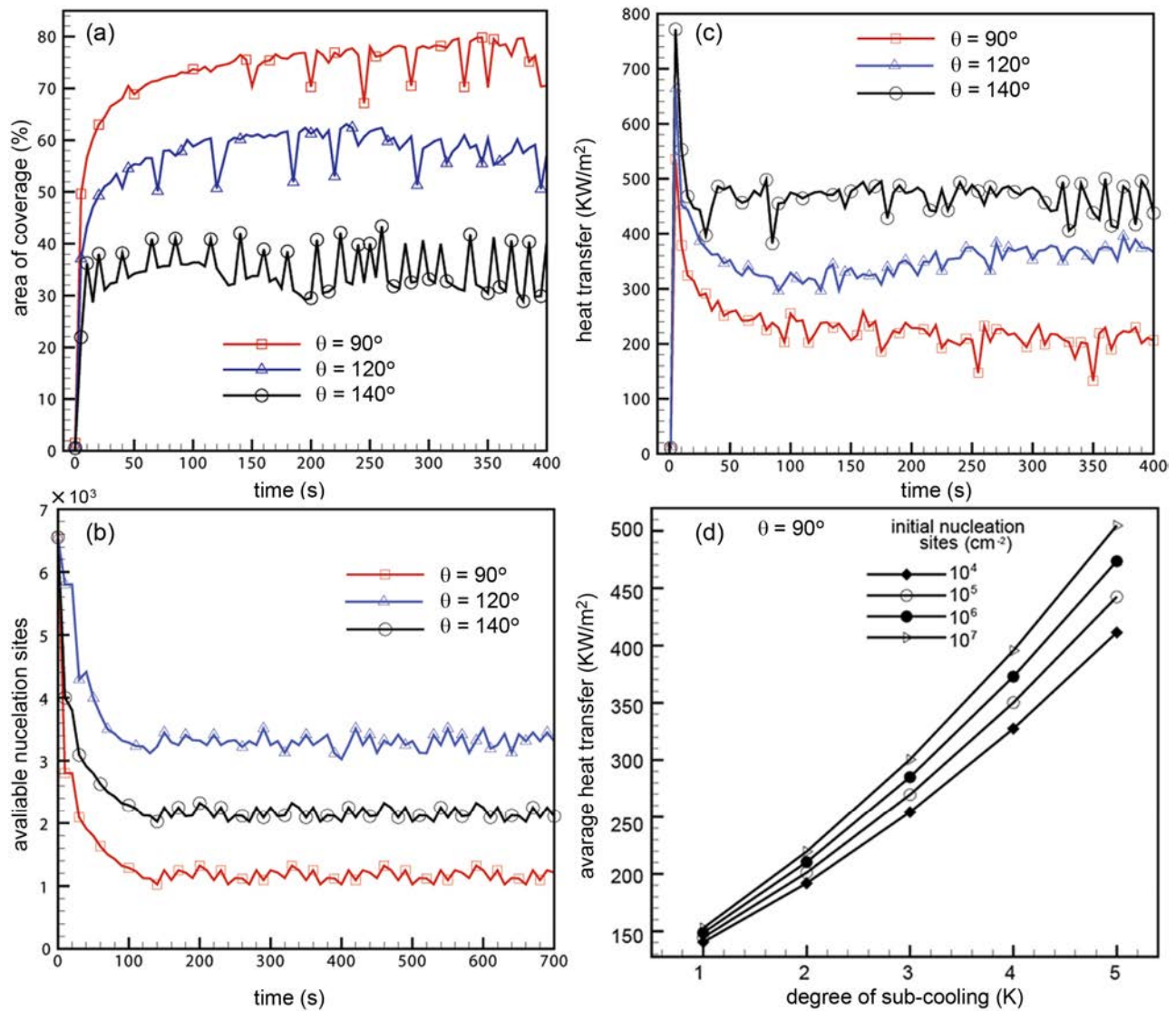

Figure 6 (a) Area of coverage versus time of condensation, (b) heat transfer fluctuation on a substrate with respect to the time (c) available nucleation site of substrate of 30 mm × 30 mm with respect to time for various contact angle of drop at 303 K and degree of sub-cooling 2 K. (d) Overall heat transfer coefficient as a function of the degree of sub-cooling with nucleation site density. Fluid considered is water at 303K and a contact angle 90°.

CONCLUSIONS

Dropwise condensation is a very efficient mode of heat transfer. The formation of drops at individual nucleation sites and heat transfer through these drops is the most acceptable mechanism of heat transfer during dropwise condensation. Although the concept of dropwise condensation was introducing more than four decades ago, comprehensive 3D model, wherein the explicit effect of contact angle on heat transfer and drop distribution has been incorporated. The small drops transfer higher heat as compared to the bigger drop per unit area. Our study reveals that the drop contact angle poses first-order effects on net heat transfer in dropwise condensation. Thus, the effect of contact angle on drop distribution, drop instabilities, available nucleation sites, and ensemble of drop needs thorough scrutiny. This manuscript fills the necessary gap in the literature by providing a comprehensive and easy-to-implement formulation. The main conclusions of the study are:

(i) The contact angel affects the conduction heat transfer through the drop in a dominant way.

(ii) Drop growth at each nucleation site in dropwise condensation model is modified according to the effect of contact angle during the drop condensation. It was shown that the smaller drop can transfer more heat per unit contact area, and heat flux can be increased even more with high contact angle fluids. New model of heat transfer through the conduction through the drop is reported.

(iii) In addition, model results reveal that the drop size distribution is strongly dependent on the solid-fluid contact angle. Large number of smaller drops is observed in high contact angel substrates. This showed that the contact angle is a critical parameter for determining the effective maximum drop radius (the size of fall-off). Hence, contact angles reduce the size of departure drops, allowing more condensing surface for nucleating drops. Higher condensation rates are achieved by hydrophobic substrates.

(iv) Early drop coalescence is observed in dropwise condensation on substrates which have high initial nucleation sites and make high contact angles with the condensing fluid.

(v) Larger surface renewal frequencies of the superhydrophobic surface, their higher drop departure frequency and large available nucleation sites, lead to an increase in the heat transfer coefficient by factor of 5~10 times than substrates with partial or higher wettability.

ACKNOWLEDGMENTS

NOMENCLATURE

A	Surface area, m^2
C_p	Specific heat at constant pressure ,W/kg K
d	Diameter of drop, m
Δl	Maximum drop height from liquid-vapour interface to condensing wall, (m)
h_{lv}	Latent heat of vaporization, J/kg
h	Heat transfer coefficient , W/m^2-K
k	Thermal conductivity of condensate, W/m-K
q	Surface heat transfer, W
r	Radius of drop, m
T	Temperature, K
ΔT	Temperature difference between the saturated vapor and condensing wall, K
V	Volume of the drop, m^3

Dimensionless quantities

Pr	Prandtl Number, $\mu C_p/k$
Bo	Bond Number, $\rho g d^2/\sigma$

Greek symbols

α	Inclination angle from horizontal, radian/degree
μ	Dynamic viscosity, Pa-s
ν	Specific volume, m^3/kg
ρ	Density, kg/m^3
σ	Surface tension of liquid, N/m
θ	Contact angle, radians/degree

Subscripts

b	Base
$crit$	Critical
int	Interface
$free$	Drop free surface
max	Maximum
min	Minimum
lv	Liquid-vapor interface
s, sat	Saturation
sl	Solid-liquid interface
v	Vapor
w	Wall

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