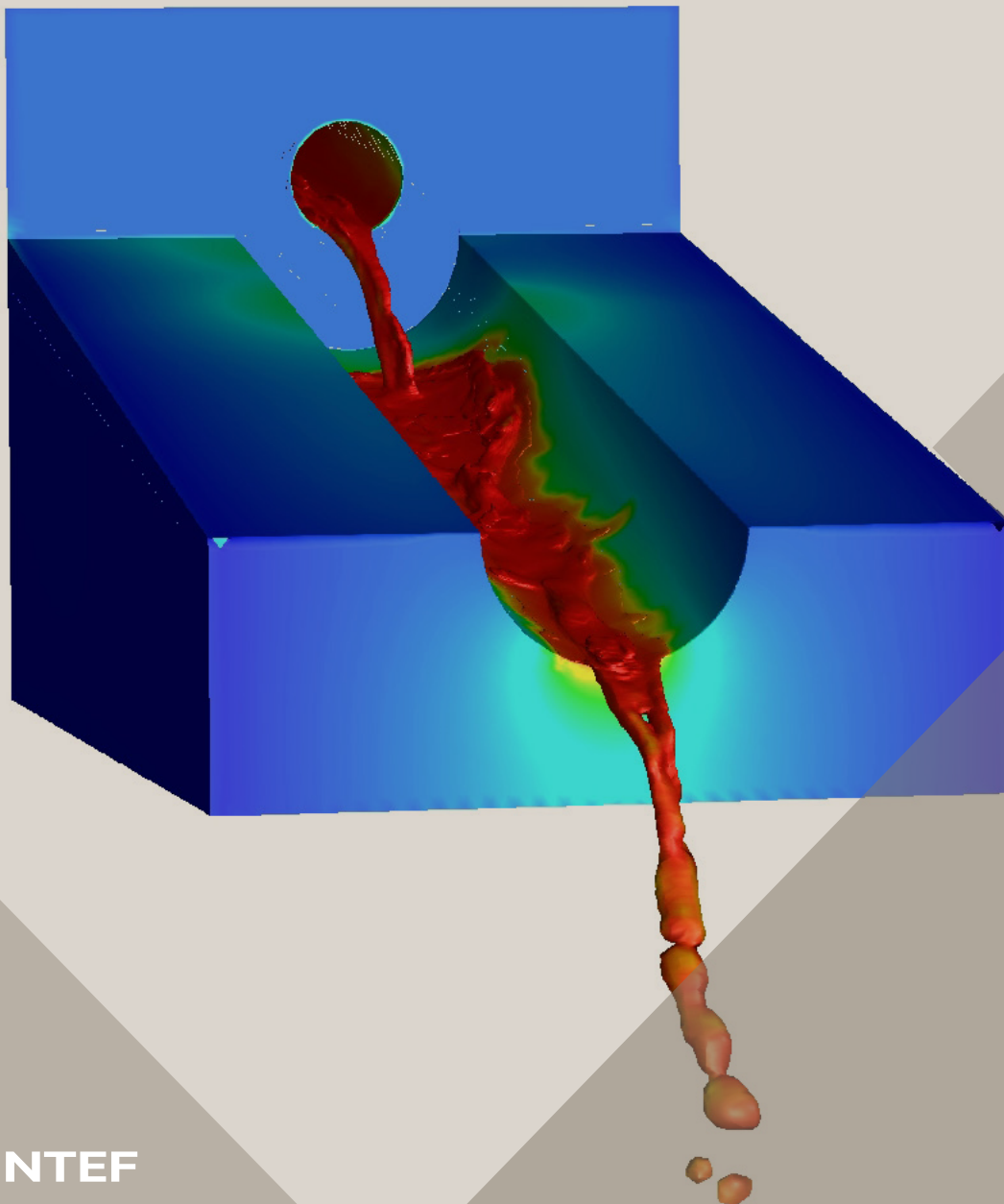


14th International Conference on CFD in  
Oil & Gas, Metallurgical and Process Industries  
SINTEF, Trondheim, Norway, October 12–14, 2020

# Proceedings from the 14<sup>th</sup> International Conference on CFD in Oil & Gas, Metallurgical and Process Industries



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Editors:

Jan Erik Olsen, Jan Hendrik Cloete and Stein Tore Johansen

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## DIRECT NUMERICAL SIMULATION STUDY ON THE FREE LIQUID AREA IN LIQUID-PARTICLE AGGLOMERATES.

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### ABSTRACT

Multiphase flows often occur in intensified industrial processes and understanding these complex processes is instrumental in their design and optimisation. In gas-phase polymerisation reactors, the heat management is improved by injecting an inert liquid. However, the injected liquid also affects the collisional behaviour of the produced particles. The liquid can create agglomerates of particles due to cohesive forces, e.g. surface tension. The formation of these agglomerates can have a drastic effect on the efficiency of the process. To determine the lifetimes of the agglomerates, it is important to predict the evaporation rate of the liquid inside such an agglomerate. The evaporation rate of the liquid is dependent on the gas-liquid interface which can be studied using Direct Numerical Simulations (DNS), specifically a combination of a Volume of Fluid method and an Immersed Boundary method. The effect of contact angle and particle configuration on the interface area is studied in this work. This study showed that the random particle configuration has a large impact on the interface area. Due to its random nature, the six investigated configurations are not sufficient to provide a meaningful average area. To determine the interface area, more different random configurations need to be investigated in order to provide a conclusive answer.

**Keywords:** Computational Fluid Dynamics, Direct Numerical Simulations, Combined Volume of Fluid Immersed Boundary Method, Contact angle model, Agglomerates .

### NOMENCLATURE

#### Greek Symbols

$\rho$  Mass density, [ $kg/m^3$ ]  
 $\mu$  Dynamic viscosity, [ $kg/ms$ ]  
 $\tau$  Stress tensor, [ $Pa$ ]  
 $\sigma$  Surface Tension, [ $N/m$ ]  
 $\varepsilon$  Fraction, [ $-$ ]  
 $\Theta$  Contact Angle, [ $-$ ]

#### Latin Symbols

$p$  Pressure, [ $Pa$ ]  
 $\mathbf{u}$  Velocity, [ $m/s$ ]  
 $t$  Time, [ $s$ ]  
 $\Delta t$  Time-step, [ $s$ ]  
 $g$  Gravitational acceleration, [ $m/s^2$ ]  
 $F$  Color function or phase fraction, [ $-$ ]  
 $\hat{\mathbf{n}}$  Interface normal vector,  $m$

$N$  Number of cells, [ $-$ ]  
 $V$  Volume, [ $m^3$ ]  
 $D$  Diameter, [ $m$ ]

#### Sub/superscripts

$g$  Gas.  
 $l$  Liquid.  
 $s$  Solid.  
 $i$  Index  $i$ .  
 $j$  Index  $j$ .  
 $d$  Droplet.  
 $p$  Particle.  
\* Intermediate.

### INTRODUCTION

Understanding complex multiphase flows is important for industrial applications, either for the design or optimisation of processes. Studying the behaviour of multiphase flows on industrial scales however, has been challenging as small scale phenomena influence the large scale behaviour. Well known complex multiphase processes are, e.g. fluid catalytic cracking, granulation, spray drying, floatation of metal ores and gas-phase polymerisation.

This work focusses on the liquid injection in fluidized bed reactors under reactive conditions, specifically the condensed-mode operation of the gas-phase polymerisation reaction (Chinh and Dumain, 1991; Havas and Lalanne-Magne, 1994). The gas-phase polymerisation reaction is highly exothermic and the reactor temperature is limited by the melting point of the produced polymer. To increase the production capacity of the reactor, the excess heat is removed by injecting an inert liquid. The role of the liquid in the condensed-mode gas-phase polymerisation reactor is to improve the heat removal capacity through evaporation. The temperature in the reactor is thus controlled by the evaporation rate of the injected liquid.

The liquid in the bed is present under three forms: vapour, droplets and in contact with polymer particles. The vapour in the reactor has a small contribution to the cooling of the reactor compared to the liquid state. The droplets in the reactor have a short life-time as collisions with particles are inevitable due to the vigorous solids mixing.

The remaining liquid is in contact with the particles. The liquid will enable the particles to stick together in a so called agglomerate. These are clusters of particles held together by the cohesion forces of the injected liquid. The heat of

reaction will gradually evaporate the liquid and reduce the size of the agglomerate.

Studying the effect of the agglomerates on the condensed-mode polymerisation process experimentally is very costly and does not allow for simple experimentation. An alternative to experiments is numerical modelling. Because computer models are often restricted with respect to either the size of the studied system or the level of detail that is resolved, a the multi-scale modelling approach has to be used to cover all time and length scales. This technique has been applied for many complex cases such as dense bubbly flows in industrial scale bubble columns and dense particle laden flows for fluidized beds (Deen *et al.*, 2004, 2012, 2014; Bauer and Eigenberger, 2001).

For example, a lab scale fluidized bed reactor can be studied using the Discrete Element Method (DEM). However, it is currently computationally too expensive to fully resolve the behaviour of the liquid inside the agglomerates. Thus the main focus of this work is to formulate closures in order to account for the effect of the liquid agglomerates. To include the effect of evaporation in agglomerates in DEM simulations, it is important to understand the time-scale of the liquid evaporation when enclosed with particles. To this end, Direct Numerical Simulations (DNS) are used to study the gas-liquid interface area in agglomerates for the prediction of evaporation rates. The effect of the number of particles in the agglomerate is studied along side the particle configuration and wetting properties.

## MODEL DESCRIPTION

The model used in this work is based on the Volume of Fluid (VOF) method and Immersed Boundary (IB) method reported by (Baltussen *et al.*, 2017). It can accurately model three-phase systems involving fluid and solid interfaces.

### Governing equations

The fluids are modelled using the one-fluid formulation, resulting in one set of mass and momentum conservation equations. The fluids are assumed to be Newtonian and incompressible.

*Continuity equation:*

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

*Momentum equation:*

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} + \mathbf{F}_\sigma \quad (2)$$

$\boldsymbol{\tau} = \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$  is the fluid stress tensor. The effects of surface tension are included using  $\mathbf{F}_\sigma$  as a volumetric source term acting on fluid interface. The density,  $\rho$ , and viscosity,  $\mu$ , are calculated using linear and harmonic averaging, respectively (Prosperetti, 2002).  $\mathbf{F}_\sigma$  is calculated using the Continuum Surface Tension (CSF) method of (Brackbill *et al.*, 1992), equation 3. To reduce the effects of parasitic currents and to increase numerical stability for high density ratio systems, a density scaling is applied for this  $\mathbf{F}_\sigma$ . This method conserves the surface tension by symmetrically distributing the acceleration due to surface tension over the interface (Yokoi, 2014).

$$\mathbf{F}_\sigma = \frac{\rho}{\langle \rho \rangle} \sigma \kappa \hat{\mathbf{n}} \quad (3)$$

In this CSF method,  $\kappa$  is the surface curvature and  $\hat{\mathbf{n}}$  the interface normal vector. The dynamics of the fluid-interface are captured using a VOF method where the fluid phase fractions are tracked with a color function ( $F$ ). The movement of the interface is captured by advecting the color function with the local fluid velocity (equation 4).

$$\frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F = 0 \quad (4)$$

Equation 4 is solved using a geometrical advection scheme based on Piecewise Linear Interface Calculation (PLIC) by Youngs (1982). To reduce numerical diffusion and maintain a high degree of mass conservation, the integration of equation 4 is based on a pseudo-Lagrangian geometric advection scheme, more information on this advection can be found in van Sint Annaland *et al.* (2005).

To calculate the normals, the phase fraction is smoothed using a polynomial proposed by Deen *et al.* (2004). However when the smoothing is performed in close proximity of the solid interface, non-physical results are obtained. This is prevented by extending the phase fraction field into the solid region (Sussman, 2001). In this work, the phase fraction extension is 4 grid-cells, more details on the implementation can be found in Patel *et al.* (2017).

The fluid-solid interactions are represented by an implicit second-order accurate IB method that applies no-slip boundary conditions (Deen *et al.*, 2009; Das *et al.*, 2016). A unidirectional quadratic interpolation polynomial is used to express the velocities near the boundaries to satisfy the no-slip boundary condition at the solid interface. A detailed explanation of this method can be found by Deen *et al.* (2009) and Das *et al.* (2016). To model the interactions of the fluid interface with the solid interface, a contact angle model is used. The contact angle is applied to the normal of the gas-liquid interface as a boundary condition. Due to the low Reynolds range used in this work, the model developed by Voinov (1976) and Cox (1986) is applied for changing the normal at the contact line. A thorough explanation on the method can be found in Patel *et al.* (2017).

### Numerical method

The VOF-IB method solves the mass and momentum conservation equations (equations 1 and 2) on a staggered grid. The diffusion term is calculated using a second order central difference scheme, which is treated implicitly except for the mixed derivatives. The convection terms in the momentum equations are discretised using a second order flux delimited Barton scheme and solved implicitly. To solve the momentum equation, a fractional step method for pressure-velocity coupling is used. The intermediate velocity is calculated in the first step based on the momentum equation, excluding the pressure gradient. In the second step, the pressure Poisson equation (equation 5) is solved to compute the pressure correction term which is then used to compute the velocities at the next time step (equation 6).

$$\nabla \cdot \left\{ \frac{\Delta t}{\rho} \nabla (\delta p) \right\} = \nabla \cdot \mathbf{u}^* \quad (5)$$

$$\mathbf{u}^{k+1} = \mathbf{u}^* - \frac{\Delta t}{\rho} \nabla (\delta p) \quad (6)$$

### Verification and Validation

The model used in this work has been validated and verified in literature. Information on the implementation and performance of the IB method can be found in Deen *et al.* (2009,

2012). An extensive explanation of the VOF method can be found in van Sint Annaland *et al.* (2005) and Baltussen *et al.* (2014). The IBM-VOF coupling was reported by Patel *et al.* (2017). Because this study will use the same methods and code implementations, the model will not be verified and validated again.

## SIMULATION AND DATA ANALYSIS

In this work, DNS was used to study the gas-liquid area of a droplet caught between a cluster of particles, by allowing the liquid to reach its stable configuration. The sections below describe the details of the simulations and the calculation of the free liquid area and the wetted solid area.

### Simulation set-up

Under normal conditions, the particles in an agglomerate have a random packing. This random configuration was obtained by the creation of a packed particle bed generated with a DEM model. The mono-dispersed particles were deposited into the domain and shaken until a solids fraction of  $\varepsilon_s = 0.55$  was obtained. This resulted in a cube of approximately 8000 particles in a close random packing.

To extract the particle positions from this packed bed, a subsection of the bed was taken and the local porosity was calculated. Next, a sphere was inserted into the subsection of which the overlap between the sphere and the particles was subtracted from its shape. By moving the subsection of the bed through the length, width and height, a set of domains was acquired having the same local porosity and volume of the inserted sphere.

The coordinates of these particles and sphere were used to set-up the solid and fluid-interfaces in the simulation domain. This effort was made to ensure that the outcome of the simulations are independent of the liquid volume and the local porosity of the particles.

The simulation time was taken such that the liquid reached a stable configuration, i.e. when the liquid interface is no longer moving. Wetting properties of the system have tremendous impact on the spreading behaviour of the liquid between particles, thus two contact angles ( $\Theta$ ) were used in the simulations. For both the contact angles, six random packings were simulated. The details of the simulations are listed below in table 1, including the particle diameter ( $D_p$ ) and liquid volume ( $V_d$ ).

**Table 1:** Simulation Details.

Property	Value	Unit
$N_x, N_y, N_z$	400	(-)
$dx, dy, dz$	$5e-6$	$m$
$dt$	$5e-7$	$s$
$\rho_g$	1	$kg/m^3$
$\mu_g$	$1e-5$	$Pa \cdot s$
$\rho_l$	$1e3$	$kg/m^3$
$\mu_l$	$1e-3$	$Pa \cdot s$
$\sigma$	$7.2e-2$	$N/m$
$V_d$	$1e-10$	$m^3$
$D_p$	$2e-4$	$m$
$\varepsilon_s$	0.55	(-)
$\Theta$	$30^\circ$ & $60^\circ$	(-)

### Data Analysis

To retrieve the gas-liquid interface area, the surface area of the interface in each cell is calculated based on the PLIC representation. By calculating the intersections of the PLIC interface with the cell edges, a polygon is formed, which is used to calculate the area. By summing the areas of all the interface cells, the total gas-liquid interface area is obtained.

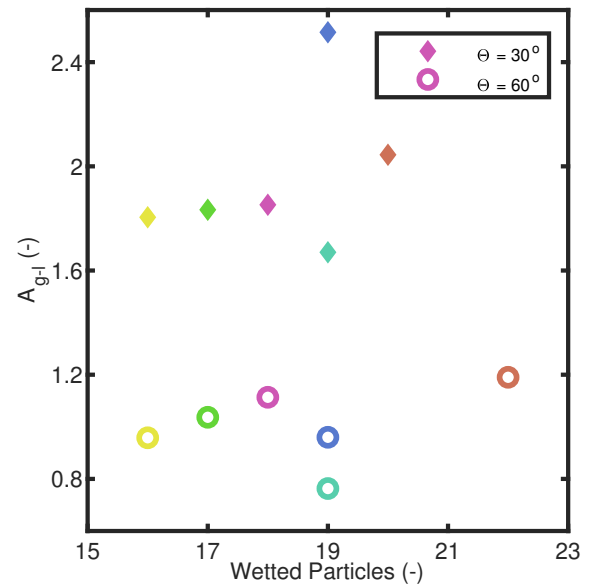
Due to the nature of the IB interface, the wetted area of the solids is not available during the simulations. To obtain the wetted area, the intersection between the solid sphere and cell is approximated using the intersections on the cell edges and IB surface. This method provides an accurate calculation of the sphere surface with less than 1% error with 5 cells per diameter of the particle. To properly model the fluid-solid interactions, 20 cells per particle diameter are used, which results in approximately an error of 0.3 % in the fluid-solid surface area calculation. To obtain the wetted area, the solid surface area per cell is multiplied with the fluid phase fraction. During the calculation of the wetted area, the particles whom are in contact with the droplet are registered, providing the number of wetted particles.

## RESULTS

Figure 1 shows the resulting gas-liquid interface area for both contact angles, versus the number of particles in contact with the liquid phase. The gas-liquid area is normalised by the area of a spherical droplet with equivalent volume. The varying colors indicate the different random particle configurations. The interface area seems to increase with increasing number of wetted particles with exception for the cases with 19 wetted particles. The difference in average area between the contact angles is expected: a lower contact angle will spread out further with a thinner liquid layer, resulting in a larger gas-liquid interface area.

Figure 2 shows the contact area between the liquid phase and particles, normalised by the area of a single particle. Similarly to the gas-liquid area, the contact area seems to be slightly dependent on the number of wetted particles, but the configurations with 19 or more wetted particles do not fit the trend. In addition, the contact angle seems to have a well defined effect on the contact area, as the data for the higher contact angle seems to be reduced with a factor 0.83.

In figures 1 and 2, there are two particle configurations with



**Figure 1:** Free liquid area in a cluster of particles.

the same amount of wetted particles (19). The figures show that there is a drastic difference in both gas-liquid interface area and wetted contact area between those two different configurations. Figures 3 and 4 show both configurations rotated

along an axis. Note that only the particles in contact with the liquid are visualised. Figure 3 has both the highest gas-liquid interface area and the highest contact area. This seems mainly due to the more concave shape of the agglomerate, where a cavity is observed, whereas the shape of the agglomerate from figure 4 is more convex. This suggests that the particle configuration has a strong influence on the wetting outcome of the liquid. To gain insight on this influence, more random particle configurations should be simulated.

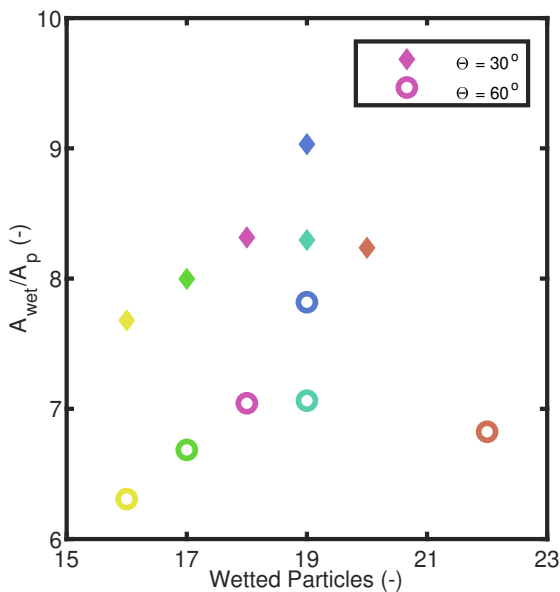
In coarse grained models, the gas-liquid interface area is used to predict the evaporation rate. We expected the gas-liquid interface area to be a function of: the liquid to particle volume ratio, the contact angle and the number of particles in the agglomerate. From the figures 1 and 4, it can be concluded that the particle configuration is also an important parameter to take into account. Due to the random nature of the particle configuration, the average gas-liquid interface area is determined by a normal distribution. The normal distribution can be used to provide an average interface area independent on the particle configuration but dependent on the other process parameters, such as the contact angle and liquid to particle volume. However, to determine the mean and variance of the distribution, the sample size needs to be larger.

**CONCLUSION**

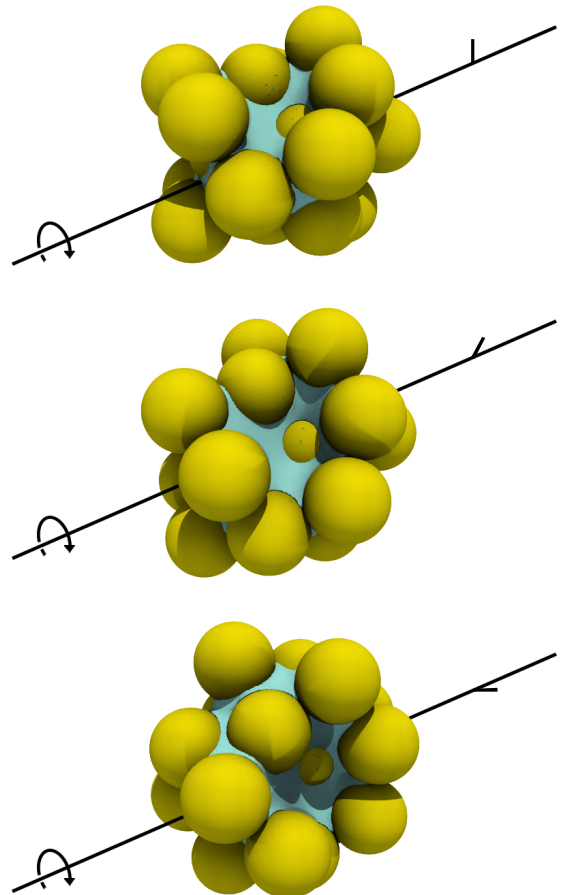
The gas-liquid area in agglomerates is dependent on the contact angle of the multiphase system, as expected. However, the random particle configuration seems to dictate the spreading outcome more than the amount of wetted particles. The random nature of this configuration suggests a normal distribution, and thus to extract an average gas-liquid interface area and its variance. With the current number of simulations, it is not possible to determine an average gas-liquid interface area independent of particle configuration.

**ACKNOWLEDGEMENT AND AFFILIATION:**

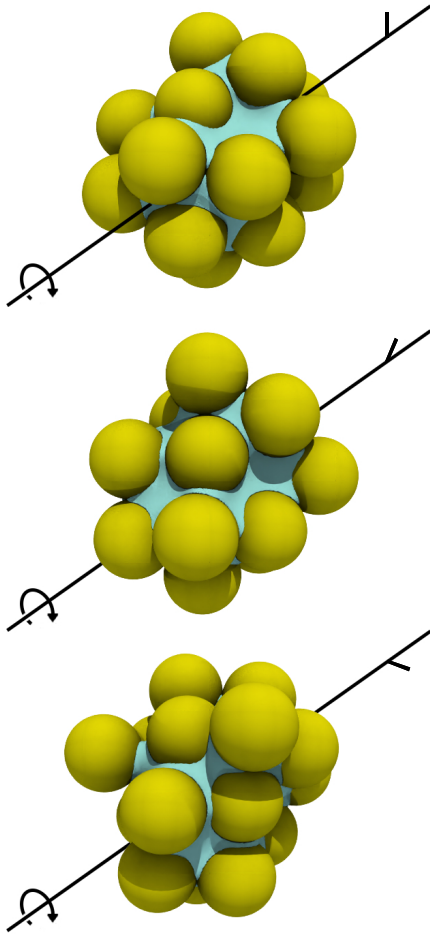
This work is part of the Research Programme of the Dutch Polymer Institute (DPI), PO Box 902, 5600 AX, Eindhoven, The Netherlands, project nr. #803.



**Figure 2:** Contact area between the liquid and the particles.



**Figure 3:** Agglomerate with 19 wetted particles rotated on an axis. This agglomerate show a concave shape, resulting in a larger gas-liquid interface area.



**Figure 4:** Agglomerate with 19 wetted particles rotated on an axis. This agglomerate shows a convex shape, resulting in a smaller gas-liquid interface area.

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