CHEMICAL ENGINEERING TRANSACTIONS

VOL. 32, 2013

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet

Chief Editors: Sauro Pierucci, Jiří J. Klemeš

**ISBN** 978-88-95608-23-5; **ISSN** 1974-9791

DOI: 10.3303/CET1332250

# A Numerical Model of Droplets Coalescence and Drainage in Fibrous Structures

Andrzej Krasinski

Warsaw University of Technology, Faculty of Chemical and Process Engineering,
Warynskiego 1, 00-645 Warsaw, Poland
A.Krasinski@ichip.pw.edu.pl

In this work the model of droplets coalescence in liquid/liquid dispersions in flow through fibrous media is proposed. It is derived for the computation cell being a cubicoid that comprises a single mesh gap and equal volumes upstream and downstream, which size corresponds to a packing factor of the filter media. The numerical approach takes into account deposition of droplets on the fibres as well as coalescence of free-flowing droplets with other ones attached to the filaments. The coalescence efficiency was calculated based on the film drainage model, while for deposition onto fibres the interception and inertial impaction mechanisms are taken into account. The computations gives efficiency of single layer of the media and enable calculation of size of droplets detaching from the fibres, so that provides a complete information about dispersion properties downstream the coalescence structure. The model describes a performance at initial states when the saturation increases and explains the quasi steady-state of operation.

## 1. Introduction

Separation of gas/liquid and liquid/liquid dispersions can be carried out in various processes, depending on properties of fluids, droplets size, concentration etc. This work focuses on liquid/liquid systems and refers to a mechanical separation, which is performed based on density difference between dispersed and continuous phase liquids. The settling velocity, induced either by gravity or enhanced by another external force (e.g. centrifugal), is strongly dependent on droplet size, which is prerequisite for high efficiency separation process and reasonable equipment size. For a very stable emulsions characterised by small size of droplets and stabilized by repulsive interaction forces between them, no significant separation by settling is usually observed. For the purpose of emulsion destabilization and droplets enlargement by merging small into larger ones, the efficient coalescence process has to be employed prior to separation.

The liquid/liquid separators with porous coalescence internals are the most economical choice for large scale process such as deoiling of water (or wastewater), dewatering of fuels, removal of caustic wash remains from petrochemical products etc. The design of the coalescence structure is a key point for high efficiency of separation – the collection of small droplets has to be maximized, while jetting and secondary redispersion have to be avoided. This requires an indigenous design of a multilayer coalescence structure.

The model developed in this work enables understanding of the influence of operating parameters as well as surface properties of the fibrous media on behaviour of dispersed phase liquid within the coalescence structure. It was developed for a basic element of single coalescence layer and comprises a single mesh gap and equal volumes upstream and downstream in form of cubicoid. The total volume corresponds to a packing factor of the filter media. Although many assumptions have been employed to simplify the mathematical formulation, the model enables good qualitative description of both initial and quasi steady-state of operation, predicts the local saturation of porous media, and provides information about the influence of process parameters and media properties on size of detached droplets.

Please cite this article as: Krasinski A., 2013, A numerical model of droplets coalescence and drainage in fibrous structures, Chemical Engineering Transactions, 32, 1495-1500 DOI: 10.3303/CET1332250

## 2. Two-phase flow through fibrous media

In subject literature several models have been developed to describe the behaviour of emulsion droplets as they move through a porous bed. Many of them are based on the theory of two-phase flow, and involve a theory of coagulation to calculate emulsion properties and degree of saturation across the structure from basic properties of coalescence media (such as porosity, fibre size), properties of liquids and local hydrodynamics. In addition, when a dispersion flows through porous structures, the observed behaviour of droplets is strongly dependent on the surface wettability of porous media by the dispersed phase liquid. Hence, the effect of surface energy of the fibres on coalescence performance was studied by many authors (Secerov-Sokolovic et al., 2004; Bansal et al., 2011), and although some discrepancies in literature, the prevailing conclusion is that for high efficiency of the process the surface of fibres has to be wetted by droplets. This affects the saturation of the coalescence media with accumulated liquid of captured dispersed phase, which adheres to the fibres. The effect was reported by Sherony and Kintner (1971), and they proposed a procedure of calculation of the apparent porosity from pressure drop for pure continuous phase and for dispersion based on the Carman-Kozeny equation. Speth et al. (2002) proposed similar approach based on measurements of pressure drop for single and two-phase flow. They derived equation, which includes the sum of total area of fibres and droplets collected within the fibrous structures as parameters contributing to the overall pressure drop for two-phase flow.

## 3. Model formulation

According to considerations presented above, it is clear that deposition of emulsion droplets takes place on fibres or they can be attached to droplets collected within the structure. Hence, in presented model a superposition of both mechanisms is included.

### 3.1 Mechanisms of droplet deposition on a fibre

As reported in literature there are two main mechanisms in typical liquid filtration processes: inertial impaction and direct interceptions. The predominant effect of inertia is observed for relatively large droplets, while for small droplets approaching 1 μm the direct interception dominates the deposition (Hazlett, 1969). Other mechanisms and effects such as Brownian diffusion or electrostatic interactions are neglected, because they are not significant in typical liquid-liquid separation processes, where the size of oil droplets is usually in the range 0.5-50 μm (Krasinski, 2012). To calculate the limiting trajectory distance for direct interception the equation derived by Bürkholz (1989) was applied:

$$y = \frac{d_f}{2} \frac{\left(1+N_R\right) ln\left(1+N_R\right) - \frac{1}{2}\left(1+N_R\right) + \frac{1}{2}\frac{1}{\left(1+N_R\right)}}{Ku} \tag{1}$$

where $d_f$ is the fibre diameter, $N_R$ the interception parameter is a ratio of droplet to fibre diameters, and the Kuwabara number is defined as follows:

$$Ku = -0.5 ln\left(1-\varepsilon\right) - 0.75 + \left(1-\varepsilon\right) - 0.25\left(1-\varepsilon\right)^2 \tag{2}$$

where $\varepsilon$ is the filter porosity. The efficiency of inertial impaction was calculated based on formula provided by Pich (1987).

### 3.2 Coalescence efficiency

During the flow of dispersion through porous media saturated with accumulated liquid of dispersed phase the free-flowing droplets can coalesce with droplets attached to fibres. In fact, not every approach will lead to merging droplets into larger ones. To estimate the tangible effect of coalescence, the film drainage model was applied. The process efficiency was calculated as a product of collection efficiency on a spherical collector proposed by Langmuir and Blodgett (1946) times coalescence efficiency □coal, which was based on simplified model of Coulaloglou (1975):

$$\eta_{coal} = exp\left(-\frac{t_d}{t_c}\right) \tag{3}$$

The model determines the coalescence efficiency from two time scales: tc which is a “contact time”, and td standing for the drainage time (often referred as coalescence time). The latter one is the time required for thinning the film between two approaching droplets to a certain value called “critical thickness”. When the critical thickness is reached the film breaks and droplets merge. The relation valid for non-deformable rigid spheres derived by Chesters (1991) was used.

### 3.3 Drainage

During the flow through fibrous media the dispersed phase particles are captured either by fibres or directly by droplets attached to them. These two mechanism contribute to growth of droplets formed within the structure. When they reach a critical size, large coalesced droplet detaches. Two independent criteria are included in the model and checked as the droplet size increases: (i) relation between the adhesion and drag forces, and (ii) stable size of a droplet at transient hydrodynamic conditions. In the model it is assumed that the droplets captured by the fibres are immediately transported along the fibres to intersections, where the liquid of dispersed phase accumulates. Such a virtual droplet is attached to the fibre located downstream (Figure 1b). In literature, two shapes of droplet on a fibre are identified: asymmetric clam-shell or axisymmetric barrel conformation. In general, barrel shapes are observed for large droplets and good wetting of fibres with droplets, while clam-shell shapes is more likely to occur for small droplets or high contact angles (Chou et al., 2011). Because the process starts from unsaturated structure (so that at the beginning clam-shell configuration seems to be preferred), and additionally the collected liquid is subject to drag force, the clam-shell shapes of attached droplets are assumed. Because the computation of shape and wetting line is based on complex FEM analysis (minimisation of free surface energy), the length of wetting line was calculated from following simplified formula:

$$P = 2\,d_{df} + d_f\,\psi \tag{4}$$

where $d_{df}$ is droplet diameter, $\psi$ is given in radians and presented in Figure 1a (the value was calculated from geometry of the system). The droplet size was defined using the equivalent sphere diameter.

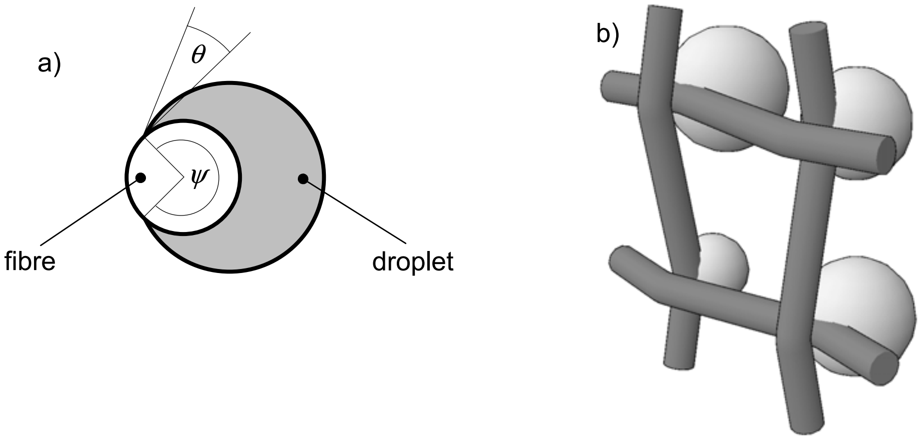


*Figure 1: a) Cross-section of the clam-shell conformation of droplet on a fibre formed prior to detachment, b) geometry of the computational cell: mesh and position of virtual droplets.*

The adhesion and drag forces acting upon a droplet attached to the fibre was calculated according to the formulae given by Sherony et al. (1978). The latter one includes the reduction of the drag on a truncated sphere due to shielding effect of the fibre:

$$F_D = \frac{\frac{15}{2}\pi\, d_{df}\, u\, \mu_c \left[1 + \frac{2}{3}\frac{\mu_c}{\mu_d}\right]}{1 + \frac{\mu_c}{\mu_d}} \tag{5}$$

where $F_D$ is given in dynes, $d_{df}$ in cm, $u$ in cm/s, $\mu_c$ and $\mu_d$ in g/cm-s and represent viscosity of continuous and dispersed phase, respectively.

An additional limit for maximum size of coalesced droplets was introduced in the model. It is based on the consideration of stable size at given hydrodynamic conditions. The relation proposed by Walstra (1993) valid for laminar flow, which is based on critical Weber number, was applied. Based on experiments the author obtained the critical value of Weber number equal 2. Bearing in mind that due to shielding effect of the fibre and contribution of adhesion force, the stresses acting upon droplets attached to the fibres differs from that for free-flowing ones, the $We_{crit}$ value has to be modified to account for this effect. In presented model the original value proposed by Walstra (1993) was used. When the stable size is exceeded it is assumed that the droplet breaks up forming two parts of equal parts. In real situation the rupture can be non-symmetrical, and this can lead to secondary redispersion. The model does not include the reasonable breakage kernel to account for redispersion and entrainment of small droplets. However, it provides information when the second criterion of drainage is fulfilled and this detrimental effect is likely to occur.

## 4. Results of calculation

Calculations were performed for liquid properties corresponding to O/W (oil in water) dispersion, namely diesel fuel no.2 in deionized water. The flow direction was perpendicular to the plane of considered mesh, characterised by two geometrical parameters: fibre diameter $d_f$ and size of the square gap $l_p$. To simplify the analysis and to study a sensitivity of the model, the monodispersed emulsion on inlet was assumed.

### 4.1 Saturation of the porous structure

A typical saturation profile during loading of clean structure is presented in Figure 2.

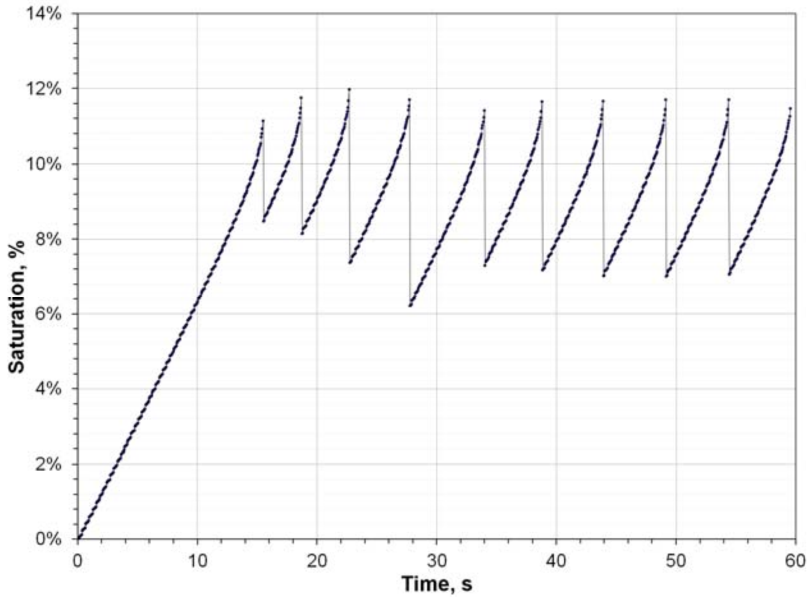


*Figure 2: Time-dependent saturation profile for packing factor 0.001, monodispersed emulsion with 5 μm, fibre diameter 10 μm, mesh gap 100 μm, superficial velocity 10 mm/s, inlet conc. 1 %vol., contact angle 30°*

A constant increase is observed until a critical saturation is reached. As a result of increased shear a coalesced droplet is detached when the stable size is exceeded or drag force surpass the adhesion. This leads to a rapid decrease of local saturation as presented in Figure 2. From this moment the quasi steady-state is achieved, and the value of local saturation is oscillating due to loading with emulsion droplets and releasing of coalesced ones.

*Table 1: Average saturation of the mesh (S) and limiting values of free area ($A_F$) against superficial velocity and contact angle for packing factor 0.001, fibre diameter 10 μm, mesh gap 100 μm, inlet conc. 1 %vol*

| | u | 1 mm/s | 5 mm/s | 10 mm/s | 50 mm/s | 100 mm/s |
|---|---|---|---|---|---|---|
| θ = 30° | S | 10.3 % | 9.97 % | 9.13 % | 8.12 % | 4.19 % |
| | $A_F$ | 0.6-30.3 % | 3.2-31.7 % | 6.5-34.1 % | 16.5-38.4 % | 36.5-46.9 % |
| θ = 60° | S | 7.32 % | 6.87 % | 6.02 % | 5.23 % | 2.11 % |
| | $A_F$ | 4.2-40.4 % | 11.5-42.7 % | 18.6-45.1 % | 32.7-50.9 % | 47.5-59.9 % |

The hold-up of dispersed phase depends strongly on hydrodynamic condition as well as on surface properties of fibrous media. At low velocity and good wetting the saturation increase can even cause a complete blocking of pores (Table 1). This can lead to so called jetting and then the redispersion is likely to occur. However, this effect is not accounted for in the model presented in this work.

### 4.2 Separation efficiency

The separation efficiency obtained for single computational cell is presented in Figure 3. The separation is calculated based on the number of collected droplets. In steady-state of operation the collected liquid is drained and large droplets are released. However, the coalesced droplets which detach from the fibers are relatively large and easy to separate, therefore they are considered as separated from continuous liquid.

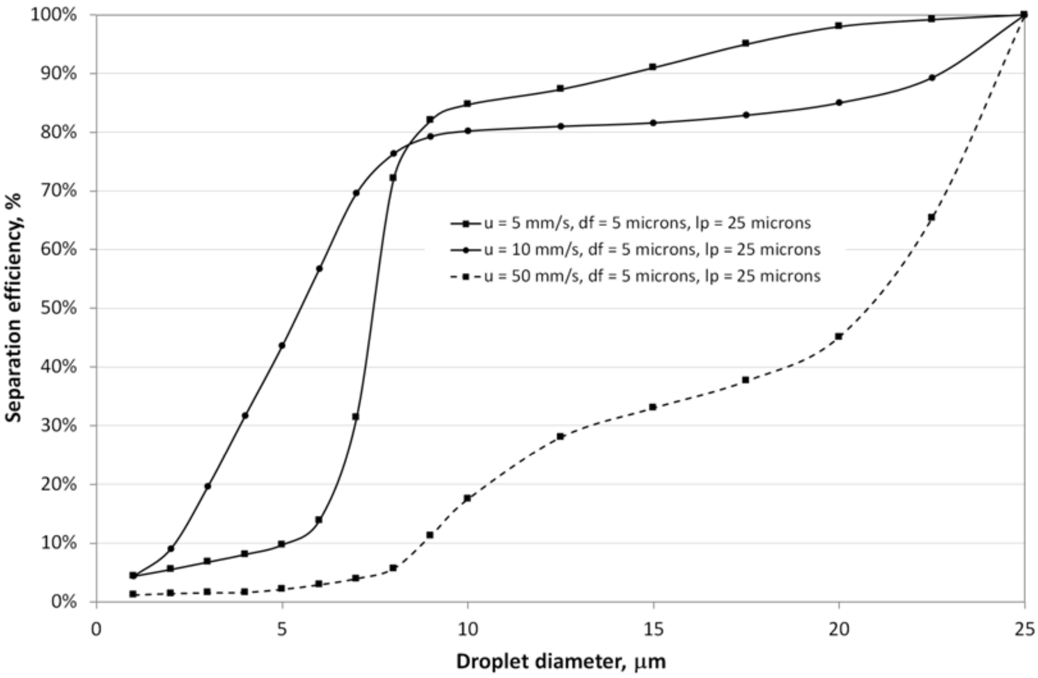


*Figure 3: Separation efficiency as a function droplet diameter and superficial velocity; calculation for filter packing factor 0.001, fibre diameter 5 µm, mesh gap 25 µm, inlet concentration 1 %vol, contact angle 30°*

The effect of inertial mechanism of deposition is observed for small droplets, even below 5 µm, when comparing efficiency curves for 5 and 10 mm/s. However, further increase of superficial velocity 50 mm/s at this range of droplets size brings about a decrease of total separation efficiency – the decrease of the coalescence efficiency prevails over the increase of inertia. When the droplets are in the range between 5 and 10 µm the effect of inertia becomes significant even for 5 mm/s and the product of collection and coalescence efficiency becomes highest, and separation performance the best. All three curves converge to 100% when droplet size approaches dimension of the pore. The results confirm that for droplets between 2 to 7 µm an optimal velocity exists as observed by Secerov-Sokolovic et al. (2004). The deficiency of the model is that it does not quantitatively include the effects of redispersion, which is detrimental for high-efficiency coalescence. Whether this phenomenon is likely to occur or not can be judged based on information, which detachment criterion is fulfilled. If the stable size is exceeded by size of droplets attached to fibres, then a redispersion is possible. This was obtained for contact angles below approximately 75° independently of velocity. For high contact angles (above 75°) then the drag to adhesion force balance controls the drainage. In such case detached droplets are expected to be of relatively uniform size. Moreover, the structure is not blocked with accumulated liquid, which easily drains off. However, in this case the separations efficiency is lower. This leads to another conclusion, which gives hints with regards to properties of fibrous media depending on the location and role performed in fibrous multilayer structure. The inlet coalescence media has to be wetted well to create locally elevated saturation and efficiently capture the droplets. The drain layer on the outlet should be moderately or weakly wetted by dispersed phase liquid to enable efficient detachment of large coalesced droplets.

### 4.3 Size of detached droplets

The calculated size of coalesced droplets that are released from the structure is presented in Table 2. A pronounced effect of fibre diameter on droplet size was obtained. One should bear in mind that in the model the droplet size is calculated based on following assumptions: the droplet is attached to one fibre only, and the flow is uniformly distributed through every pore. When the external layer of the coalescence structure is considered, these assumptions are usually not justified, and size of droplets observed in experiments are larger (Krasinski, 2012). Nevertheless, the model gives valuable trends related to influence of material properties and process conditions on size of coalesced droplets.

*Table 2: Mean size of detached droplets (in μm) as a function of fibre diameter and contact angle; calculations for superficial velocity10 mm/s, packing factor 0.001, $l_p = 10\,d_f$; superscripts indicates the detachment criterion: S – stable size of droplets, D-A – drag to adhesion force ratio*

| | | $d_f$ | 5 μm | 10 μm | 25 μm | 50 μm | 100 μm |
|---|---|---|---|---|---|---|---|
| θ | 30° | | $52.7_{S}$ | $108_{S}$ | $263_{S}$ | $496_{S}$ | $1063_{S}$ |
| | 75° | | $73.2_{D\text{-}A}$ | $146_{D\text{-}A}$ | $366_{D\text{-}A}$ | $729_{D\text{-}A}$ | $1457_{D\text{-}A}$ |

## 5. Summary and conclusions

The model of droplets coalescence in liquid/liquid dispersions in flow through fibrous media is proposed, which includes deposition of droplets on the fibres due to the interception and inertial impaction mechanisms as well as coalescence of free-flowing droplets with other ones attached to the filaments. The coalescence efficiency was calculated based on the film drainage model, while for deposition onto fibres are taken into account. The model gives a valuable insight into droplets coalescence in fibrous media and enables understanding, how operation parameters and media properties affect the separation performance and size of coalesced droplets. Although model needs the validation with experimental data and possible tuning of some parameters, it gives reasonable tendencies, which are consistent with observed phenomena and confirm commonly accepted design rules applied for coalescing filters.

### Acknowledgments

This work was supported by Polish National Science Centre, grant no. N N209 029340.

### References

Bansal S., von Arnim V., Stegmaier T., Planck H., 2011, Effect of fibrous filter properties on the oil-in-water-emulsion separation and filtration performance, J. Hazard. Mat., 190, 45-50.

Bürkholz A., 1989, Droplet Separation, VCH Verlagsgesellschaft, Weinheim.

Chesters A.K., 1991. The modeling of coalescence processes in fluid-liquid dispersions: A review of current understanding, Chem. Eng. Res. Des.: transactions of the IChemE, A 69, 259-270.

Chou T.H., Hong S.J., Liang Y.E., Tsao H.K., Sheng Y.J., 2011, Equilibrium Phase Diagram of Drop-on-Fiber: Coexistent States and Gravity Effect, Langmuir, 27, 3685-3692, DOI: 10.1021/LA2000969.

Coulaloglou C.A., 1975, Dispersed phase interactions in an agitated flow vessel, Ph.D. Thesis, Illinois Institute of Technology, Chicago.

Hazlett R.N., 1969, Fibrous bed coalescence of water: steps in the coalescence process, Ind. Eng. Chem. Fund., 8, 4, 625-632.

Krasinski A., 2012, Experimental verification of the coalescence performance in flow through multilayer fibrous media, 11th World Filtration Congress Proceedings, Session PL02 - Solid-Liquid Separation II.

Langmuir I., Blodgett K.B., 1946, A mathematical investigation of water droplets trajectories, U.S. Army Air Forces Technical Report No. 5418, Washington DC, USA.

Pich J., 1987, Filtration - Principles and Practices, Marcel Dekker, New York, USA.

Secerov-Sokolovic R.M., Sokolovic S.M., 2004, Effect of the nature of different polymeric fibers on steady-state bed coalescence of an oil-in-water emulsion, Ind. Eng. Chem. Res., 43, 6490-6495.

Sherony D.F., Kintner R.C., 1971, Coalescence of an emulsion in fibrous bed: Part I. Theory, Can. J. Chem. Eng., 49, 314-320.

Sherony D.F., Kintner R.C., Wasan D.T., 1978, Coalescence of Secondary Emulsions in fibrous beds, Surf. Coll. Sci., 10, 99-161.

Speth H., Pfenning A., Chatterjee M., Franken H., 2002, Coalescence of secondary dispersions in fiber beds, Separation and Purification Technology, 29, 113-119.

Walstra P., 1993, Principles of emulsion formation, Chem. Eng. Sci., 48, 2, 333-349.