Mathematical modelling of surface tension effects in liquid wall films

Jakov Baleta*, Milan Vujanović and Neven Duić

Faculty of Mechanical Engineering and Naval Architecture, Department of Energy, Power Engineering and Environment, University of Zagreb, Ivana Lučića 5, Zagreb 10 002, Croatia
Email: jakov.baleta@fsb.hr
Email: milan.vujanovic@fsb.hr
Email: neven.duic@fsb.hr
*Corresponding author

Abstract: Behaviour of liquid wall films finds its application in many industrial areas – internal combustion engines, air blast atomisers, heat exchanger ducts, etc. Given assumptions regarding thin liquid films, Navier-Stokes equations are converted to wall film governing equations. The main limitations of a continuous finite volume approach of the film model are at boundary edges of the liquid phase. To overcome those issues, mathematical model for description of surface tension effects was developed and implemented into the computational fluid dynamics (CFD) code. Further area where surface tension force effects are important is the behaviour of liquid film encountering a sharp edge. The analytical force balance approach from Friedrich was incorporated into the existing numerical framework. The improved model of liquid wall film behaviour developed within this paper is the important step in improvement of the accuracy of physical models used in CFD, necessary to comply with stringent requirements of the industry.

Keywords: wall film; computational fluid dynamic; surface tension; droplet spreading; capillary force; Eulerian approach; analytical force balance; film rupturing.


Biographical notes: Jakov Baleta is a Researcher at the Department of Energy, Power Engineering and Environment, Faculty of Mechanical Engineering and Naval Architecture. He has completed his graduate studies in Thermal Engineering with highest honour (summa cum laude) in 2013, and for outstanding achievement during the study, he was awarded with the medal of the Faculty. His areas of research interest are rational use of energy in buildings and industry, with a focus on heat pumps, energy analysis of HVAC systems and the development of mathematical models of computational fluid dynamics problems in the treatment of exhaust gases of internal combustion engines.

Milan Vujanović is a Researcher and Team Leader of CFD Combustion Research Group at Department of Energy, Power Engineering and Environment, Faculty of Mechanical Engineering and Naval Architecture,
University of Zagreb. His research is in the areas of modelling and simulation of turbulent combustion, pollution formation, multiphase flows and sprays, and also in the areas of sustainable energy, environmental protection and climate change. He holds lecturers within courses “Combustion and Radiation Modelling”, and “Numerical Methods in Continuum Mechanics”. He has over 40 publications in Scientific Journals, Books and International Conferences Proceedings to his credit.

Neven Dušić is a Professor in Energy Planning, Policy and Economics since 2001, Department of Energy, Power Engineering and Environment, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb. He is co-Editor of Energy Conversion and Management, subject Editor of Energy, Editorial Board member of Applied Energy, member of regional editorial board of *Thermal Science Journal* and Editor-in-Chief of *Journal of Sustainable Development of Energy, Water and Environment Systems*. His research covers areas of energy planning of energy systems with high penetration of renewables, sustainable communities, energy policy, energy economics, mitigation of climate change, energy efficiency and combustion engineering.

This paper is a revised and expanded version of a paper entitled ‘Modelling and implementation of surface tension effects into CFD wall film module’ presented at 1st South East European Conference on Sustainable Development of Energy Water and Environment Systems – SDEWES, Ohrid, Republic of Macedonia, 29 June–3 July, 2014.

1 Introduction

Liquid film flow sheared by an external air flow field is a physical phenomenon encountered in many engineering applications such as burners, rocket nozzles, mist eliminators, heat exchangers, steam turbine blades and especially internal combustion (IC) engines. In IC engines, it has been observed that unburned fuel that goes directly into the manifold causes an increase in emissions of unburned hydrocarbons in petrol engines and larger product of soot in compression-ignited engines. Also, injection of precursor substance into exhaust gases before the catalyst leads to the formation of liquid wall film owing to unsteady engine working conditions (Birkhold et al., 2007). The above-mentioned examples show great importance of the correct prediction of wall film behaviour as a part of the effort to comply with upcoming stringent environmental regulations (European Union, 2007).

Assumptions of thin liquid film lead to the implementation of the wall film model as a 2D finite volume method on the air flow–wall boundaries. The current wall film model in the commercial CFD code Fire contains mathematical description of physical phenomena in the form of three conservation laws, namely conservation of mass, conservation of momentum and conservation of energy. However, surface tension effects, which are of great importance at the late film spreading stages when the inertial forces are negligible (Horvat, 2006) and also in cases when shear-driven film comes at a sharp expanding corner (Friedrich et al., 2008), are not taken into account.
Mathematical modelling of surface tension effects in liquid wall films

The continuum surface force (CSF) method of Brackbill has been employed extensively over the last 13 years to model surface tension in various fixed (Eulerian) mesh formulations for interfacial flows, in particular in the volume-of-fluid (VOF), level-set (LS) and front tracking (FT) interface representation techniques (Francois et al., 2006). The main drawback of the above-mentioned approaches is that they are unsuitable for the finite area Eulerian approach owing to computational demands. They are usually used on small-scale interfaces such as impinging droplet or few droplet collisions. Another approach for describing surface tension was made by Bai (1996) who developed the solution procedure where capillary forces are taken into account through the capillary pressure term. It is suitable to incorporate this pressure term into momentum equation of wall film and details of the procedure are given in the following section.

Although the behaviour of thin liquid film over solid surfaces is covered by numerous numerical, experimental and theoretical investigations, the same cannot be stated for physics of liquid films flowing around the sharp corner. To the best of the authors’ knowledge and insights gained from the thorough literature review, there were only five investigations of mentioned phenomena, which were concerned with the construction of theoretical model.

Owen and Ryley (1985) were the first to consider flow of thin liquid films around corners. More specifically, they made theoretical analysis to examine radial stress distribution within a uniformly thin liquid film flowing around a sharp bend of fixed radius. For that purpose, linear velocity profile for film was assumed and viscous effects were neglected, as well as film surface disturbances. Separation criterion was derived based on the force balance for an infinitesimal volume of the film turning around the corner. They also conducted experimental investigation, which seemingly confirmed validity of the model for films thinner than 100 µm.

The second approach was offered by O’Rourke and Amsden (1996) and it is the most simple one, since it disregards surface tension and gravity forces, taking into account only pressure difference acting on the film from the gas and the wall side (Goniva et al., 2010). This approach lacks thorough experimental validation, and the comparison with currently available measurements is not promising.

Maroteaux et al. (2002) introduced different ways for describing film separation by carrying out the analysis of film surface instabilities, which appear owing to liquid film inertial forces. Thus, the analogy with Rayleigh-Taylor instabilities was utilised. Following the method of Jain and Ruckenstein (1976) that describes instabilities on stagnant nano-film, they modify it to encompass thicker films in the range of 100 µm. However, this method encountered serious criticism (Gubaidullin, 2007) and discrepancies from experimental measurements (Steinhaus et al., 2007), and will not be taken into account for implementation.

The recent work of Friedrich et al. (2008) has focused on the drawbacks of previous three approaches to overcome them. They assumed that film will either maintain its flow around the corner or will rupture, thereby forming the liquid ligament if critical conditions are met. Separation criterion was derived from momentum balance on the control volume surrounding this ligament. Forces taken into account were surface tension, film inertia and gravity. Inertia tends to keep previous direction of the film flow and thus separates it from substrate, whilst surface tension and gravity oppose that action and tend to keep the film on the substrate. From those observations, they derived very intuitive conclusion that, when inertial forces overcome surface tension and gravity, film
separation will occur. Although this approach overpredicts the onset of film separation (Bacharoudis et al., 2012), it is considered as fairly reliable (Bacharoudis et al., 2013).

Finally, the most recent approach found in the literature is that of Bacharoudis et al. (2014) that combines the force balance approach with film wave characteristics. It not only differs from all existing models by its complexity, but also eliminates their weaknesses. However, it only gives prediction of film separation for the edge angle of 90°, which makes it unsuitable for practical application.

Taking into account the above-mentioned discussion, the purpose of this paper is implementation of surface tension effects on the film interface, as well as the separation criterion from Friedrich et al. (2008) in the CFD code Fire.

The film surface tension effects that are present at boundary edges of the liquid phase play a crucial role in slowing down the film progression. These effects are not currently accounted for within the existing model and the approximation of constant film height over the control volume does not allow reconstructing characteristics of the interface. In this way, scattering of liquid film causes high numerical diffusion, which does not correspond to the physical reality. The threshold value can be set by the user, and only those cells where the film is higher than this value are considered as active. Current approach is not acceptable and, therefore, the second object of this work is improvement of the existing model by incorporating a proper mathematical description of surface tension effects.

The rest of the paper is organised as follows. First, the research methodology is explained together with the mathematical apparatus. Afterwards, the paper is divided into two separate parts taking into account implementation of surface tension effects in two different areas both occurring inside liquid wall films. Hence, each of the two separate parts contains overview of numerical simulation settings and results, together with discussion. Finally, conclusion of the work is presented, which summarises conducted work and gives recommendations for further research.

2 Methodology

Equations of continuum mechanics are based on the conservation laws for mass, momentum and energy. The general form of the time-averaged conservation equation for any dependent variable $\phi$ of the continuous phase in the differential form is:

$$\frac{\partial}{\partial t} (\rho \phi) + \frac{\partial}{\partial x_j} (\rho \phi u_j) = \frac{\partial}{\partial x_j} \left( \Gamma_{\phi} \frac{\partial \phi}{\partial x_j} \right) + S_{\phi},$$

where $\rho$ is the density, $u_j$ Cartesian velocity, $\Gamma_{\phi}$ diffusion coefficient and $S_{\phi}$ is the source term of the dependent variable $\phi$. The source term $S_{\phi}$ is used for the coupling of the liquid and the gaseous phase.

Fundamental assumptions and simplifications of the wall film model incorporated in the commercial CFD code Fire are listed here:

- gas and wall film flow are treated as separate single phases
- the coupling of two phases is achieved by a modified set of boundary conditions based on semi-empirical relations
the film thickness is very small in relation to the mean diameter of the gas flow, so no adaptation of the volume grid to the film surface is necessary

• owing to the thin film and its small velocity, wall friction and interfacial shear stress dominate the film behaviour – a momentum equation could be dropped for a steady state

• wall temperature is below the Leidenfrost point

• the wavy surface of the film is modelled as a mean film thickness with a superimposed film roughness

• mean film surface is assumed to be parallel to the solid wall.

The above-mentioned assumptions lead to the implementation of the wall film model as a 2D finite volume method on the air flow–wall boundaries.

The film thickness equation is the basic governing equation for the wall film flow. It represents a slightly modified formulation of the continuity equation where, instead of mass, the wall film thickness is conserved property. Cartesian formulation of the film thickness equation is:

$$\frac{\partial \delta}{\partial t} + \frac{\partial \delta u_1}{\partial x_1} + \frac{\partial \delta u_2}{\partial x_2} = \frac{1}{\rho A} (S_{mf} - S_{mf'})$$

where $\delta$ is the film thickness, $\rho$ is the film density, $u_1$ and $u_2$ are film velocity components, $S_{mf}$ and $S_{mf'}$ are source terms and $A$ is the surface of the film. If we assume that the source terms are provided, equation (2) can be solved explicitly if the velocity components are known beforehand.

Film momentum equation describes the dynamics of liquid film interaction with its environment – wall, air stream above the film, impinging droplets, etc. Equation (3) gives mathematical formulation of wall film momentum conservation law:

$$\frac{dM_i}{dt} + \int_{\partial L} \rho u_i (n_i - V_j) \hat{n}_i \, dL = \int_L p \delta \hat{n}_i \, dL + mg_i + \Gamma_i + S_{mf},$$

where $M_i$ is the film momentum, $\rho$ is the film density, $u_i$ is the film velocity, $V_j$ is the wall velocity, $\hat{n}_i$ is normal to the face cell facing outwards, $L$ is the length of the face cell boundary, $\delta$ is the film thickness, $\rho$ is the film pressure, $m$ is the film mass, $g_i$ is the gravity vector, $\Gamma_i$ is the term that takes into account all shear stresses and $S_{mf}$ presents various source and sink terms, such as film entrainment, spray droplets impingement and film evaporation.

Inclusion of surface tension effects into the pressure term of momentum equation was made by calculating the capillary pressure. This force drives the surface towards a minimal energy state characterised by a configuration of minimum surface area, and is represented by the combined action of liquid surface tension $\sigma$ and film surface curvature $C$ (Horvat, 2006):

$$p_\sigma = -\sigma C.$$  

As shown in O’Brien and Schwartz (2006) and Schwartz and Weidner (1995), the mean curvature of the free-surface can be approximated using the following expression:
\[ C = \left( \frac{1}{R_1} + \frac{1}{R_2} \right) - \left( \frac{\delta}{R_1^2} + \frac{\delta}{R_2^2} \right) + \nabla \cdot \nabla \delta. \]  \hspace{1cm} (5)

On quality computational meshes surface area patches are rather small, so that they could be considered as flat, which means that the first two terms of equation (5) could be neglected. Thus, film surface curvature could be approximated only with the Laplacian of film thickness.

Using schematic representation of wall film cells given in Figure 1, the Laplacian of film thickness could be numerically approximated as follows:

\[ \Delta \delta = \nabla \cdot \nabla \delta = \frac{1}{S} \sum_{i=1}^{n_{edges}} n_i \nabla \delta \cdot L = \frac{1}{S} \sum_{i=1}^{n_{edges}} n_i \frac{\delta_i - \delta_j}{AB_i} \cdot L, \]  \hspace{1cm} (6)

where \( S \) is the surface patch area, \( L \) is the length of the neighbour edge, \( n_i \) is the unit normal on common edge facing outwards and \( AB_i \) is the length between cell centres A and B. Equation (6) was incorporated into the pressure term of momentum equation of the existing numerical framework.

**Figure 1** Schematic representation of wall film cells (see online version for colours)

Film rupturing model is based on the work of Friedrich et al. (2008) as stated in the Introduction. A 2D control volume that embraces liquid film ligament shown in Figure 2 is considered. For this control volume, linear momentum conservation law will be written taking into account inertial forces, surface tension and gravity.

As the film approaches the corner, its momentum tends to separate it from the corner, while surface tension and gravity oppose it. The momentum flux entering the control volume can be expressed as:

\[ -\rho_f \dot{V}_f \cdot u_f \sin \theta, \]  \hspace{1cm} (7)

where \( \rho_f \) is the liquid film density, \( \dot{V}_f \) is the film volumetric flow, \( u_f \) is the mean film velocity and \( \theta \) represents inclination of the surface from the horizontal. Surface tension force acts on both sides of the ligament and can be written as:

\[ -\sigma w_f \sin \theta, \]  \hspace{1cm} (8)

on the upper side and as:

\[ -\sigma w_f \]  \hspace{1cm} (9)
on the lower side. $\sigma$ is the surface tension and $w_f$ is the film width. To calculate film ligament length for the evaluation of gravitational forces, experimental correlation of Arai and Hashimoto (1985) is used:

$$L_b = 0.0388 h_f^{0.5} Re_f^{0.6} We_{rel}^{0.5}$$  \hspace{1cm} (10)

where $L_b$ is the ligament length, $h_f$ is the film thickness and $Re_f$ and $We_{rel}$ are film Reynolds and Weber number defined, respectively, as follows:

$$Re_f = \frac{\rho_f u_f h_f}{\mu_f}$$  \hspace{1cm} (11)

$$We_{rel} = \frac{\rho_g h_f (U_g - u_f)^2}{2\sigma}.$$  \hspace{1cm} (12)

where $\rho_g$ represents gas phase density, $\mu_f$ is the liquid film dynamic viscosity and $U_g$ is the gas phase velocity. Finally, after defining film volumetric flow:

$$\dot{V}_f = u_f w_f h_f,$$  \hspace{1cm} (13)

linear momentum balance per unit width is given here:

$$\rho_f u_f^2 h_f \sin \theta = \sigma \sin \theta + \sigma + \rho_f g h_f L_u \cos \theta.$$  \hspace{1cm} (14)

**Figure 2**  Force balance on film ligament

Source: Friedrich et al. (2008)

Force ratio, which also represents the separation criterion, is obtained by dividing equation (14) with right-hand side terms:

$$\text{force ratio} = \frac{\rho_f u_f^2 h_f \sin \theta}{\sigma \sin \theta + \sigma + \rho_f g h_f L_u \cos \theta}.$$  \hspace{1cm} (15)

This criterion represents a Weber number modified to include effects of gravity and surface tension on the bottom surface of the film. If it exceeds unity, liquid film separation will occur.
It should be noted that current models found in the literature are giving only separation criterion without any description of separated liquid characteristics, such as separated film mass fraction or particle size distribution of separated droplets. This remains pending problem with the high potential for experimental and theoretical research. The developed models were integrated into the commercial CFD code via user-functions written in the FORTRAN programming language.

3 Liquid film interface

3.1 Test case

To test the numerical scheme and to check if the capillary pressure effects can be predicted properly, there is a need for a simple case where only capillary force effects are relevant and for which there is an analytical solution. Thus, the spreading of an isothermal droplet on a solid surface is simulated. The droplet is driven with Laplace (capillary) pressure as dominant force and other forces being absent or negligible. Similar tests were obtained by Diez et al. (1994), who proposed analytical solution using lubrication theory, which neglects convective terms in momentum equation, and compared the proposed solution with experimental results. The problem can be observed as two dimensional because of axial symmetry. They showed that the normalised film thickness $h/h_0$ can be expressed as a single function of the scaled radial position $r/r_s$, irrespective of the time level. In this way, the non-dimensional profile of droplet throughout the spreading stage is obtained. This profile is the basis for validation of implemented mathematical model of surface tension.

3.1.1 Numerical simulation settings

The simulation domain with relevant boundary conditions is shown in Figure 3. A three-dimensional computational mesh with dimensions of $5 \times 5 \times 0.1$ mm$^3$ with 20,000 orthogonal hexahedron cells was used for the simulation. Wall boundary condition was defined at the bottom of the domain, whilst a static pressure outlet was imposed at all other sides. The domain pressure was 1 bar and temperature was equal to the droplet temperature. Pressure velocity coupling of momentum and continuity equation was obtained using the SIMPLE/PISO algorithm. The central difference discretisation scheme was used for the convective term in the continuity equation with a blending factor of 1, whilst a MINMOD Relaxed with a blending factor of 0.5 was used for the convective terms in momentum equations. Turbulence model was deactivated, since quiescent air is necessary for comparison with analytical expression. Energy equation was also deactivated together with the gravity in order that the only relevant force stays capillary pressure, which tends to spread given droplet shape into the state of minimal surface energy.

Simulation starts from a drop, which initially takes the shape of a rotational paraboloid, shown on the right part of Figure 3, with volume of 0.12 mm$^3$ and thickness at the centre of 0.08 mm. Second simulation was conducted with the cube-shaped droplet to see whether incorporated model will spread this artificial shape into rotational paraboloid. The spatial and time discretisation increments were 0.05 mm and $10^{-5}$ s, respectively. The simulated time was 0.4 s since spreading of the droplet practically remained unchanged around and after 0.4 s.
3.2 Results and discussion

This section presents results and discussion regarding two simulation cases of droplet spreading. Diez et al. (1994) showed that the droplet assumes parabolic non-dimensional profile, which is conserved during all stages of the spreading process. This way it is reasonable to begin validation of the implemented model by assuming initial droplet shape of rotational paraboloid to see if non-dimensional profile of Diez et al. (1994) is conserved during the numerical simulation of droplet spreading. Further confirmation of the model comes from the initialisation of some artificial droplet shape that is highly unlikely to be encountered in nature. This shape should be again spread into the shape of minimal surface energy, i.e., parabolic droplet, owing to activity of capillary force.

3.2.1 Parabolic droplet

Qualitative depiction of droplet evolution is presented in Figure 4. As can be seen, droplet shape changes only after 1 ms. The reason behind this phenomenon is that only relevant force is capillary pressure, which produces fairly small spreading velocities whose effects on the droplet spreading are visible only after 1 ms. Further time evolution shows that droplet shape does not change much between 0.25 s and 0.4 s, since the wall film thickness gradients on the edge of the droplet tend to zero. On the same picture could also be noticed that the behaviour of the droplet during the whole period of the simulation remains symmetrical, which is qualitatively in agreement with analytical results of Diez et al. (1994).

Quantitative comparison of simulation results and non-dimensional analytical droplet profile given in Figure 5 shows that the present numerical predictions are in good agreement with the analytical expression from Diez. It can be seen that the initial non-dimensional droplet profile is conserved during the whole process of the establishment of steady state, which is the first confirmation of model physics. However, the model does not include correction of the film curvature at the film front owing to the wettability effects represented by (dynamic) contact angle. These effects are omitted from modelling owing to the relatively large spatial discretisation, which prevails in most of the practical applications where wall film phenomena are important.
3.2.2 Cube-shaped droplet

Simulation of the second case starts from a quadratic drop with uniform thickness of 0.8 mm. The goal was final confirmation of the incorporated model by studying whether this shape will also be spread into the rotational paraboloid.

Qualitative evolution of the droplet shape depicted in Figure 6 reveals that, under the influence of the strong film thickness gradient, droplet spreading is the most intense during the first 0.1 s of the simulation. After this period, relative increase in the area occupied by the droplet is much lower. Final shape of the droplet achieved after steady state was established around 0.5 s and reveals a slight asymmetry in its shape. The reason behind this is not inaccuracy within the developed model, but rather relatively coarse computational grid whose resolution was not adequate to smooth out initially asymmetric quadratic shape. Closer look at Figure 6 reveals that the gradient of film thickness is uniform along droplet radius, which confirms validity of the implemented model.
Figure 6 Qualitative representation of cube shaped droplet evolution (see online version for colours)

Dimensional and non-dimensional evolution of droplet profile in Figure 7 shows that it continuously propagates towards parabolic shape with exception of profile captured at 0.01 s. Although the general trend of the droplet spreading should include decrease in the central film thickness, purple curve on Figure 7 clearly states that this is not the case. The reason for this lies behind the pressure velocity interpolation procedure, which brings non-physical increase in film thickness. However, owing to small propagation velocities encountered in problems where surface tension is the driving force, solution smooths itself towards the end of simulation, which is also depicted in the same figure. Finally, the left part of Figure 7 clearly shows that there is no significant movement of droplet front between 0.25 s and 0.5 s, which is in accordance with the previously given qualitative observation.

Figure 7 Quantitative representation of cube shaped droplet profile (see online version for colours)

This case together with the previous one gives final confirmation of the implemented model, indicating that the numerical modelling of the capillary pressure is reasonable in terms of trade-off between accuracy of results and computational demands.
4 Film separation

4.1 Numerical simulation settings

To verify film separation criterion from Friedrich et al. (2008), simulation of liquid film sheared by air flow was conducted on geometry with dimensions given in Figure 8. A three-dimensional computational mesh with 420,000 orthogonal hexahedron cells and corner section with slope of 60° measured from the horizontal was used for the simulation. To properly describe evolution of liquid film sheared by air flow, mesh was refined until the corner section with cell size below 1.5 mm. Air enters the domain with 20 m/s through the inlet with dimensions of 100 × 20 mm². Turbulence quantities on the inlet were 0.001 m²/s² for turbulent kinetic energy and 0.0033 m for turbulent length scale. Outlet was defined as constant pressure outlet of 1 bar. The wall boundary condition was imposed at the bottom, top and on the domain sides. Pressure velocity coupling of momentum and continuity equation was obtained using the SIMPLE/PISO algorithm. The central difference discretisation scheme was used for the convective term in the continuity equation with a blending factor of 1, and for the convective terms in momentum equations the same scheme with a blending factor of 0.5 was used. Turbulence was modelled using advanced k-\( \omega \)-f model (Hanjalić et al., 2004). Liquid film of water was introduced using feeder located 20 mm from the inlet with volumetric flow rate of 41.5 cm³/s. Time discretisation step was reduced to \( 10^{-4} \) s to achieve stable calculation.

4.2 Results and discussion

Verification of film rupturing criterion was carried on just on the qualitative basis in this stage of research. Separation criterion in the form of force ratio described in mathematical model section was implemented into the commercial CFD code Fire. Since there is no model in the literature that describes properties of ruptured film, i.e., percentage of ruptured mass and particle size distribution of separated droplets, authors made some assumptions that they presume as fairly reasonable:

- when force ratio is above unity, the whole film mass will detach, otherwise film will continue with propagation along the wall
- normal particle size distribution of separated droplets is assumed with expected value of droplet radius equal to the half of film thickness according to O’Rourke and Amsden (1996).

Qualitative depiction of film separation is presented in Figure 9. Cells where separation occurs are marked red inside the software, and it can be seen that they are located at the edge of the slope as expected. On that position, film properties were calculated and inserted into the separation criterion to check whether the code produces correct values. Thus, verification of the implemented model was obtained through qualitative check of cell position where separation occurred and through manual calculation of separation criterion for activated cells. This is a reasonable approach since only separation criterion is implemented in the code and it is the result of semi-empirical considerations. There are no further physical implications following from the criterion, which could be observed in the simulations.
5 Conclusions

After literature review, the existing numerical framework was extended by incorporation of the appropriate surface tension model that takes into account the trade-off between computational demands and accuracy of the solution. Thus, effects resulting from capillary action are modelled as a part of a pressure term of the wall film momentum equation. Simulation results conducted with the new model were compared with analytical non-dimensional droplet profile. Two simulation studies were conducted with different initial droplet shape to test whether model conserves theoretical droplet profile.
during all stages of droplet spreading and whether would some artificial initial droplet shape take form of minimum surface energy, i.e., rotational paraboloid, under the action of surface tension. Agreement with theoretical expression is satisfactory and gives confidence for commercial application of the implemented model. In this paper was shown that incorporation of surface tension effects into the existing wall film model can increase its capabilities in prediction of wall film propagation with a high accuracy.

Furthermore, the existing framework was extended by incorporation of the suitable film separation criterion. This criterion was verified with relatively simple approach described in the previous section. The pending problem still remains proper mathematical description of percentage of separated film mass and particle size distribution of generated droplets, which is going to be object of the future work. Results of the conducted numerical study support the feasibility of commercial application of implemented models.

As a part of the global pollution problem, increasingly strict legislation on allowed emissions from the industry and transport sector forces manufacturers to design more efficient and ‘cleaner’ equipment. Direct consequence is the increased complexity of the design process, which makes usage of advanced design tools, one of which is CFD. The improved model of liquid wall film behaviour developed within this paper may be a valuable contribution in continuous process where constant improvement of accuracy of the physical model used in CFD is mandatory to comply with the ever-increasing requirements of the industry.

Acknowledgement

The authors wish to express sincere gratitude to Professor Željko Tuković from the University of Zagreb for fruitful discussions regarding mathematical modelling of surface curvature as an important term for calculating pressure coming from surface tension.

References


