

SPH Simulation of Rivulet Dynamics on Surfaces with Various Wettabilities

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ABSTRACT

Rivulet dynamics is involved in different scientific problems and industrial applications from production of microchips, to rain flow on structural systems such as wind turbine blades and aircraft wings. In the latter case for example, rivulet flow leads to accumulation of ice on airfoil surface that may affect the aircraft performance. Hence, understanding the dynamics of rivulets is important in solving various scientific problems. In this paper the results of a numerical simulation based on smoothed particle hydrodynamic (SPH) method will be reported on dynamics of rivulets under the effect of various air shear speeds and different surface morphologies. The simulation results will be compared and validated with experiments to shed more lights in understanding the mechanism of shear driven rivulet flow on solid substrates.

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INTRODUCTION

A narrow stream of liquid falling down a solid substrate (e.g. rain on window pane) is called a rivulet. Rivulets pattern can be affected by their flow rate [1]. The onset of rivulet formation is sequence of droplets that merge into a linear straight narrow film. Rivulets start to meander with instability at their interface with air at higher flow rates [2]. Oscillating rivulets may be formed by increasing the flow rate [2]. Rivulet flows are influenced by a number of parameters such as flow velocity, the morphology and the temperature of the surface on which they are moving.

Rivulet dynamics is involved in diverse scientific problems and industrial applications such as production of microchips, the flow of surface active materials in chemistry [3] and rain flow on structural systems such as wind turbine blades, power lines and air crafts [4]. In the case of aircrafts for example, during the flight, rain droplets hit the airfoil surface which then create rivulets due to wind shear effects. At sub-zero temperatures, ice may be accumulated on the airfoil surface which decreases the aerodynamic efficiency of the aircraft [4]. Hence, developing better de-icing or anti-icing systems for aircrafts is crucial in aerospace industry [4].

Mathematical description of rivulet dynamics is complicated due to the existence of free boundary interfaces which must be determined as a part of the solution for the governing equations. Additionally, linearized equations are not sufficient to study the phenomenon if the film unit depth goes to zero. Lubrication theory or long-wave-theory is one of the methods to study thin film flow on a solid surface [5, 6, 7]. In this method, the governing equations and boundary conditions

are simplified to a system that usually contains a single nonlinear partial differential equation that is formulated in terms of the local film thickness [5]. Other unknowns such as fluid temperature and velocity are determined by functional solution of the initial differential equation. In this case the free boundary complication can be eliminated from the system [6]. Marshall and Ettema [7] used lubrication approximation in their experiments with low Reynolds number to investigate the effect of gravity and shear flow on rivulets. The authors showed that for low speed shear flows (less than 5 m/s) shear driven flow and gravity effects have nearly the same influence on rivulets behavior. However, at high sheer speeds of 10 m/s there is a large difference between the flows driven by wind shear and the flow of rivulets under the effect of gravity. In addition in the latter case, they presented that the effect of microgravity and terrestrial gravity is also considerably different in rivulet flow.

As mentioned before, surface morphology is one of the factors that should be taken into consideration while studying rivulets behavior. Gajewski [8, 9] conducted experiments with rivulets on three different surfaces: aluminum, copper and brass while heating [8] and cooling [9] these surfaces. It was shown that lowering the temperature improves the hydrophilic behavior of the metal surface, thus, the rivulet width increases. In addition when the number of electrons on the last metal shell is higher, the metal shows more hydrophilic properties [9]. This is the reason that the worst wetting property is for copper, the rivulet is the narrowest on this plate and the contact angle is the highest. In contrast, among these metals the best wetted surface is aluminum, it has the widest rivulet flow and the contact angle is the lowest on this plate [9].

Simulation of thin film flow patterns, flowing down inclined and horizontal planes was performed by Diez *et al.* [3, 10]. To analyze the rivulets wave lengths, the effect of capillary force and fluid-solid interactions were considered in their model. Fluid inertia found to be the main cause of rivulets meandering behavior [11]. Saber *et al.* [12] obtained analytical results for rivulet thickness and wetting rate at break up by assuming the fluid flowing down or climbing on a vertical or inclined surface while the surface was subjected to the interfacial shear flow.

Up to now a complete understanding of rivulet dynamics especially under the effect of different surface wettabilities has not yet been achieved. Being able to predict the rivulet behavior under the effect of these two important parameters is of utmost importance for understanding the underlying physics of rivulet dynamics under practical conditions, i.e. in-flight icing. This paper consists of numerical simulation of rivulets dynamics under the effect of different air shear speeds and various surface wettabilities based on smoothed particle hydrodynamic method.

METHODOLOGY

Smoothed Particle Hydrodynamics (SPH) used in this study is a numerical technique which discretizes the continuum through a set of nodes to approximate its dynamics by using interpolation points. The main idea of SPH like the other mesh-free methods is to treat nodes as material particles carrying physical properties. This method was originally developed to simulate astrophysical problems [13, 14]. Later on it was modified as a leading mesh-free method with wide variety of applications in fluid mechanics [15, 16].

In this method, the equations of motion can be easily derived for the nodes. Particle representation of SPH yields to a simultaneous conservation of mass, linear and angular momentum, energy and entropy (without applying artificial viscosity) [15]. Unlike the grid-based methods, the derivatives of quantities can be determined analytically in SPH. In addition, the absence of convective term in the governing equations makes the numerical computations easier. Due to the Lagrangian nature of SPH, handling deformations and complex geometries, describing moving boundary conditions or irregular interfaces, and tracking the time-history of the variables will be comparatively simple.

In this study, the main reason for preferring SPH over grid-based models is the ability of this technique to easily track the moving boundaries which yields more accurate simulation of interfaces [17, 18, 19]. The principle features of SPH are described in details in [20, 21, 22, 23]. The general procedure of SPH can be summarized in two steps; decomposing the continuum into a set of particles (without connectivity) and using finite summation instead of integral representation for approximating particle attributes.

SPH Theory and Implementation

The attributes of each particle in SPH depend on the objects being simulated. Some of the common characteristics for a particle are its position, mass, size, velocity, acceleration and etc.

For any field $A(r')$ in the fluid represented by a set of particles like $i \in [1, \dots, N]$, the smoothed interpolated version, $A_s(r)$ can be defined through a kernel $W(r - \hat{r}, h)$ [24];

$$A_s(r) = \int A(r') W(r - \hat{r}, h) d\hat{r} \quad (1)$$

where $W(r - \hat{r}, h)$, is a smoothing kernel. This kind of kernel is nonparametric weight function which is used as an approximation for the Dirac delta function in the identity transform definition. It enables us to estimate the value of the quantity at each point based on the values at the neighboring points. The width of the kernel (h) approximates a Dirac delta function in the limit $h \rightarrow 0$. The main characteristics of an SPH kernel are [15];

$$\lim_{h \rightarrow 0} W(r - \hat{r}, h) d\hat{r} = \delta(r - \hat{r}) \quad (2)$$

$$\int W(r - \hat{r}, h) d\hat{r} = 1, \text{ over the domain} \quad (3)$$

$$W(r - \hat{r}, h) \geq 0, \text{ inside the domain} \quad (4)$$

$$W(r - \hat{r}, h) = 0, \text{ outside the domain} \quad (5)$$

Based on [25, 26, 27], for an even and normalized kernel, SPH interpolation is of the second order. In order to improve stability, Müller *et al.* [26, 27] proposed to apply three kernels for the quantity interpolations that can be practically used for all of the simulation quantities. These easy and fast computable kernels are zero at the origin. To prevent clumping effect for pressure calculations W_{spiky} can be used [28]. Noting that clumping occurs when particles are so closed to each other that unrealistic clusters are produced due to numerical instability [28]. $W_{viscosity}$ is also recommended for viscosity, as it inhibits increase of particles relative velocity due to their positive Laplacian. These kernels are;

$$W_{poly6}(r, h) = \begin{cases} \frac{315}{64\pi h^9} (h^2 - |r|^2)^3, & 0 \leq |r| \leq h \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

$$W_{spiky}(r, h) = \begin{cases} \frac{15}{\pi h^6} (h - |r|)^3, & 0 \leq |r| \leq h \\ 0, & \text{otherwise} \end{cases}$$



$$W_{viscosity}(r, h) = \begin{cases} \frac{15}{2\pi h^3} \left(-\frac{|r|^3}{2h^3} + \frac{|r|^2}{h^2} + \frac{h}{2|r|} - 1 \right), & 0 \leq |r| \leq h \\ 0, & \text{otherwise} \end{cases} \quad (8)$$

By providing sufficient points and choosing smooth kernel, the integral in [equation \(1\)](#) can be approximated by this summation;

$$A(r) = \sum_j m_j \frac{A_j}{\rho_j} W(r - r_j, h) \quad (9)$$

As the distribution of the points is more regular, the accuracy of this summation will be better than in Monte-Carlo method. In addition, it can be shown that in 3D modeling, the minimum number of neighbors are ~ 33 [29]. For example, by applying this definition, the smoothed estimate of the density at particle i can be found using;

$$\rho_i = \sum_j m_j W(r_i - r_j, h) \quad (10)$$

Also, the gradient and Laplacian of the smoothed function $A(r)$ are, respectively;

$$\nabla A(r) = \sum_j m_j \frac{A_j}{\rho_j} \nabla W(r - r_j, h) \quad (11)$$

$$\nabla^2 A(r) = \sum_j m_j \frac{A_j}{\rho_j} \nabla^2 W(r - r_j, h) \quad (12)$$

Each particle in SPH should have at least a position and velocity. These particles are moved by applying forces and calculating the acceleration. Other attributes can change over time as well, which represents the objects dynamic.

Fluid dynamics is about the study of fluid motion in response to the forces such as gravity, pressure and shear. In SPH, direct applying of force balance is necessary for finding velocities and positions of the particles in a transient process. It should be mentioned that the SPH method was first introduced as a new method for solving the equations of motion of a compressible fluid. The equations in this work are from the adaptation of the method for incompressible flow described by Monaghan [30]. In order to make a compressible fluid behave like an incompressible fluid, the pressure should increase in a way that the density becomes high. Thus, it will be difficult to compress the fluid any further. [Equation \(9\)](#) is the base to find the particle body forces and the acceleration a_i of the fluid particle i can be applied for each property in the following Lagrangian form of hydrodynamic equations [29];

$$\frac{d\rho}{dt} = -\rho \nabla \cdot v \quad (13)$$

$$\frac{dv}{dt} = -\frac{1}{\rho} \nabla P \quad (14)$$

where ρ , P and v represent density, pressure and velocity, respectively.

For sufficiently small time steps, $d\rho_i/dt = \sum_j m_j v_{ij} \nabla_i W_{ij}$ which is the particle form of [equation \(13\)](#) is recommended for density calculation, because [equation \(10\)](#) may underestimate particles densities at fluid surfaces [23]. Also for [equation \(14\)](#) by using [equations \(9\)](#) and [\(11\)](#), we can have;

$$\frac{\nabla P_i}{\rho_i} = \sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij} \quad (15)$$

where $\nabla_i W_{ij}$ is the gradient of W with respect to particle i , considering particle j as its neighbor. The specific pressure format is applied for the summation in [equation \(15\)](#), because using only $\sum_j m_j \left(\frac{P_i}{\rho_i^2} \right) \nabla_i W_{ij}$ for the pressure gradient does not result in force symmetry. Based on Monaghan [16], the proposed form of governing equations, can be written as;

$$\frac{d\rho_i}{dt} = \sum_j m_j v_{ij} \nabla_i W_{ij} \quad (16)$$

$$\frac{dv_i}{dt} = - \sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W_{ij} + F_i \quad (17)$$

The term Π_{ij} is an artificial viscosity which is usually added to control the shocks. The definition of this term based on [15, 31] is;

$$\Pi_{ij} = \begin{cases} \frac{-\psi \bar{c}_{ij} \mu_{ij} + \beta \mu_{ij}^2}{\bar{\rho}_{ij}} & \text{if } v_{ij} \cdot r_{ij} < 0 \\ 0 & \text{if } v_{ij} \cdot r_{ij} > 0 \end{cases}, \quad \mu_{ij} = \frac{h v_{ij} r_{ij}}{r_{ij}^2 + \eta^2} \quad (18)$$

where ψ and β are viscous constants (usually set to 1 and 2, respectively), η is a constant used to avoid numerical divergences, and finally c identifies the mean speed of sound for particle i [32, 33];

$$c_i = \sqrt{\frac{\gamma P_i}{\rho_i}} \quad (19)$$

γ is the ratio of specific heat and c_i represents the speed of sound through the fluid represented by particle i . Then, the acceleration a_i of the fluid particle i can be obtained by calculating the force density fields;

$$a_i = 1/\rho_i (f_i^{pressure} + f_i^{viscosity} + f_i^{surface\ tension} + f_i^{gravity} + f_i^{external}) \quad (20)$$

$$f_i^{pressure} = - \sum_j m_j \frac{P_j + P_i}{2\rho_j} \nabla W(r_{ij}, h) \quad (21)$$

$$f_i^{viscosity} = \mu \sum_j m_j \frac{v_j - v_i}{\rho_j} \nabla^2 W(r_{ij}, h) \quad (22)$$

$f_i^{external}$ are the external body forces for the system.

$f_i^{surface\ tension}$ will be explained in the next sections.

For SPH, particle pressure has a significant effect in the calculations. The common constitutive equation for pressures P_i is computed by;

$$P_i = k(\rho_i - \rho_0) \quad or \quad P_i = B \left(\left(\frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right) \quad (23)$$

where k is the stiffness of the fluid and ρ_0 is the rest density. For compressible fluid, by using derivative of equation of state with respect to density, relation between the fluid bulk modulus of elasticity in [equation \(23\)](#) and the speed of sound (c), can be found as follows;

$$c^2(\rho) = \frac{\partial P}{\partial \rho} = \frac{B\gamma}{\rho_0^\gamma} \rho^{\gamma-1} \quad (24)$$

Applying Lagrangian projection method for enforcing incompressibility is shown to be very slow due to its implicit solution [19, 26, 34, 35, 36], therefore by assuming weak compressibility, [equation \(23\)](#) can be used as a faster option even for incompressible fluids [37]. Monaghan however, used a different equation of state, for water [15];

$$P_i = B \left(\left(\frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right) , \quad c_i = \sqrt{\frac{\gamma(P_i + B)}{\rho_i}} , \quad B = \frac{200gH}{\rho\gamma} \quad (25)$$

where H is the maximum depth of water. This equation as we expect produces large changes in pressure for small changes in density.

There are some other attributes that play an important role for applying boundary conditions or stability of this numerical method. The color attribute in SPH is a quantity that is zero everywhere except at the liquid particle which is equal to one and it can be obtained as follows;

$$C_i = \sum_j \frac{m_j}{\rho_j} C_j W(r_{ij}, h) \quad (26)$$

This color attribute is set to zero for all air particles [27]. The gradient of the color field is;

$$\nabla C_i = \sum_j \frac{m_j}{\rho_j} C_j \nabla W(r_{ij}, h) \quad (27)$$

In general, large deviation in the magnitude of the color gradient shows that the particle is located at the fluid surface. This definition helps adding the surface tension force which tends to make the surface smooth. For surface tension, force is defined by [27, 38];

$$f_i^{surface\ tension} = -\sigma \nabla^2 C_i \frac{n_i}{|n_i|} \quad n_i = \nabla C_i \quad \nabla^2 C_i = \sum_j \frac{m_j}{\rho_j} C_j \nabla^2 W(r_{ij}, h) \quad (28)$$

This equation can cover the important effects of surface forces between the liquid and gas phases, however in case of forces on the liquid-solid interface, some additional procedures are suggested in the literature [38, 39, 40, 41]. Based on [39, 41] for the surface particles near the contact line of fluid and solid, it is recommended to use additional force term (parallel to the wall). The magnitude of this force per unit length is $(\sigma \cos \theta_D)$ where θ_D is the dynamic contact angle. For the particles located next to the contact line, instead of using $\frac{\nabla C_i}{|\nabla C_i|}$ for calculation of unit normal vector, it is proposed to use [39];

$$\hat{n} = \hat{n}_{wall} \cos \theta_D + \hat{n}_{contact\ line} \sin \theta_D \quad (29)$$

where $\hat{n}_{\text{contact line}}$ is the unit vector parallel to the wall and $\hat{n}_{\text{wall}}$ is the unit normal vector directed into the wall.

Time Stepping

Another important issue in SPH technique is the collision between particles. The velocity of each particle should be adjusted to inhibit particle interpenetrations and mixing. To do so, the XSPH variant [15, 16] is useful especially for high speed flow. The variant is calculated by using;

$$\Delta v_i = \varepsilon \sum_j \frac{m_j v_{ij}}{\bar{\rho}_{ij}} W_{ij} \quad (30)$$

where ε is a constant between 0 and 1. The variant should be added to the velocity when advancing the particle position in the time integration algorithm. However it does not affect the velocity used for other SPH computations.

To find the positions and velocities of the particles, using a standard and stable time integration method such as Verlet or leap-frog is inevitable. In this work, Verlet algorithm [42] is used. The main idea is to write one forward and one backward for the time variable in Taylor expansions. In this method, positions, velocities and accelerations at the next time are obtained from the same quantities at the current time.

$$r^{(n+1)}_i = r^{(n)}_i + v^{(n)}_i \Delta t + \frac{1}{2} a^{(n)}_i \Delta t^2 \quad (31)$$

$$v^{(n+\frac{1}{2})}_i = v^{(n)}_i + \frac{1}{2} a^{(n)}_i \Delta t \quad (32)$$

$$v^{(n+1)}_i = v^{(n+\frac{1}{2})}_i + \frac{1}{2} a^{(n+1)}_i \Delta t \quad (33)$$

The time step size is determined by Courant condition which implies that the time step should be smaller than the amount of time it takes for sound to travel through that fluid over a specific distance. In SPH this specific distance is the smoothing length. For adjusting time steps, the Courant condition for our problem is [43, 44, 45];

$$\Delta t = \min \left(\frac{Ch}{\max(1, \text{maximum of velocity})}, \sqrt{\frac{h}{\text{maximum of acceleration}}}, \frac{Ch}{\text{maximum of sound speed}} \right) \quad (34)$$

where C is the Courant safety factor.

By applying this condition and choosing the smallest time steps based on the flow velocity, the sound velocity and the velocity determined by the acceleration, the positions of particles in each time step can be controlled, so they do not travel too far in just one time step [19]. Therefore, for each time step, the procedure includes; finding the neighbors of each particle, calculation of the density for each particle, calculation of pressure and other attributes for each particle, calculation and summation of all acceleration terms for each particle, and applying Verlet method and then calculation of the new velocity and positions (to update position, XSPH variant should be calculated too).

In SPH algorithm, it is shown that computation time is significantly reduced by performing the summation only over the particles within the kernel width. This effective optimization method is widely used in literature [15, 16, 21, 30, 46]. The common algorithm for this method includes; creating cell grids in the domain (cells of width $2h$), tracking particles location and their corresponding cells, and summation only over the particles in the neighbor cells.

In this optimization for summation [47], each cell contains a reference to a list of all particles that map to the spatial location associated with the cell. In each time step, after searching for the particles in the adjacent cells, location and list of the particles in each grid should be updated. Obviously for a 3D grid cell, the maximum number of the neighboring cells is 26.

Boundary and Initial Conditions

Boundary conditions are not shown explicitly in SPH algorithm. Dynamic particles method [48] is used in this work in which particles have the same equations of continuity and state as the fluid particles, however their position remains unchanged. Because there are no extra considerations or special equations for these boundary particles, this method is computationally simple, with considerable less time for simulation. Validity of using dynamic boundary particles is extensively studied in literature [17, 28, 49, 50]. In this work, dynamic particles method is used for solid boundary condition and three layers of these fixed particles are placed outside the boundaries.

It should be noted that the simulation in this work is based on the experimental work of the authors mentioned in [51]. As indicated in [51], the test plate is located inside a wind tunnel. Water comes to the substrate from a surface-hole (see Fig. 1.) with the diameter of 1 mm and will be subjected to various air speeds ranging from 5 to 20 m/s. For all of the cases considered in this work, fluid particles are initially placed inside of the surface hole with the density equal to the rest density. Then for $t > 0$, all of the particles at the edge of the hole get a constant velocity (rate= 2 ml/min) and also air particles will have constant velocity at the edge of the sample depending on the simulations ($u_{\text{air}} = 5, 10$ and 20 m/s).