Droplet formation in microfluidic T-junction generators operating in the transitional regime. II. Modeling

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This is the second part of a two-part study on the generation of droplets at a microfluidic T-junction operating in the transition regime. In the preceding paper [Phys. Rev. E 85, 016322 (2012)], we presented our experimental observations of droplet formation and decomposed the process into three sequential stages defined as the lag, filling, and necking stages. Here we develop a model that describes the performance of microfluidic T-junction generators working in the squeezing to transition regimes where confinement of the droplet dominates the formation process. The model incorporates a detailed geometric description of the drop shape during the formation process combined with a force balance and necking criteria to define the droplet size, production rate, and spacing.

In this paper we seek to develop a robust model that describes the entire operation of a T-junction generator in the transition regime so that one can predict the size of droplets formed, the spacing between droplets, and the frequency of formation. An analysis of the three stages suggests that the scaling law that describes the size of the droplets has the form

$$\frac{V_{\text{drop}}}{w_c^2h} = \alpha_{\text{lag}} + \alpha_{\text{fill}} + \beta \varphi,$$

where the volume is normalized by $w_c^2h$, $\alpha_{\text{lag}}$ is the volume added during the lag stage, $\alpha_{\text{fill}}$ is the filling stage, and $\beta$ is the dimensionless necking time. These parameters are generally obtained through empirical fitting; however, our goal in this study is to develop mathematical expressions for these three parameters based on theoretical arguments.

The model formulation begins with a general geometric description of the three-dimensional (3D) shape of the droplet throughout the formation process. This geometric description is used to calculate the evolution of the volume of the droplet during the three stages of the formation process. First, the contribution of the lag stage $\alpha_{\text{lag}}$ is calculated as the volume added as the interface recovers in the side channel. Second, the filling volume $\alpha_{\text{fill}}$ is calculated, which includes a different force balance that predicts the penetration depth and includes viscosity and geometric influences. Third, the necking parameter is calculated using a control volume analysis, which also includes an alternative criterion for pinchoff based on our own experimental observations in the transition regime. In addition to the droplet volume, equations are derived for the spacing and frequency so that the entire operation of the generator is defined. The predictive capabilities of the model are verified by performing a detailed experimental analysis to validate the model across several different T-junction designs and flow conditions.

II. MODEL DEVELOPMENT

A. Model limits and constraints

The model developed herein applies to droplet formation in the squeezing-to-transition regime where the breakup process is governed by the squeezing pressure generated as the interface extends into the cross-flowing stream [3–5]. Fluid
The general description of the shape of the droplet during the formation cycle is shown in Fig. 2, which follows the description provided by van Steijn et al. but modified into a more general form applicable to the transition regime [11].
characterized by the extent of the protrusion at the filling stage for two cases where $L_{\text{lag}}$ and the volume is defined by $V_{\text{lag}}$. $L_{\text{lag}}$ is a complicated relationship between the flow conditions and geometry [1]. An adequate description is not available at the moment for $L_{\text{lag}}$; thus, in the present model, $L_{\text{lag}}$ is taken directly from experimental measurements and substituted into Eq. (3).

2. Filling stage

The filling stage ends when forces on the droplet balance and the neck of the droplet starts to collapse toward the inner corner of the T-junction. In concurrence with observations and the neck of the droplet starts to collapse toward the inner corner of the T-junction. In concurrence with observations made by Christopher et al. and van Steijn et al., our own interpretation of the experimental evidence also advocates that the final size of the droplet at the end of the filling stage has the characteristic shape described in Fig. 4 [3,11]. Again, the front half of the droplet is defined by a half circle of diameter $b_{\text{fill}}$ and the back half is defined by a quarter circle of diameter $R_{\text{fill}}$. Two cases exist depending on the geometry of the T-junction: the neck radius is confined (i) by a virtual channel wall created by the interface at $b_{\text{fill}}$ or (ii) by the inlet channel. This condition is defined as $R_{\text{fill}} = \max(w_d,b_{\text{fill}})$.

The final volume at the end of the filling stage can be calculated by applying Eq. (2) to the two shapes. For $w_d \leq b_{\text{fill}}$ the result is

$$\phi_{\text{fill}} = \frac{3}{8}\pi(b_{\text{fill}}^*)^2 - \frac{b_{\text{fill}}^*}{2}\left(1 - \frac{\pi}{4}\right)(\pi b_{\text{fill}}^* + (b_{\text{fill}}^* - \Lambda^*)) \quad (4a)$$

For $w_d > b_{\text{fill}}$, the calculation is slightly different as the back part is defined by a half circular segment [12]:

$$\phi_{\text{fill}} = \frac{\pi}{8}(b_{\text{fill}}^*)^2 + \frac{1}{4}(\Lambda^*)^2(\theta - \sin \theta) - \frac{h_{\text{fill}}^*}{4}\left(1 - \frac{\pi}{4}\right)(\pi b_{\text{fill}}^* + \Lambda^*\theta), \quad (4b)$$

$$\theta = 2 \arccos \left(1 - \frac{b_{\text{fill}}^*}{\Lambda^*}\right).$$

The remaining unknown in the preceding equations is $b_{\text{fill}}^*$, which is determined by a force balance on the droplet in Sec. II.

3. Necking

During the necking period additional fluid is being pumped into the droplet as the neck collapses. The increase in size of the droplet during this stage is related to the time that the neck remains open and the flow rate of the dispersed phase. Only a portion of the continuous phase flow collapses the neck and this depends on this correlates with the fraction of the flow that is blocked by the interface [1].

The factor $\beta$ essentially represents the dimensionless necking time $\beta = \Delta t_{\text{sq}}^\ast / \Delta t_{\text{sq}}. v_{\text{fill}}^2 h / Q_c$. To determine $\Delta t_{\text{sq}}^\ast$, van Steijn et al. applied conservation of mass to the continuous phase in order to describe the changing shape of the neck in terms of the radius $R_n$ [11]. As the neck collapses the radius becomes larger and the neck approaches the inside corner of the T-junction; once it reaches a critical distance $2d_{\text{pinch}}$, the rate of collapse increases exponentially. Therefore, the shape of the neck at the point of collapse needs to be known to calculate $\beta$.

Consider the deformable control volume consisting of the continuous phase surrounding the neck as shown in Fig. 5. The change in shape of the control volume during the squeezing process is related to the relative inflow and outflow of the continuous phase across any boundary, which in this case reduces to [13]

$$\frac{dV_C}{dt} = Q_c \left(1 - \frac{A_{\text{hp}}^*}{h_{\text{fill}}^*}\right). \quad (5)$$

The dimensionless bypass area is given as

$$A_{\text{hp}}^* = A_{\text{gap}}^* = (1 - \tilde{b}^*)h_{\text{fill}}^* + \left(1 - \frac{\pi}{4}\right)\left(h_{\text{fill}}^*\right)^2 / 2, \quad (6)$$

where $\tilde{b}^*$ is the average penetration depth during the necking stage $b^* = (b_{\text{fill}}^* + b_{\text{inlet}}^*)$. Nondimensionalizing Eq. (5) and integrating with respect to time from the initial filling volume...
FIG. 5. (Color online) Sequence of traces showing the boundary of the droplet as it evolves during the squeezing stage. At first the neck shape follows a quarter circle until it becomes pinned within the dispersed phase channel at a distance $w_d$; it then follows the shape of a circular segment. The control volume around the neck is highlighted in light gray (green). At the bottom, the detailed geometry and flow parameters of the control volume are shown.

$V_{\text{fill}}^*$ to the final pinch volume $V_{\text{pinch}}^*$, the factor $\beta$ can be recovered:

$$\beta = \left( V_{\text{pinch}}^* - V_{\text{fill}}^* \right) \left( 1 - \frac{A_{\text{bp}}}{h^*} \right)^{-1}. \quad (7)$$

Here the assumption is made that $1 - A_{\text{bp}}/h^*$ represents the fraction of the continuous phase actually squeezing the neck and not bypassing it through the gap [1].

Applying Eq. (2) to the 2D area of the control volume at the end of the filling period we obtain

$$V_{\text{fill}}^* = (1 - b^*)R_{\text{fill}}^* + \left( 1 - \frac{\pi}{4} \right) \left( R_{\text{fill}}^* \right)^2 + \frac{\pi h^*}{4} \left( 1 - \frac{\pi}{4} \right) R_{\text{fill}}^*. \quad (8)$$

To describe the evolution of neck shape, van Steijn et al. used a quarter circle to approximate the shape of the neck throughout the necking process. However, we found that this approximation consistently underestimated the necking time in the transition regime. At first the neck does in fact follow a quarter-circle shape; however, once the continuous phase penetrates into the side channel a distance $w_d$ it remains pinned at this distance while the neck radius continues to grow, resulting in a longer necking period (refer to Fig. 5). At this point, a better description of the neck shape is a half-circular segment [12]. Using the definition of variables in Fig. 5, the back of the droplet is described by

$$d^* = b_{\text{pinch}}^* + \Lambda^*, \quad a^* = \sqrt{d^* (2 R_{\text{pinch}}^* - d^*)}, \quad \theta = 2 \arccos \left( 1 - \frac{b_{\text{pinch}}^*}{R_{\text{pinch}}^*} \right). \quad (9)$$

$$2r_n^* - \varepsilon^* = R_{\text{pinch}}^* - \sqrt{(R_{\text{pinch}}^* - b_{\text{pinch}}^*)^2 + (a^* - \Lambda^*)^2},$$

where $R_{\text{pinch}}^*$ is calculated for a specific $2r_n^*$ by iterating the set of equations above. The final pinch volume for the half-circular segment is then given as

$$V_{\text{pinch}}^* = (1 - b_{\text{pinch}}^*)a^* + (1 + \Lambda^*)a^* - \frac{(R_{\text{pinch}}^*)^2}{4} \left( \theta - \sin \theta \right) + \frac{h^* \theta}{4} \left( 1 - \frac{\pi}{4} \right) R_{\text{pinch}}^*. \quad (10)$$

Experimental observations showed that for the geometries considered in this study $b_{\text{pinch}}^*$ increases by approximately 20% after the filling stage to the end of necking, capped by the far wall ($b_{\text{pinch}}^* \leq 1$). Therefore, in the following calculations involving the second stage of formation the following expression is used: $b_{\text{pinch}}^* = \min(1.2 b_{\text{fill}}^*, 1)$.
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FIG. 6. (Color online) Diagram indicating the forces acting on the emerging droplet in the filling stage. As the droplet grows it obstructs the continuous phase, resulting in a pressure difference across the droplet as well as shear stress on the interface. These two forces are countered by the interfacial tension force, which resists deformation. At some point the droplet reaches a maximum size characterized by the dimension \( b \), where the pressure and shear forces exceed the surface tension force and the neck begins to thin.

Once \( V^*_{\text{pinch}} \) is known it is substituted into Eq. (6) to determine the necking factor \( \beta \). So far the two factors \( \alpha \) and \( \beta \) have been defined; however, there are still two unknown quantities \( b_{\text{fill}}^* \) and \( 2r_{\text{pinch}} \) that need to be defined.

C. Force balance on the emerging droplet

Following the estimates put forth by Garstecki et al. and Christopher et al., three primary forces govern droplet formation: the interfacial tension resisting deformation, the tangential shear acting on the interface, and the squeezing pressure across the droplet (refer to Fig. 6) [3,4]. Necking begins once the stabilizing capillary force is overwhelmed by the shear and pressure forces. The penetration depth \( b_{\text{fill}}^* \) defines this point.

The capillary force is associated with the Laplace pressure difference between the upstream and downstream ends of the emerging droplet interface. Based on the droplet shape at the end of the filling phase (refer to Fig. 4), the upstream interface has a curvature \( k_u = 2/b + 2/h \), while the downstream curvature is \( k_u = 1/R_u + 2/h \). The sum of these two Laplace pressures, multiplied by the area over which the force is applied, \( A \sim bh \), gives the resulting capillary force \( F_c \approx -\gamma h \). The viscous shear force acting on the droplet may be estimated as the average shear stress on the interface multiplied by the exposed area \( A \sim bh \) and is given as \( F_{\tau} \approx \tau_{\text{avg}}bh \). The partial blockage of the continuous phase flow by the emerging interface creates a pressure drop across the droplet. The resultant force is the difference between the upstream and downstream pressures multiplied by the exposed area \( A \sim bh \): \( F_p \approx \Delta P_{u-d} bh \). The filling stage ends when the three forces sum to zero:

\[
F_c + F_{\tau} + F_p = 0. \tag{11}
\]

Initial models by Garstecki et al. and Christopher et al. estimated the pressure drop through a simple scaling analysis based on the Hagen-Poiseuille relation in a thin gap [3,4]. Here the same approach is taken to quickly estimate the relative magnitude of the shear and pressure forces. Approximating the shear rate on the droplets as the average velocity through the gap \( w_{\text{gap}} = (w_c - b_{\text{fill}}) \) divided by the height \( t_{\text{int}} \approx \mu_c h_{\text{gap}}/h \), the resulting shear force becomes

\[
F_{\tau} \approx \frac{\mu_c b_{\text{fill}}}{w_{\text{gap}} h} Q_c. \tag{12}
\]

The pressure drop can be approximated using the lubrication analysis for pressure drop between two parallel plates \( \Delta P_{u-d} \approx 12 Q_c \mu_c b_{\text{fill}}/(w_{\text{gap}} h)^2 \) resulting in a pressure force give by [13]

\[
F_p \approx \frac{12 \mu_c b_{\text{fill}}^2}{w_{\text{gap}}^2 h^2} Q_c. \tag{13}
\]

Taking the ratio of the two forces in order to estimate their importance we obtain

\[
\frac{F_c}{F_p} \approx \frac{w_{\text{gap}}}{12b_{\text{fill}}^2} = \frac{(w_c - b_{\text{fill}})}{12b_{\text{fill}}}. \tag{14}
\]

Under typical conditions for droplet generation in the T-junction (\( Ca = 0.0001–0.02 \) and \( b^* = 0.6–1 \)), the shear stress force is only 0–5% of the pressure force. Therefore, it is safe to neglect the contribution of shear stress from the force balance on the emerging interface.

To accurately predict \( b_{\text{fill}}^* \) the remaining issue is to develop a model that captures the pressure drop across the droplet correctly. This is not straightforward as the flow profile through the gap is quite complex since the region is comprised of three walls obeying the no-slip conditions and the fourth is the interface where the shear and velocity between the two phases must be continuous. In addition, the shape of the interface creates a curved boundary in both the out-of-plane and in-plane orientations, resulting in a 3D flow profile throughout the gap, which does not lend itself to a simple analytical solution. For this reason, a semianalytical solution was developed based on asymptotic limits to the flow profile using the assistance of numerical simulations.

III. PRESSURE DROP CALCULATION

Tchikanda et al. numerically modeled pressure and shear driven flow in open rectangular microchannels with one boundary being a curved interface. Their intended application was the design of evaporative microfluidic cooling devices with parallel liquid-vapor flows [14]. The authors performed 2D numerical simulations to obtain the flow field for various gap shapes and then developed analytical solutions by blending asymptotic results for limits of channel aspect ratio and interface curvature. For example, when the gap is large and the interface is flat, the flow resembles that between two parallel plates. If the interface is curved and the gap is small then flow is primarily through the two disjoint corners (see Fig. 7).

Tchikanda et al. provide separate solutions for shear and pressure driven flow that may be combined due to the linearity of the Navier-Stokes equations in the lubrication limit [14]. The analytical solutions are easy to apply and are accurate to within a few percent compared to the numerical solutions.
The authors provide solutions in terms of the dimensionless average velocity in the area occupied by the fluid:

$$
\bar{u}^* = \frac{Q \cdot \mu}{Ah^2 \left(-\frac{\partial P}{\partial z}\right)}
$$

(15)

where $h$ is the height of the channel, $A$ is the area of the conduit, $\mu$ is the viscosity, $Q$ is the flow rate, and $-\partial P/\partial z$ is the pressure gradient. Integrating the pressure gradient over a uniform conduit of length $L$, the equation can be rearranged into a format similar to the Hagen-Poiseuille law [13]:

$$
\frac{\Delta P}{Q} = R_{\text{hyd}} = \frac{L}{\bar{u}^* Ah^2 \mu},
$$

(16)

where $R_{\text{hyd}}$ is the hydrodynamic resistance and $L/\bar{u}^* Ah^2$ is the geometric component.

Using the notation of Tchinkada et al., the geometry of the gap corresponds to an interface with a contact angle of $0^\circ$ [14]. The relevant dimensions for the gap geometry are shown in Fig. 7. The nondimensional area is then given as

$$
A_{\text{gap}}^* = (1 - b^*)h^* + \frac{1}{2}(h^*)^2 \left(1 - \frac{\pi}{4}\right).
$$

(17)

The average dimensionless velocity is provided as a blend of asymptotic solutions $u_{1*}$ and $u_{2*}$, given by the following expression:

$$
\bar{u}^* = \left[ \left( \frac{u_{1*}^2 u_{2*}^2}{m_1} \right)^{m_1} + \left( u_{2*}^2 \right)^{m_1} \right]^{1/m_1}.
$$

(18)

The expression approaches $u_{1*}$ in the limit of $u_{1*} \gg u_{2*}$ and $u_{2*}$ in the opposite limit of $u_{1*} \ll u_{2*}$. The shape of the blend is controlled by the fitting parameter $m_1$. The first asymptote $u_{1*}$ corresponds to a wide aspect ratio gap $\lambda_{\text{gap}} = h^*/(1 - b^*)$ or flow between two infinite plates (top and bottom of the microchannel) $u_{1*}^2 = 1/12$. The second asymptote approaches two limits. The first is when the gap is very shallow and the interface is flat; the second is when the crest of the meniscus is in contact with the wall and flow is only through the corners:

$$
u_{2*}^2 = \left[ \frac{1}{a^{m_2} \lambda_{\text{gap}}^{2m_2}} \right]^{1/m_2},
$$

(19)

where $u_{2*} = 0.0027$ is the corner asymptotic limit.

We repeated the numerical simulations and found different optimum fitting parameters $m_1 = 1.25$, $m_2 = 0.90$, $m_3 = 1.88$, and $a = 7.90$ for our geometry. With this curve fit the average error compared to the numerical results is less than 1.5%. The shape of the average mean velocity function including the two asymptotes is shown in Fig. 8.

Two additional effects are absent in the approximation by Tchinkada et al. that are present in the situation of the bypassing flow. First, the solutions correspond to a conduit with a uniform cross section. Curvature of the droplet in the $x-z$ plane creates a nonuniform gap profile. Second, the analysis assumes a zero-shear boundary at the interface, which is appropriate for conditions where the continuous phase viscosity is much greater than the dispersed phase viscosity ($\eta \rightarrow 0$). Higher viscosity ratios act to modify the shear stress condition on the interface, resulting in an increase in resistance to flow through the gap. We performed numerical simulations and developed additional factors $\lambda_{\text{eff}}$ for the curvature and $g(\eta, \lambda_{\text{gap}})$ for the viscosity contrast that modify Eq. (16).

### A. Effective pressure drop length

The interface curvature in the $x-z$ plane creates a constantly varying gap profile along the length of the droplet. The pressure drop generally scales with the cube root of the smallest dimension; therefore, one expects that the effective length over which the majority of the pressure drop occurs in the gap will vary with the penetration depth $b^*$. Such a dependence was derived by Stone in his study of lubrication flow through shallow curved gaps [15]. Because of the complex shape of the droplet, a solution to the pressure drop requires a full 3D analysis of the flow field. For this reason a numerical study of the flow field through the gap was performed using COMSOL Multiphysics 4.1.

Simulations were performed for different droplet sizes $b^* = 0.5–1$ and channel heights $h^* = 0.2, 0.35$, and 0.5. Only one half of the droplet was simulated due to symmetry along the $x-z$ plane as shown in Fig. 9. Five channel lengths were added before and after the droplet to ensure that the flow field is properly realigned at the entrance and exit.
No-slip conditions were applied to all microchannel walls and a no-shear condition was applied to the interface of the droplet. A symmetry boundary condition (no shear) was applied at the plane of symmetry. At the entrance and exit pressures were fixed. For each simulation the pressure drop was measured at two planes just before and after the droplet (the total distance between planes is 1.5$b$). Additionally, the average velocity in the channel was measured to calculate the total flow rate and determine $\bar{u}^*$. The goal here is to still utilize the curve fits provided by Tchiknada et al. because of their inherent simplicity and accuracy while adding the influence of the out-of-plane curvature. This is accomplished by calculating the equivalent length of channel of the uniform cross section for the minimum gap, which will produce the same pressure drop as the 3D numerical simulation. Mathematically this relationship is given as the ratio of the pressure drop from the 3D numerical simulations to the pressure drop from the asymptotic model ($L_{\text{eff}}^* = L_{\text{eff}}^*/u_c = 1.5b^*\Delta P_{3D}/\Delta P_{\text{avg}}$). Figure 10 plots the ratio $\Delta P_{3D}/\Delta P_{\text{avg}}$ as a function of $b^*$ for a range of $h^*$ for droplets following the shape of $w_d \leq b_{\text{fill}}$. Normalizing the 3D result by the asymptotic model causes all of the data to collapse onto a single curve. The relationship for $L_{\text{eff}}^*$ can be described by a blend of limiting solutions consisting of a linear relationship $L_1^* = −2.66b^* + 2.88$ and an asymptote $L_{\text{drop}}^*$:

$$L_{\text{eff}}^* = L_{\text{drop}}^* \left( \frac{(L_1^* L_2^*)^k}{(L_1^*)^k + (L_2^*)^k} \right)^{1/k}.$$  (20)

For the case $w_d \leq b_{\text{fill}}$ the coefficients are $L_1^* = 1.3$, $k = 6$, and $L_{\text{drop}}^* = 1.5b_{\text{fill}}^*$; for $w_d > b_{\text{fill}}$, $L_2^* = 1$, $k = 3$, and $L_{\text{drop}}^* = L_{\text{fill}}^*$. 

### B. Viscosity contrast effect

Simulations were performed in two dimensions emulating the cross-sectional view of the microchannel at the minimum gap point. A pressure gradient was applied in the continuous phase while no pressure gradient was applied in the portion of the dispersed phase. Thus flow in the dispersed phase is caused by the drag at the interface created by the bypassing continuous flow. This situation approximates the actual conditions prevalent in the gap during droplet formation. Generally, $Q_c > Q_d$ and the continuous phase must flow through a smaller area $\sim(1 - b^*)$ then the dispersed phase $\sim b^*$. Thus the average velocity in the gap region is typically an order of magnitude higher than the velocity within the droplet, so that as an approximation, one can consider the flow in the drop to be stagnant in comparison. For the boundary conditions, no slip is applied along all the microchannel walls and continuity at the interface boundary.

Simulations were performed for gaps varying between $b^* = 0.6$ and 1 and viscosity contrasts between $\eta = 1/100$ and 1. Figure 11 plots the relative change in resistance to flow as compared to the no-shear case for different viscosity contrasts. The trend is a nonmonotonic function that generally increases as the gap closes ($b^* = 0.5–1$). Peculiarly, a small decrease in the relative pressure drop occurs around $b^* = 0.95$ presumably due to the unique geometry and competing boundary conditions on the flow within the gap region. A two-step fit is applied to the function approximating the first part $\lambda_{\text{gap}} < 2$ with a linear curve fit $g(\eta, \lambda_{\text{gap}}) = a(\eta)\lambda_{\text{gap}} + 1$

![FIG. 10. Effective pressure drop length $L_{\text{eff}}^*$. Data correspond to $h^* = 0.2 (\diamond)$, 0.35 (□), and 0.5 (○).](image)

![FIG. 11. Effect of viscosity contrast on the pressure drop from the 2D numerical simulations. Data correspond to $\eta = 0.1 (\diamond)$, 0.2 (□), 0.33 (△), 0.5 (+), and $\eta = 1 (\ast)$.](image)
and the second $\lambda_{gap} > 2$ as a constant. The slope of the linear function scales proportionally with the viscosity contrast and has the form $a(\eta) = 0.1\eta (R^2 = 0.96)$. The piecewise function that defines the effect of the viscosity contrast is thus given by

$$g(\eta, \lambda_{gap}) = \begin{cases} 
0.1\eta\lambda_{gap} + 1, & \lambda_{gap} < 2 \\
0.2\eta + 1, & \lambda_{gap} \geq 2.
\end{cases}$$

(21)

This relationship is used to modify the pressure drop calculation provided by Tchinkada et al. and account for the effect of viscosity contrast.

C. Reconstituted force balance

By integrating Eq. (16) the pressure difference over the droplet can be calculated as

$$\Delta P_{a-d} = \frac{L_{eff} Q_{\text{gap}} \mu_c}{h^2 (A_{\text{gap}} u_{\text{gap}})} g(\eta, \lambda_{gap}).$$

(22)

Substituting into Eq. (11) and neglecting the shear stress contribution, the force balance in dimensionless terms becomes

$$\frac{h^*}{Ca^2} = \frac{1}{2} \frac{L_{eff} g(\eta, \lambda_{gap})}{(A_{\text{gap}} u_{\text{gap}})} \frac{b_{\text{fill}}^*}{R_{\text{fill}}^2}.$$  

(23)

For the case $w_d \leq b_{\text{fill}}$, $R_n = b_{\text{fill}}$; for $w_d > b_{\text{fill}}$, $R_n = w_d$ when calculating the force balance. This shows that the controlling parameter for the fill volume is $h^*/Ca$. Equation (23) is iterated until a convergent solution for $b_{\text{fill}}^*$ is found. Once $b_{\text{fill}}^*$ is known it is substituted back into Eq. (4a) or (4b) to calculate $\alpha_{\text{fill}}$. A comparison with experiment indicates that a prefactor of $C = 1/2$ fits well—a peculiar value as it suggests that the surface tension force is underestimated by a factor of 2 or the pressure force is overestimated by a factor of 2. The reason for this is not quite known, but there are several explanations that can be suggested. First, the force balance in the streamwise direction is not the only contribution to the deformation of the emerging interface as a force in the cross-stream direction also exists. This force is caused by the pressure difference between the front and back of the droplet, resulting in the cancellation of out-of-plane curvature effects. It is well known that the curvature of the front cap increases relative to the back cap when droplets travel in microchannels [16]. If we presume that this effect also occurs during drop formation then it would contribute to an increase in the surface tension force. Most likely a combination of these effects produce the prefactor of 1/2 and untangling them would require a detailed numerical study, which is beyond the scope of this current work. Nevertheless, the penetration depth is well described by Eq. (23) when a prefactor of 1/2 is used, as will be shown later on.

From the force balance a criterion can also be found for the point where the system changes from purely squeezing into the transition regime. Considering the limit for the squeezing regime to be when the interface reaches the far wall during the first stage, Eq. (23) may be rearranged to determine the critical $Ca$ for the squeezing regime:

$$Ca_{eq} \leq \frac{1.7e^{-3}(h^*)^3}{g(\eta, \lambda_{gap})}.$$  

(24)

This result shows that the critical limit for squeezing is very sensitive to the height of the microchannel. Furthermore, squeezing occurs for very low $Ca_{eq} = 2.05e^{-4}$ values ($h^* = 0.5$ and $\eta = 0$), suggesting that, in practice, T-junction generators always operate in the transition regime to some degree.

IV. CALCULATION OF THE PINCHOFF POINT

In order to incorporate the observed $Ca$ and viscosity dependence on $2r_{\text{pinch}}^*$ an alternative approach was taken. The idea is that pinchoff occurs when the Laplace pressure difference between the front and back of the droplet generates a backward flow that exceeds some multiple $m$ of the bypassing flow $Q_c A_{\text{gap}}/h^*$. The Laplace pressure driven fluid flow around the drop may be approximated by

$$\Delta P_{LP} = \gamma \left( \frac{1}{R_n} + \frac{1}{r_n} \right) - \gamma \left( \frac{2}{b_{\text{pinch}}} + \frac{2}{h} \right),$$

(25)

where the pressure created by the bypassing flow is given as

$$\Delta P_{LP} = \frac{L_{eff} h^* g(\eta, \lambda_{gap})}{h^2 (A_{\text{gap}} u_{\text{gap}})} m Q_c A_{\text{gap}}^* / h^*.$$  

(26)

Ignoring the smaller term of $1/R_n$ and rearranging Eqs. (25) and (26), the critical neck thickness is given as

$$2r_{\text{pinch}}^* = \frac{h^*}{1 + \frac{h^*}{b_{\text{pinch}}} + \frac{m Ca}{2h^*} \frac{L_{eff} g(\eta, \lambda_{gap})}{u_{\text{gap}}}}.$$  

(27)

In the case of $Ca \rightarrow 0$, then $b^* \rightarrow 1$ and the limit from van Steijn et al. is recovered for the squeezing regime [10]. Comparisons with experiments show that the optimum fitting parameter is $m = 1$. This means that the sudden collapse of the neck occurs when the back pressure matches the hydrodynamic pressure from the bypassing flow. Overall the alternative model for the neck is more robust since it includes the interfacial tension and viscosity in $Ca$ as well as the resistance to fluid flow through the gutters around the drop through $\bar{u}^*$.

V. OPERATIONAL PARAMETERS

In this section the other important operational parameters are calculated, including the volume of oil injected between the droplets, droplet spacing, and the frequency of formation. The total volume of oil injected can be broken down into three contributions: (a) oil that bypasses the droplet during the lag stage when the interface is inside the dispersed channel, (b) oil that bypasses the emerging interface during the drop filling stage, and (c) oil that continues to bypass the droplet during the squeezing stage:

$$V_c = V_{\text{cap}} + V_{\text{fill}} + V_{\text{neck}}.$$  

(28)
The volume is related to the length of each stage and the oil flow rate, which is assumed to remain constant throughout the three stages:

$$V_c = \Delta t_{\text{lag}} Q_c + \Delta t_{\text{fill}} Q_c + \Delta t_{\text{neck}} Q_c.$$  \hfill (29)

Note that during the necking stage $Q_c$ is used because all of the flow either collapses the neck or bypasses the droplet and thus eventually contributes to the spacing. The length of each stage is given as $\Delta t_{\text{lag}} = \alpha_{\text{lag}} w_c h / Q_d$, $\Delta t_{\text{fill}} = \alpha_{\text{fill}} w_c h / Q_d$, and $\Delta t_{\text{neck}} = \beta w_c h / Q_c$. The nondimensional form becomes

$$V_c^* = \frac{\alpha_{\text{lag}} + \alpha_{\text{fill}}}{\phi} + \beta.$$  \hfill (30)

The rate of production and droplet spacing are additional parameters that are important in the design of a droplet generator and can be derived using arguments similar to those that were employed in the calculation of the droplet volume.

$$t_{\text{drop}} = \Delta t_{\text{lag}} + \Delta t_{\text{fill}} + \Delta t_{\text{sq}}.$$  \hfill (32)

The normalized frequency is then the reciprocal of this equation:

$$f^* = \frac{\phi}{\alpha_{\text{lag}} + \alpha_{\text{fill}} + \phi \beta}.$$  \hfill (33)

For the reader’s benefit, the complete set of equations is concisely presented in Ref. [17].

**VI. MODEL SUMMARY**

Plots for the parameters $b_{\text{fill}}^*$, $2r_{\text{pinch}}^*$, $\alpha_{\text{fill}}$, and $\beta$ for various conditions and T-junction designs are provided Figs. 12–15.
The most important parameters governing droplet formation are the T-junction geometry \((w_c, w_d, h)\) and the term \(h^*/Ca\) as it governs \(b^*_{\text{fill}}\) and \(2r^*_{\text{pinch}}\).

Consider Fig. 12, which shows the calculation for \(b^*_{\text{fill}}\) for different \(h^*\) and two different viscosity ratios \(\eta = 0\) and 1. The plot shows that the relationship between \(b^*_{\text{fill}}\) and \(h^*/Ca\) is nonlinear and as well as a modest dependence on \(h^*\) and a weak dependence on viscosity contrast. Overall, \(b^*_{\text{fill}}\) increases with \(h^*/Ca\) until it becomes capped at the wall \(b^*_{\text{fill}} = 1\). Often this critical point is associated with the transition into the purely squeezing regime of droplet formation, as predicted by Eq. (24).

Figure 13 plots the ratio of critical neck thickness against \(b^*_{\text{fill}}\). The profile is nonlinear with an inflection point at \(b^*_{\text{fill}} = 0.833\), which is caused by the relation \(b^*_{\text{pinch}} = 1.2b^*_{\text{fill}}\) and the limit \(b^*_{\text{pinch}} \leq 1\). To the left of the inflection point \(b^*_{\text{fill}}\) is still free and the critical neck thickness increases; however, it then decreases towards the inflection point because the gap closes, thus increasing the resistance to flow around the droplet. To the right of the inflection point \(b^*_{\text{pinch}}\) is capped at \(b^*_{\text{pinch}} = 1\) and all of the variables in Eq. (27) are constant, except for the \(Ca\) term, which continues to decrease so that Eq. (27) approaches the limit \(2r^*_{\text{pinch}} \rightarrow h^*/(1 + h^*)\).

Both \(\alpha_{\text{fill}}\) and \(\beta\) are primarily governed by the geometry of the T-junction generator, with the width ratio \(\Lambda^*\) having a stronger influence than the height-to-width ratio \(h^*\), as shown in Figs. 14 and 15. As expected, the fill volume \(\alpha_{\text{fill}}\) decreases with \(b^*_{\text{fill}}\), which corresponds to higher \(Ca\). What may be a surprise is that the dimensionless necking time \(\beta\) actually increases with higher \(Ca\) (seen in the plot as decreasing \(b^*_{\text{fill}}\)). There are two contributions to this effect: (i) the emerging interface blocks less of the crossflow, so a smaller fraction of the continuous phase is directed to collapsing the neck and (ii) higher \(Ca\) results in a lower \(2r^*_{\text{pinch}}\) value, which means the neck is open longer.

To illustrate the changing performance of a T-junction generator with higher operational speeds (i.e., higher \(Ca\)), the variation in \(V^*_{c}\), \(V^*_{d}\), and \(f^*\) is plotted in Fig. 16 for a standard generator design (\(\Lambda^* = 0.5\) and \(h^* = 0.3\)) while keeping the flow ratio constant \(\varphi = 0.3\). At lower speeds (\(Ca \rightarrow 0\)) droplets are larger and spaced farther apart, which also means that they are produced at a comparatively lower rate. As \(Ca\) increases smaller droplets are formed closer together and the rate of production increases accordingly. This example clearly shows the complex operational behavior of a T-junction generator within the squeezing-to-transitional regimes.

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VII. MODEL VALIDATION

The theoretical model was validated by comparing it to experimental data for T-junctions with \( \Lambda^* = 0.34-1 \) and \( h^* = 0.3-0.6 \) under conditions ranging from \( \eta = 0.12 \) to 1.7 and \( \text{Ca} = 0.001 \) to 0.008. Details on the experimental procedures were presented in the preceding paper [1]. This set of data covers a wide range of conditions that are typically associated with the transition between squeezing and dripping (\( b_{\text{fill}}^* = 0.7 - 1 \)). All data that are presented were first screened to verify that the flow rates are constant during the formation process. This was accomplished by the tracking droplet velocity \( u_d \) as it is directly proportional to the total flow rate \( Q_c + Q_d \) and by monitoring oscillations in droplet size \( V_d \) and spacing \( \lambda \) as these two metrics are sensitive to the relative flow rate \( \phi \). During the screening process we included only data with <5% variance in all three metrics. Therefore, we are confident that the condition of relatively constant flow is satisfied.

The effectiveness of the model is measured by a series of parity plots that compare the predicted penetration depth, droplet volume, oil volume, and production frequency produced by the model to that measured in the experiments. Perfect parity exists when the data fall along the solid black line in the following figures.

Figure 17 presents the overall accuracy for the calculation \( b_{\text{fill}}^* \) from the new force balance for all the experiments. Generally, the predictions are very good as most of the data fall within an error range of \( \pm 10\% \), which is deemed acceptable given the potential errors involved in measuring all the parameters from the videos. Figure 18 demonstrates the importance of including \( L_{\text{eff}}^* \) and \( g(\eta, \lambda_{\text{exp}}) \) in the force balance. One could see that the omission of these two effects results in a systematic overestimation of the penetration depth.

Figure 19 presents a comparison between predicted and measured pinchoff. Good agreement is found, although there is some scatter due to the difficulties measuring the exact moment of collapse. Predictions for \( V_d^*, V_c^*, \) and \( f^* \) are provided in Figs. 20–22, with an excellent correlation between the experimental and model results as all data fall within \( \pm 10\% \) of parity. This suggests that the model developed herein is successful in predicting the performance of the T-junction generator in the squeezing-to-transition regime without excessive use of correlations. These results verify that the alternative model is able to accurately predict the performance of the T-junction generator in the squeezing-to-transition regime.

VIII. CONCLUSION

In this paper II of our two-part series [1], we presented a physical model for the formation of droplets in a microfluidic T-junction generator operating in the squeezing-to-transition regime. The model consists of three parts. The first is a geometric description of the droplet shape and neck during the formation process in the transition regime. This was followed by an alternative force balance to calculate the initial fill volume that includes hydrodynamic resistance of the gap by incorporating the analytical approximations of Tchikanda et al. [14]. Additional modifications to the resistance calculation were developed that account for the 3D shape of the droplet and the effect of the viscosity contrast between the two fluids. Finally, a modified pinchoff criterion was developed based on experimental observations that includes the shape of the gap and the strength of the Laplace pressure driven flow. The model captures the strong influence of the flow ratio, Ca, and geometry on droplet formation.
Good agreement was found between the model and experiments for the droplet size, frequency, and spacing across all the conditions considered, with most data falling within 10% of the predicted values. Additionally, $h^*/Ca$ was identified as an important parameter for defining the flow in the squeezing-to-transition regime as it determines the degree of squeezing pressure created on the emerging droplet interface. Although the current model was validated with only liquid-liquid systems, it should translate just as well to gas-liquid systems.

Despite the success, more testing is required to define the applicability of the model. This includes extending the range of experiments into $\Lambda^* > 1$, $Ca > 0.005$, and $\eta \gg 1$ to determine the limits of the assumptions that were applied. Future extensions of the model into the dripping regime must include the shear stress in the force balance. Still, in its current form, the model is sufficiently robust to enable the efficient design of T-junction generators without the ambiguity of trial and error methods. Other applications for the model may also include direct integration into real-time control systems or as a subroutine in a larger droplet network trafficking model [18,19].

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