

The dynamics of liquid slugs forced by a syringe pump

Reza Miraghaie, M. Abouali, C. Breward, I. Chan,
A. Ellis, J. Fehribach, M.B. Gratton, K. Matusik

Math-in-industry, Claremont Colleges, 2009

1 Introduction

Microfluidic processes for chemical synthesis have become popular in recent years. The small scale of the chemical reactions promise greater control over reaction conditions and more timely creation of products. The small scale of microfluidics poses its own set of problems, however. At the microscale, the dominant fluid forces are viscous resistance and surface tension. The effects of viscosity and scale reduce the Reynolds number and make mixing difficult. Much work has been done to control mixing at the microscale [2], [4], [5], [6].

This problem is concerned with a different microfluidic problem: delivering reactants to the site of reaction. A common setup is to attach syringes full of reactant to a reaction chamber by narrow hydrophobic tubing. Using a stepper motor, a controlled dose of liquid may be injected into the tube. The hydrophobosity causes the dose to curve outward on the sides, becoming a “slug” of reactant with air in front and behind. The syringe at the rear is then switched for one full of air, and air pressure is used to drive the slug to the reaction site.

If too much pressure is applied, the slug will arrive with a significant back pressure that will be relieved through bubbling in the reaction site. This causes the formation of a foam and is highly undesirable. We present a simple model based on Boyle’s law for the motion of a slug through a tube. We then extend this model for trains of slugs separated by air bubbles. Last, we consider the case of a flooded reaction site, where the forward air bubble must be pushed through the flooding liquid.

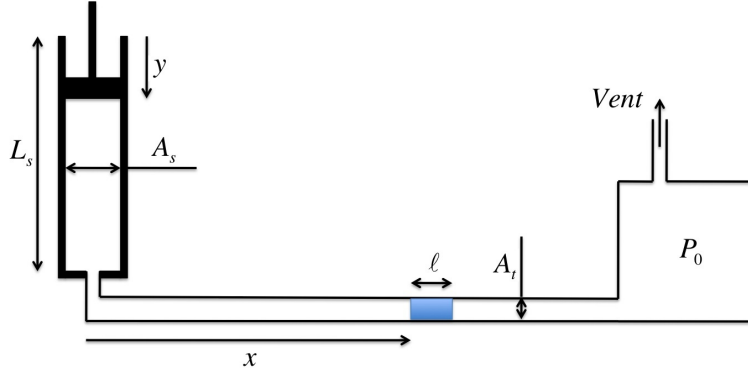


Figure 1: Schematic of a single slug moving along a tube.

2 Single slug model

We consider a single slug of aqueous solution at a location $\hat{x}(t)$ and of length ℓ in a hydrophobic tube.¹ In front of the bubble, there is a volume of gas

$$V_f = A_t(L_t - (\hat{x} + \hat{\ell})), \quad (1)$$

where A_t is the cross-sectional area of the tube and L_t is the length of the tube. The volume of gas behind the slug is

$$V_b = A_s[L_s - \hat{y}(t)] + A_t\hat{x}, \quad (2)$$

where A_s is the area of the syringe and L_s is the length of the syringe. The function $\hat{y}(t)$ is the location of the syringe piston and is specified by the user. See Fig. 1 for a schematic

and Table 1 for a summary of notation and scale.

Initially,

$$\hat{x}(0) = 0 \quad (3)$$

$$\hat{y}(0) = 0 \quad (4)$$

$$\frac{d\hat{x}}{dt} = 0, \quad (5)$$

corresponding to a slug at rest backed up against the mouth of a syringe whose piston is fully extended. These give initial volumes of

$$V_f^o = A_t(L_t - \hat{\ell}) \quad (6)$$

$$V_b^o = A_sL_s. \quad (7)$$

¹Variables with hats or in capital letters are dimensional quantities.

Quantity	Value		Description
L_t	5	m	Length of tube
r_t	2.5×10^{-4}	m	Radius of tube
A_t	10^{-7}	m ²	Cross-sectional area of tube
L_s	5×10^{-2}	m	Length of syringe
A_s	4×10^{-7}	m ²	Cross-sectional area of syringe
P_{atm}	10^5	Pa	Atmospheric pressure
$\hat{\ell}_i$	10^{-2}	m	Length of i th slug
\hat{d}_i	10^{-2}	m	Distance between slugs i and $i + 1$
ρ	10^3	kg/m ³	Density of slug
μ	10^{-3}	Pa/s	Dynamic viscosity of slug
γ	10^{-1}	N/m	Surface tension of slug
θ	150°		Contact angle of slug with tube

Table 1: Relevant physical scales for problem parameters

When $y > 0$, the gas in the bubble behind the slug is compressed. Assuming the system is isothermal, the new pressure is given by Boyle's law as

$$P_b = P_{\text{atm}} \frac{V_b^o}{V_b}. \quad (8)$$

Converting this pressure to a force by multiplying by the facing surface area of the slug and using Newton's law gives

$$A_t(P_b - P_f) = m \frac{d^2 \hat{x}}{d\hat{t}^2} + c \frac{d\hat{x}}{d\hat{t}}, \quad (9)$$

for forward pressure P_f , slug mass m and a damping c due to viscosity discussed shortly. As the gas in front of the slug is open to the atmosphere, $P_f = P_{\text{atm}}$, and so

$$A_t P_{\text{atm}} \left(\frac{V_b^o}{V_b} - 1 \right) = \rho A_t \hat{\ell} \frac{d^2 \hat{x}}{d\hat{t}^2} + c \frac{d\hat{x}}{d\hat{t}}. \quad (10)$$

Nondimensionalizing according to Table 2 yields

$$\left(\frac{1}{1 + \delta(x - y)} - 1 \right) = \alpha \frac{d^2 x}{dt^2} + \beta \frac{dx}{dt}. \quad (11)$$

The parameters α and β represent scaled mass and damping, respectively. The ratio δ sets the strength of piston depression to compression.

Symbol	Definition	Scale	Note
x	\hat{x}/L_t	$O(1)$	Location of slug in tube
y	$\hat{y}A_s/(A_tL_t)$	$O(1/\delta)$	Displacement of piston.
t	\hat{t}/T	Arb.	Imposed timescale
δ	$(A_tL_t)/(A_sL_s)$	$\approx 1/4$	Ratio of tube volume to syringe volume
ℓ_i	$\hat{\ell}_i/L_t$	$O(10^{-3})$	Relative length of slug i
d_i	\hat{d}_i/L_t	$O(10^{-3})$	Relative separation slugs i and $i+1$
α_i	$(\rho\hat{\ell}_iL_t)/(P_{\text{atm}}T^2)$	$O(10^{-3})$	Inertia parameter
β_i	$(8\pi\mu\hat{\ell}_iL_t)/(A_tP_{\text{atm}}T)$	$O(1)$	Damping parameter
p_*	P_*/P_{atm}	1.01	Overpressure

Table 2: Nondimensionalization of model variables and parameters. Variables shown with hats or in capital letters have dimension.

2.1 Frictional resistance to motion

The motion of the slug is retarded by frictional effects, including viscous loss inside the slug, losses from turning flow at the free surfaces of the slug, and losses from the moving contact line between the slug and tube. This last effect is small, as the tube is hydrophobic so the contact line may move with minimum impediment. The second effect is more important in slugs with small ℓ and for large Re . We will focus on the first effect, the viscous loss inside the flow set up in the slug through motion.

The Reynolds number is

$$\text{Re} = \frac{U^o \sqrt{A_t/\pi} \rho}{\mu} = O(10) \quad (12)$$

for lengthscale $L = \sqrt{A_t/\pi}$ and velocity scale $U^o \approx 4$ cm/s. At this moderate value, the fluid follows Poiseuille flow set up by the motion on the slug through the tube with no-slip conditions. Standard references, e.g. [1] give the average fluid velocity down the tube as

$$\bar{u} = \frac{\Delta P A_t}{8\pi\mu\hat{\ell}}. \quad (13)$$

This speed must match $\frac{dx}{dt}$ for the slug to be coherent. Using (10), the left-hand side is the pressure drop across the slug times the area, equivalent to $\Delta P A_t$. Neglecting inertia, we have

$$A_t (P_b - P_f) = (8\pi\hat{\ell}) \frac{dx}{dt}. \quad (14)$$

Nondimensionalizing, we obtain

$$\beta = \frac{8\pi\mu\hat{\ell}L_t}{A_t P_{\text{atm}} T}. \quad (15)$$

For $T = 1$ s, $\beta \approx 0.4$.

2.2 Simplified models

The model (11) suggests two simplifications: removal of inertia, and the removal of damping. We consider each in turn.

The inertia parameter α is small for modest timescales, about 10^{-3} . If this term is dropped, the remaining ODE is a first order differential equation with nonlinear forcing:

$$\left(\frac{1}{1 + \delta(x - y)} - 1 \right) = \beta \frac{dx}{dt}. \quad (16)$$

In this model, the slug's motion is monotonic, with x increasing from zero to its equilibrium value (given below) without overshooting its final position. However, the assumption that α is negligible depends on the timescale T . As $\alpha \propto T^{-2}$, rapid depression of the piston will cause alpha to be large and oscillatory behaviour to be possible.

As the mass α is small and β is modest, to a rough approximation the gas is incompressible. In this situation, the dimensional position of the slug is just

$$\hat{x} = \frac{A_s}{A_t} \hat{y}. \quad (17)$$

This is also the equilibrium location of a slug in (11), the point at which $P_b = P_f$ and there is no longer any forcing. Another insight from this limit is that the size of β determines the magnitude of the pressure jump across a slug. Very viscous slugs behave like solid stoppers, allowing the back bubble to become highly pressurized. Nearly inviscid slugs move quickly as the back pressure changes. Two factors main factors control β : the length of the slug $\hat{\ell}$ and the timescale T of the forcing. Long slugs and rapid motion of the piston result in larger β values and hence larger pressure drops across a slug.

2.3 Phase-plane analysis

We wish to know under what conditions a slug may overshoot its equilibrium position (17) depending on the relative sizes of α , β and δ . Notably the parameters α and β vary with the timescale over which the the plunger

is depressed and also with the length of the slug. We proceed by using standard phase-plane analysis of the linear o.d.e. (11).

If we write $u = \dot{x}$, where a dot denotes differentiation with respect to time, we find that the phase-plane equation for (11) is

$$\frac{du}{dx} = \frac{-\delta(x-y) - \beta u[1 + \delta(x-y)]}{\alpha u(1 + \delta(x-y))}. \quad (18)$$

Therefore a singular point exists when $u = 0$ and $x = y$. In order to examine the phase-plane local to the singular point we put $x = y + X$ and $u = U$ with $|X|, |U| \ll 1$. At leading order the phase plane equation becomes

$$\frac{dU}{dX} \approx \frac{-\delta X - \beta U}{\alpha U} \quad (19)$$

and consequently we find that the nature of the singular point is determined by the sign of $\beta^2 - 4\delta\alpha$. In particular when $\beta^2 > 4\delta\alpha$ the singular point is a stable node. This particular case corresponds to overdamping - the slug will come to rest at the singular point and it will not overshoot the equilibrium position $x = y$. On the other hand, if $\beta^2 < 4\delta\alpha$ then the singular point is a stable spiral point; this corresponds to underdamping - the slug will oscillate about the singular point at $x = y$ before coming to rest. That is to say in this case the slug will overshoot the equilibrium position.

Observe that the critical value $\beta^2 = 4\delta\alpha$ is equivalent to a critical length

$$\hat{l}_{\text{crit}} = \frac{4\rho A_t^3 P_{\text{atm}}}{64\pi^2 \mu^2 A_s L_s} \quad (20)$$

If the slug length exceeds this value then the slug will be overdamped, if the slug length is below this value then the slug will be underdamped. Interestingly the dynamic behaviour of the slug is independent of the timescale T over which the plunger is depressed. Substituting orders of magnitude estimates for the values of each parameter reveals $\hat{l}_{\text{crit}} \approx 0.03\text{m}$.

2.4 Results

Figure 2 shows the position $x(t)$ of the slug as it moves through the tube given a linear depression $y(t)$ of the syringe pump. The slug very quickly accelerates up to a constant speed until the plunger reaches the end of the syringe. The pressure either side of the slug then begins to equalise so the slug decelerates until it comes to rest in the equilibrium position y_{eq} . Figure 3 shows the corresponding velocity profile. The discontinuity in the gradient corresponds to the point at which the plunger reaches the bottom of the syringe when the pressure behind the slug begins to decrease as the volume behind it increases.

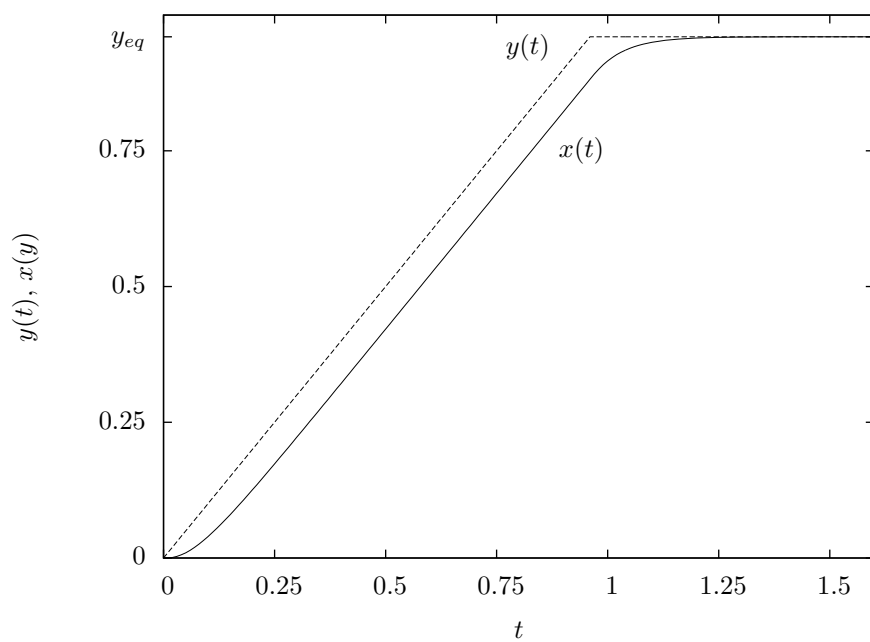


Figure 2: The position $x(t)$ for a single slug in a tube for which the reaction chamber is empty. The dashed line shows the syringe compression $y(t)$.

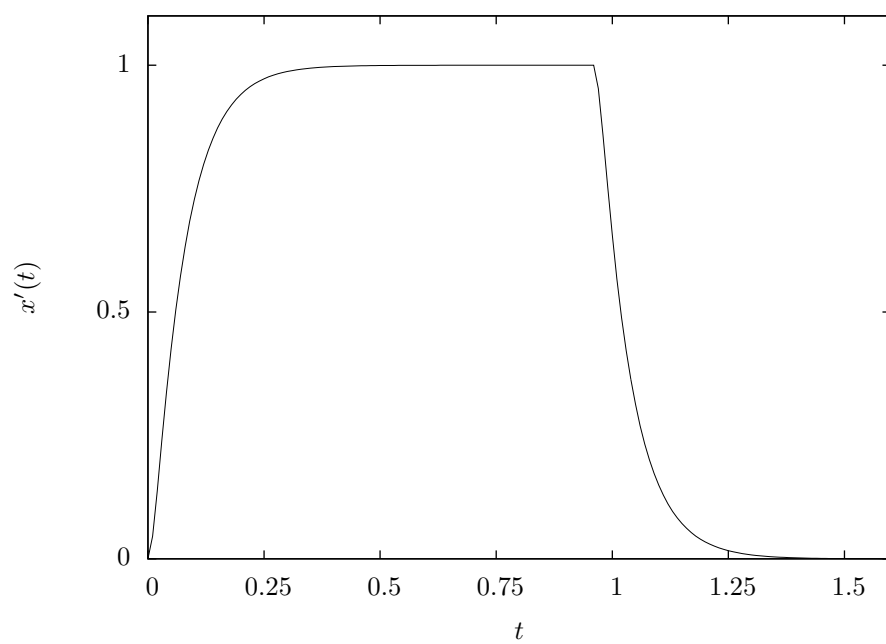


Figure 3: The velocity $x'(t)$ for a single slug in a tube for which the reaction chamber is empty corresponding to figure 2.

3 Flooded reaction chamber

The reaction chamber at the end of the tube is a cylinder of radius $r_c = 1.5 \times 10^{-3} \text{m}$ and height $l_c = 5 \times 10^{-3} \text{m}$. The tube carrying the slug enters parallel and level to the bottom, as shown in Fig. 1. When $5 \mu\text{L}$ of fluid arrive, the reaction chamber is *flooded*. Any new slugs that are to be forced into the chamber will have a forebubble of gas that must be forced through the liquid blocking the end of the tube. To model this, we replace atmospheric pressure in (10) with an expression for the pressure in the forebubble P_f .

The compressibility of the gas gives

$$P_f = \frac{V_f^o}{V_f} P_{\text{atm}} = \frac{(1 - \ell)}{(1 - x - \ell)} P_{\text{atm}},$$

provided that the forebubble is at atmospheric pressure initially. However, P_f cannot increase forever. Eventually, the high pressure will deform the liquid/air interface at the mouth of the reaction chamber. The meniscus here will bend into the chamber, eventually pinching-off into a bubble. The pressure above atmospheric pressure required to bend this interface backward (see [1]) is given by

$$\Delta P = 2\gamma\kappa,$$

where κ is the curvature of the interface. Near pinch-off, $\kappa \approx 1/r_t$, provided that the Reynolds number of the gas is $O(1)$ [3]. Thus,

$$P_* - P_{\text{atm}} = 2\gamma/r_t \approx 10^3 \text{ Pa}. \quad (21)$$

This overpressure P_* is only different from P_{atm} by a factor that is a hundredth of an atmosphere.

As the slug moves forward, P_f increases to P_* . At P_* , bubbles begin to form in the reaction chamber. These bubbles have pressure P_* and volume $V_{\text{bub}} \approx \frac{4}{3}\pi r_t^3$. The pressure in P_f stays at P_* , but the volume V_f decreases as gas mass is lost through bubbling. This leads to the piecewise defined forepressure

$$P_f = \min \left(P_*, \frac{(1 - \ell)}{(1 - x - \ell)} P_{\text{atm}} \right). \quad (22)$$

Defining $p_* = P_*/P_{\text{atm}}$ as the dimensionless overpressure, we arrive at

$$\left[\frac{1}{1 + \delta(x - y)} - \min \left(p_*, \frac{1 - \ell}{1 - x - \ell} \right) \right] = \alpha \frac{d^2 x}{dt^2} + \beta \frac{dx}{dt}. \quad (23)$$

The equilibrium location (17) no longer holds for this model, as equilibrium

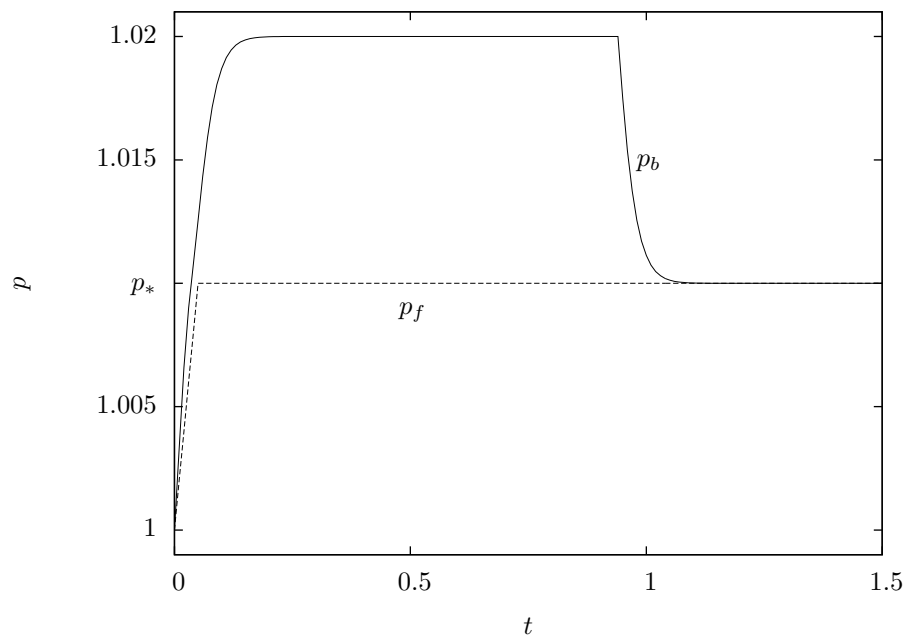


Figure 4: The back pressure p_b and forward pressure p_f of a slug heading toward a flooded reaction chamber. The pressure p_* is the value at which bubbling occurs.

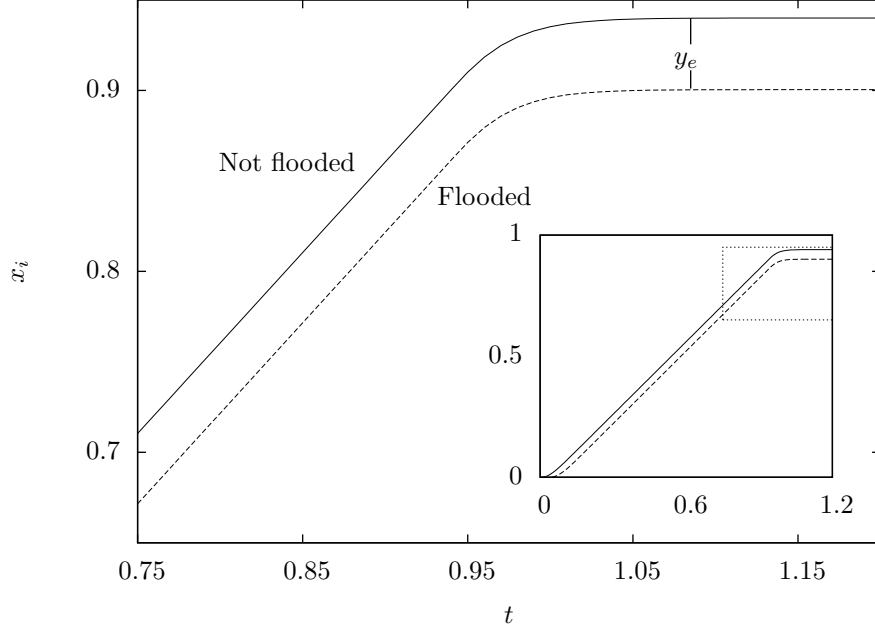


Figure 5: The position $x(t)$ for identical slugs with and without a flooded reaction chamber. The pumping protocol $y(t)$ is the same for both simulation, resulting in a visible miss of the target by a distance y_e for the slug with a flooded chamber.

is now achieved when the fore and back pressures are both P_* . A simple correction is to add an amount y_e to $y(0)$, where

$$y_e = \frac{A_s L_s}{A_t L_t} + 1 - \ell - (1 - x - \ell)/p_* - \frac{A_s L_s}{A_t L_t}/p_* \quad (24)$$

is the distance the piston must be depressed to just pressurize all of the gas to P_* . The new equilibrium is given by

$$\hat{x} = \frac{A_s}{A_t} (\hat{y} + \hat{y}_e). \quad (25)$$

3.1 Bubbling frequency

We may estimate the frequency of bubbling when pushing the gas in the forebubble through a flooded reaction chamber by assuming that bubbles

form as soon as enough mass of gas has been forced into the reaction chamber liquid. This is an approximation that assumes a monodisperse bubble size and an infinitely fast relaxation of the air/liquid interface between the reaction chamber fluid and the forebubble.

Under these assumptions, we estimate the rate of bubble formation as the rate of mass loss in the forebubble divided by the mass per bubble. The rate of mass loss is given by taking the ideal gas law

$$P_* V_f = \frac{r\Theta}{M} m_f,$$

for gas constant r , temperature Θ , molar mass M , and mass m_f , and differentiating in time to obtain

$$\frac{dm_f}{d\hat{t}} = \frac{P_* M}{r\Theta} \frac{dV_f}{d\hat{t}}. \quad (26)$$

The rate of volume loss is given by differentiating (1). Combined with the above, we obtain

$$\frac{dm_f}{d\hat{t}} = -\frac{P_* M A_t}{r\Theta} \frac{d\hat{x}}{d\hat{t}}. \quad (27)$$

To find the mass per bubble, we assume that all bubbles will have an identical radius $r_t = \sqrt{A_t/\pi}$, the radius of the tube through which they are blown. The pressure in each bubble must be P_* . This follows from the estimation of P_* as the pressure required to bend the meniscus backward. In that case, we may again use the ideal gas law to see that

$$m_{\text{bub}} = \frac{P_* M A_t}{r\Theta} \frac{4}{3} r_t. \quad (28)$$

We have used a bit of elementary geometry to rewrite the volume of the bubble in terms of A_t . Combining (27) and (28), we obtain the frequency of bubble formation as

$$\phi_{\text{bub}} = -\frac{3}{4r_t} \frac{d\hat{x}}{d\hat{t}}. \quad (29)$$

While varying the speed of the slug will vary the rate of bubble formation as shown, the number of m_{bub} -sized bubbles that will form will be dictated by the mass of gas that must be expelled from the forebubble:

$$N_{\text{bub}} = \frac{m_f}{m_{\text{bub}}} = \frac{3P_{\text{atm}}(L_t - \hat{\ell})}{4P_* r_t}, \quad (30)$$

where we assume that the forebubble has an initial pressure P_{atm} .

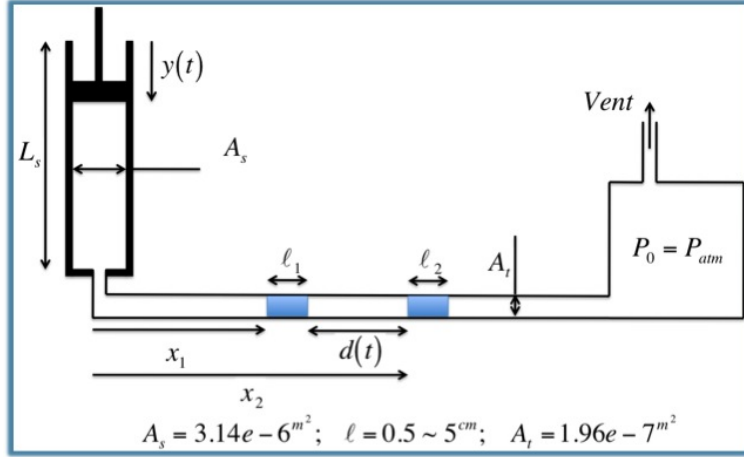


Figure 6: Schematic of a two-slug system.

3.2 Results

Figure 5 shows the position $x(t)$ of a slug when the reaction chamber is flooded alongside a plot of the position when the reaction chamber is empty. We see that the behaviour is largely the same except now, in the flooded case, the slug comes to rest a distance y_e short of the previous equilibrium position. This is because the forcing stops when the back pressure p_b reaches the bubbling pressure $p_* > p_{Atm}$. This is highlighted by figure 4 which shows the back pressure p_b and forward pressure p_f as a function of time. The forward pressure appears to linearly approach p_* , at which point bubbling in the flooded chamber occurs and so the forward pressure is maintained at this value. The back pressure increases to a value greater than p_* while the plunger is being depressed. When the plunger reaches the end of the syringe the back pressure drops smoothly as the gas behind the slug expands and the slug moves rightwards. It finally reaches the value p_* at which point the slug reaches its equilibrium position.

4 Multiple slugs in a tube

A sketch of the two-slug problem is shown in figure 6. In this case we define a back volume behind the first slug as

$$V_{b_1} = A_t \hat{x}_1 + A_s (L_s - \hat{y}) \quad (31)$$

which includes the volume of the syringe². Similarly, a volume in front of the first slug and behind the second slug is defined as

$$V_{b_2} = A_t(\hat{x}_2 - \hat{x}_1 - \hat{l}_1) \quad (32)$$

where \hat{l}_1 is the length of the first slug. The corresponding pressures are again assumed to satisfy Boyle's law and hence:

$$P_{b_1} = \frac{V_{b_1}^0 P_{\text{atm}}}{A_t \hat{x}_1 + A_s(L_s - \hat{y})}, \quad (33)$$

and

$$P_{b_2} = \frac{V_{b_2}^0 P_{\text{atm}}}{A_t(\hat{x}_2 - \hat{x}_1 - \hat{l}_1)}, \quad (34)$$

where $V_{b_1}^0, V_{b_2}^0$ are the initial volumes behind each slug.

The motion of each slug is driven by the pressure across it so the equations of motion are

$$A_t P_{\text{atm}} \left(\frac{V_{b_1}^0}{A_t \hat{x}_1 + A_s(L_s - \hat{y})} - \frac{V_{b_2}^0}{A_t(\hat{x}_2 - \hat{x}_1 - \hat{l}_1)} \right) = m_1 \ddot{\hat{x}}_1 + c_1 \dot{\hat{x}}_1, \quad (35)$$

and

$$A_t P_{\text{atm}} \left(\frac{V_{b_2}^0}{A_t(\hat{x}_2 - \hat{x}_1 - \hat{l}_1)} - 1 \right) = m_2 \ddot{\hat{x}}_2 + c_2 \dot{\hat{x}}_2. \quad (36)$$

Observe that this system assumes that the reaction chamber that has not yet been flooded.

We nondimensionalise in a similar way as before, together with now defining $V_{b_1}^0 = A_s L_s$ and $V_{b_2}^0 = A_t \hat{d}_1$ where $\hat{d}_1 = (x_1^0 - x_2^0 - l_2^0)$ is the initial distance between the slugs. Nondimensional parameters $l_1 = \hat{l}_1/L_t$, $d_1 = \hat{d}_1/L_t$ are also introduced alongside $\alpha_i = \rho \hat{l}_i X / (P_{\text{atm}} T^2)$, $\beta_i = 8\pi \hat{l}_i \mu X / (A_t P_{\text{atm}} T)$ for $i = 1, 2$. Consequently we reach

$$\left[\frac{1}{\delta(x_1 - y) + 1} - \frac{d_1}{x_2 - x_1 - l_1} \right] = \alpha_1 \ddot{x}_1 + \beta_1 \dot{x}_1 \quad (37)$$

and

$$\left[\frac{d_1}{x_2 - x_1 - l_1} - 1 \right] = \alpha_2 \ddot{x}_2 + \beta_2 \dot{x}_2 \quad (38)$$

²Recall that variables with hats or in capital letters are dimensional quantities.

as a coupled system of o.d.e.'s for the two slug problem. This is easily generalised to multiple slugs, for which the system of o.d.e.'s is:

$$\begin{aligned} \left[\frac{1}{1 + \delta(x_1 - y)} - \frac{d_1}{x_2 - x_1 - \ell_1} \right] &= \alpha_1 \frac{d^2 x_1}{dt^2} + \beta_1 \frac{dx_1}{dt} \\ \left[\frac{d_{i-1}}{x_i - x_{i-1} - \ell_{i-1}} - \frac{d_i}{x_{i+1} - x_i - \ell_i} \right] &= \alpha_i \frac{d^2 x_i}{dt^2} + \beta_i \frac{dx_i}{dt} \\ \left[\frac{d_{n-1}}{x_n - x_{n-1} - \ell_{n-1}} - p_f(x_n; p_*) \right] &= \alpha_n \frac{d^2 x_n}{dt^2} + \beta_n \frac{dx_n}{dt} \end{aligned} \quad (39)$$

where

$$p_f(x_n; p_*) = \begin{cases} \min \left(p_*, \frac{1-\ell}{1-x_n-\ell_n} \right) & \text{flooded} \\ 1 & \text{not flooded} \end{cases} \quad (40)$$

These equations therefore also include the foaming effect of having a flooded reaction chamber as discussed in section 3.

4.1 Results

Figure 7 shows the position of two slugs of equal length as they move through the tube toward an empty reaction chamber. The distance between the slugs becomes slightly compressed whilst the plunger is being depressed and then they move along together with an equal speed. After the plunger has reached the end of the syringe, the distance between the slugs relaxes to its equilibrium value and the slugs remain separated at a fixed distance. The velocity profile is highlighted in figure 8.

Figure 9 then shows the position of two slugs for the case when the length of the first slug is twice the length of the second slug. Similarly, figure 10 again shows the velocity profile. The behaviour is qualitatively exactly the same as in the previous case.

5 Recommendations

The model (11) should predict the position of the slug as a function of the piston position. Using the length criterion (20) will ensure that motion is monotonic. The pumping protocol $y(t)$ may be selected so as to avoid fragmenting slugs.

The principle difficulty lies in avoiding foaming in the reaction chamber. Foaming is caused by pushing the gas in V_f , the forward bubble, through

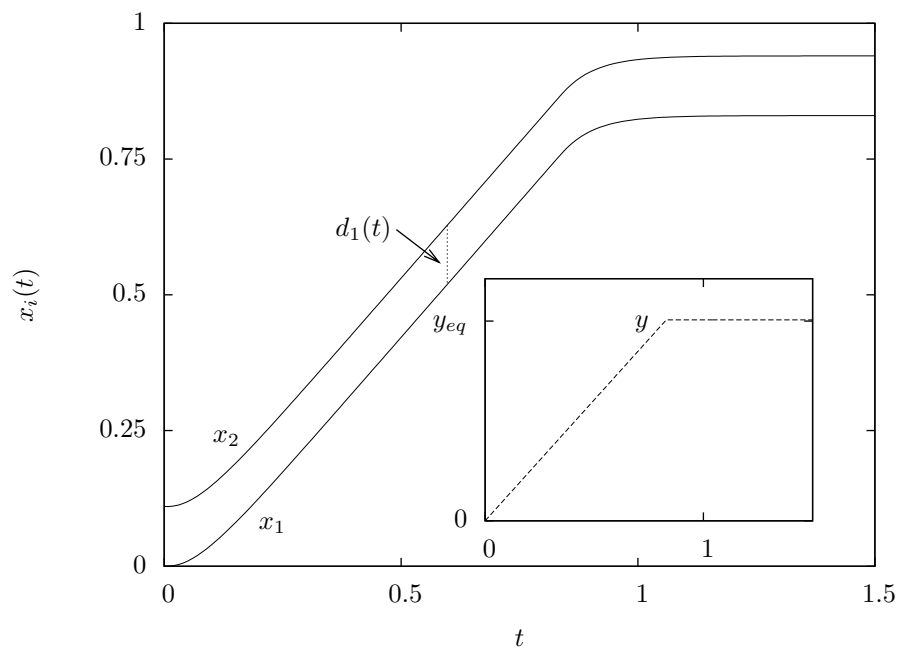


Figure 7: Position $x(t)$ for two slugs of equal length. Again, the reaction chamber is assumed to be empty and the dashed line shows the syringe compression $y(t)$.

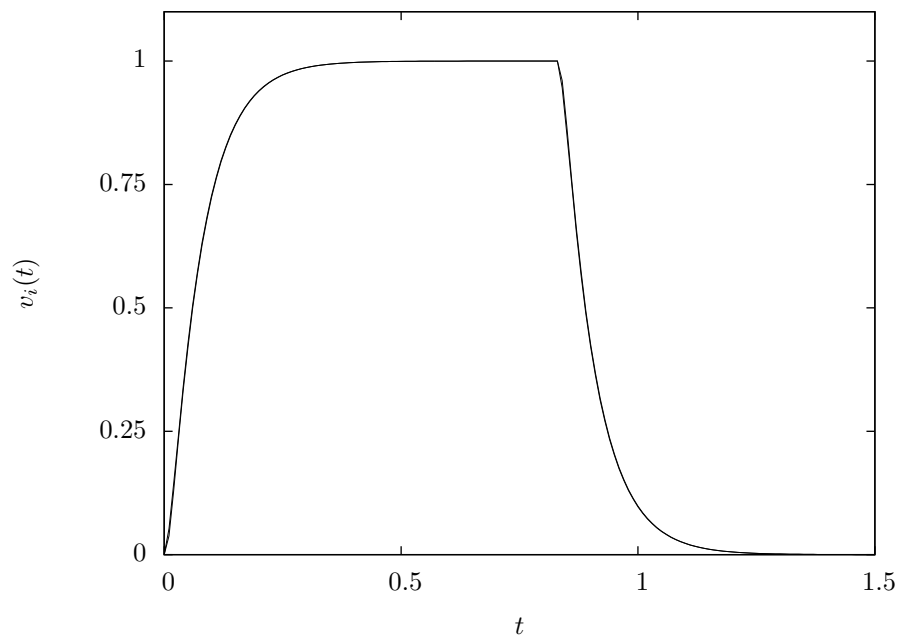


Figure 8: Velocity $\dot{x}(t)$ for two slugs of equal length corresponding to figure 7.

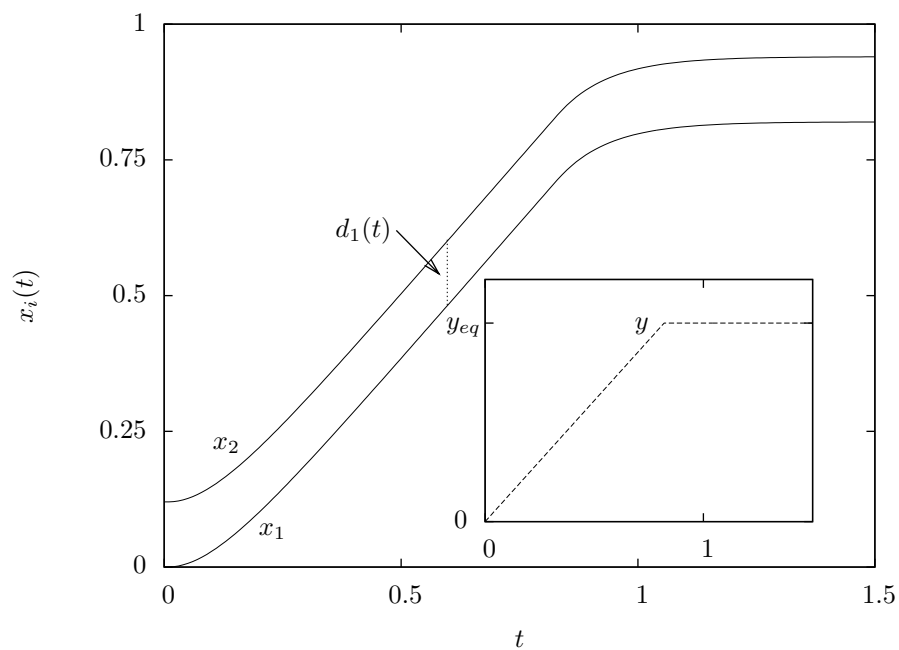


Figure 9: Position $x(t)$ of two slugs for the case where $l_1 = 2l_2$. The dashed line shows the syringe compression and the reaction chamber is assumed to be empty.

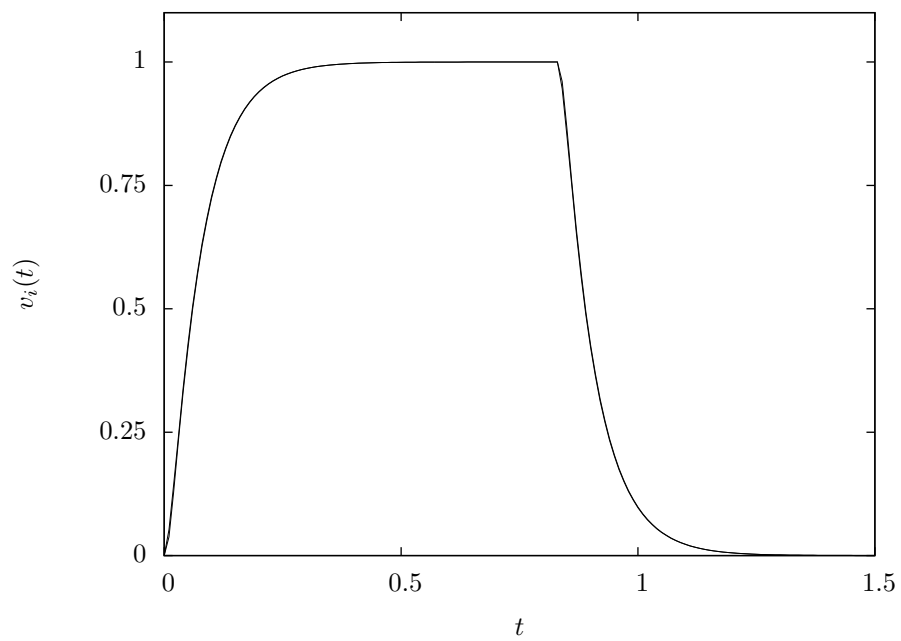


Figure 10: Velocity of the two slugs for the case where $l_1 = 2l_2$ corresponding to figure 9. Despite the differences in slug size, both experience very similar motion.

the liquid in flooding the chamber. There are two general ideas to reduce foaming.

First, the volume of air at P_{atm} that must be forced through the liquid must be kept to a minimum. If there are multiple tubes into the reaction chamber, slugs in each tube should be queued up at the edge of their tubes before any slug is allowed in to flood the chamber. If multiple slugs are to be delivered along a single tube, these slugs should be grouped into a “train” of slugs so that the bubble between adjacent slugs is small. The dynamics of such trains was discussed in Section 4. Adding a small amount of air-permeable membrane tubing to the end of the tube would also allow gas to vent rather than being forced through liquid in the reaction chamber.

Second, the pressure behind a slug must not be allowed to rise too far beyond P_* . At the instant of absorption of a slug into the reaction chamber, the pressure behind the slug must be greater than P_* as there must have been a pressure gradient across the slug. Thus, this overpressure will be relieved by bubbling through the front liquid. The higher the back pressure is above P_* , the more violent this bubbling will be. Using the model in 3.1 will allow an operator to determine the overpressure between slugs and design $\hat{y}(\hat{t})$ to compensate.

Most of the model parameters may be estimated through simple experiments. The damping β may be related to the pressure drop across a slug through (11). When a slug moves at a constant speed (e.g. the middle regime of Fig. 2, $\dot{x} = \dot{y}$, and so $x - y \rightarrow C$ for some constant C). Thus

$$\beta = \frac{1}{\dot{x}} \left(\frac{1}{1 + \delta C} - 1 \right).$$

The bubbling pressure P_* may be measured by flooding the reaction chamber, then pushing air into a dry tube. When bubbles begin to form in the reaction chamber, P_* has been reached. Noting the depression of \hat{y} at the time of bubbling gives

$$P_* = \left(\frac{A_s L_s + A_t L_t}{A_s L_s + A_t L_t - A_s \hat{y}} \right) P_{\text{atm}}.$$

The inertial parameter α may be calculated directly.

In conclusion, we have determined the dynamics of a single slug moving towards an empty reaction chamber giving the final equilibrium position of the slug. A phase-plane analysis then determined a condition on the size of the slug needed to ensure that it comes to rest without oscillating about the equilibrium position. The effect of a flooded reaction chamber

was then considered. In this case it is impossible to avoid bubbling due to the design of the device. We found that it is possible, however, to reduce the bubbling by minimising the back pressure behind the slug. Finally, the dynamics of multiple slugs with or without a flooded reaction chamber has been investigated.

References

- [1] G. K. Batchelor. *An Introduction to Fluid Dynamics*. Cambridge University Press, 1967.
- [2] Chien, R-L; and Wallace Parce, J. Multi-port flow control system for lab-on-a-chip microfluidic devices. *Fresenius J. Anal Chem*, 371:106–111, 2001.
- [3] J.F. Davidson and B.O.G. Schüler. Bubble formation at an orifice in a viscous liquid. *Trans. Instn Chem. Engrs*, 38:144–154, 1960.
- [4] De, A; Mukhopadhyay, A; and Puri, I. Lattice boltzmann method simulation of electroosmotic stirring in a microscale cavity. *Microfluid Nanofluid*, 4:463–470, 2008.
- [5] Lu, L-H; Ryu, K.S.; and Liu, C. A magnetic microstirrer and array for microfluidic mixing. *J. Microelectromechanical systems*, 11:462–469, 2002.
- [6] Matthew, G.; Mezic, I.; Grivopoulos, S.; Vaidya, U.; and Petzold, L. Optimal control of mixing in stokes fluid flows. *J. Fluid Mech*, 580:261–281, 2007.