A broadly-applicable unified closure relation for Taylor bubble rise velocity in pipes with stagnant liquid

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Abstract

Taylor bubble velocity in slug flow is a closure relation which significantly affects the prediction of liquid holdup (or void fraction) and pressure gradient in mechanistic models of slug flow for oil and gas pipe applications. In this work, we use a validated Computational Fluid Dynamics (CFD) approach to simulate the motion of Taylor bubbles in pipes; the interface is tracked with a Level-Set method implemented in a commercial code. A large numerical database is generated covering the most ample range of fluid properties and pipe inclination angles explored to date ($Eo \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$, and $\theta \in [0^\circ, 90^\circ]$). A unified Taylor bubble rise velocity correlation is extracted from that database. The new correlation predicts the numerical database with 8.6% absolute average relative error and a coefficient of determination $R^2 = 0.97$, and other available experimental data with 13.0% absolute average relative error and $R^2 = 0.84$ outperforming existing correlations and models.

Keywords: Taylor bubble, slug flow, terminal velocity, inclined pipes

1. Introduction

Two-phase slug flow is a common occurrence in wells, riser pipes and pipelines of crude oil and natural gas systems. Current predictive tools for two-phase flow

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are based on either the mixture model or the mechanistic two-fluid model [11].

5 In the latter, slug flow is modeled as a sequence of fundamental units, also called slug units. Each unit contains a long bullet-shaped bubble, known as Taylor bubble, and a liquid portion with smaller homogeneously distributed bubbles, known as liquid slug. Thorough studies about the modeling of two-phase slug flow can be found in [8, 24, 68]. The mechanistic model requires the use of clo-
 10 sure relations to capture the transfer of mass, momentum and energy between the phases, in the respective conservation equations, so that integral flow parameters such as liquid holdup (or void fraction) and pressure gradient can be predicted. However, these closure relations typically carry the highest uncertainties in the model, since they are obtained empirically or through the use of
 15 overly simplified assumptions. In particular, significant discrepancies have been found between experimental data and closure relations for the Taylor bubble velocity in slug flow, which has been determined to strongly affect the pressure gradient and liquid holdup predicted by the mechanistic models of [2, 53, 57].

Taylor bubble velocity, v_{TB} , in slug flow is generally modeled based on the drift flux approach of [49],

$$v_{TB} = C_0 \cdot v_m + v_d, \quad (1)$$

where v_d is the *drift velocity* of the bubble in a stagnant liquid, and $C_0 \cdot v_m$ is
 20 the contribution of the mixture velocity, v_m , which is the sum of the liquid and gas superficial velocities, $v_m = v_{SL} + v_{Sg}$. The *distribution parameter*, C_0 , is a dimensionless coefficient that depends on the velocity profile in the liquid, and is approximately the ratio of the maximum to the mean velocity. The present article is focused on the velocity and dynamics of the Taylor bubble in stagnant
 25 liquid, i.e., the second term of the RHS of equation 1, v_d .

Taylor bubble's dynamics are influenced by the viscous, inertial, gravitational, and interfacial forces acting on it. Assuming that the liquid transport properties are dominant ($\rho_g/\rho_L \ll 1$, $\mu_g/\mu_L \ll 1$, where the subscripts g and L indicate the gas and liquid phases, respectively, ρ is the density, and μ is
 30 the dynamic viscosity), dimensional analysis indicates the following four dimen-

Table 1: Ranges of Mo for various oils [12]

	ρ_L [kg/m ³]	σ [N/m]	μ_L [Pa·s]	Mo
Heavy oil	1100	0.03	2	$5 \cdot 10^3$
High viscous oil	1100	0.03	0.15	$2 \cdot 10^{-1}$
Medium viscous oil	1000	0.03	0.03	$3 \cdot 10^{-4}$
Light oil	900	0.03	0.007	$1 \cdot 10^{-6}$
Very light oil	800	0.03	0.001	$5 \cdot 10^{-10}$

sionless pi -groups are sufficient to determine the bubble dynamics: the Froude number, $Fr = v_{TB}/\sqrt{gd}$, where g is the gravitational acceleration and d is the pipe diameter, is the ratio of the bubble inertia to the gravitational forces; the Eötvös number, $Eo = \rho_L g d^2 / \sigma$, σ is the surface tension, is the ratio of the grav-
 35 itational to interfacial forces; the Morton number, $Mo = g \mu_L^4 / \rho_L \sigma^3$, sometimes called the property number; and the inclination angle, θ , measured from the horizontal. Note, however, that the choice of the pi -groups is not unique; for example, the inverse viscosity number, N_f , a combination of Eo and Mo , can also be employed. Thus, Buckingham Pi -Theorem assures that the four pi -groups
 40 are related by a unique function of the form $Fr = f(Eo, Mo, \theta)$. In this article, a proposed correlation for this function is presented for an ample range of fluid properties and pipe inclination angles: $Eo \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$, and $\theta \in [0^\circ, 90^\circ]$.

Table 1 shows the range of Mo for different types of oil. In this work, we
 45 focus on the upper range of the spectrum since ample work has been done using water, which has similar properties to very light oil, as will be described later. Furthermore, the oil and gas industry is currently moving towards the production of heavier oils, with the associated need to predict their behavior.

2. Literature review

50 The literature for Taylor bubbles rising in vertical tubes ($\theta = 90^\circ$) filled with a stagnant liquid is extensive. [20] and [23] studied analytically the limiting problem of negligible viscous force and surface tension where Fr is found to be constant. [75] performed a wide range of experiments and proposed a general graphical correlation of Fr as a function of EO and Mo , identifying regions
55 where some governing forces can be neglected (see figure 1). [77] investigated experimentally the influence of liquid viscosity and surface tension on the bubble velocity, and proposed a velocity correlation for vertical tubes. [73] reported a correlation with three different regions based on N_f for the vertical drift velocity and horizontal drift velocity, v_d^v and v_d^h , respectively. [71] performed experiments
60 and, together with the available published data, obtained a correlation for $Fr = f(N_f, EO)$. They composed bi-power laws for two separate flow regions: large N_f , $N_f > 200$, and small N_f , $N_f < 10$, and connected them through a logistic dose response curve [55, 33]:

$$Fr = \frac{0.34}{(1 + (14.793/EO)^{3.06})^{0.58}} \left/ \left(1 + \left(\frac{N_f}{31.08(1 + (29.868/EO)^{1.96})^{0.49}} \right)^a \right)^b \right. \quad (2a)$$

$$a = -1.45(1 + (24.867/EO)^{9.93})^{0.094} \quad (2b)$$

$$b = -1.0295/a. \quad (2c)$$

CFD numerical simulations have also been used to study slug flow mainly
65 with 2D axisymmetric domain. [18], and [46] focused on the flow ahead and around the bubble. [4] analyzed a wide range of Taylor bubbles in vertical stagnant liquid columns using 2D axisymmetric simulations ($EO \in [6, 900]$, $Mo \in [4.72 \cdot 10^{-5}, 104]$, $N_f \in [3.5, 517]$). [3] studied the hydrodynamics of pairs of consecutive Taylor bubbles in stagnant liquid. [37] studied experimen-
70 tally and numerically the terminal velocities of clean and contaminated drops, as well as Taylor bubbles, in vertical pipes. In their terminal velocity correlation, they modified the coefficients of the correlations given by [29], who obtained the functional form of that empirical correlation through a force balance on the Taylor drop. The latter was deduced with a scaling analysis based on the field

75 equations for two phases and the jump conditions at the interface. The range of applicability of their correlation is $Eo \in [4.8, 228]$ and $Mo \in [1 \cdot 10^{-12}, 1 \cdot 10^4]$. [60] performed simulations using VOF, including some limiting cases for inviscid liquid ($Mo = 0$, $N_f = \infty$), and zero surface tension ($Eo = \infty$). Other 2D vertical axisymmetric studies were done by [13], [67] and [34].

80 The effect of the pipe inclination angle on the Taylor bubble dynamics has also been studied in the literature. Table 2 shows the Eo and Mo number ranges of these studies as well as the inclination angles covered, and tables 3 and 4 enumerate the correlations found in the literature for the Taylor bubble terminal velocity in inclined pipes. [77] described qualitatively the effect of tube inclination in closed tubes. [7] was the first to propose a correlation for 85 inclined pipes. He claimed that v_d^h can be different from zero in pipes with one end opened and partially filled with liquid and gas. In the open end, liquid drains out and gas enters the pipe, which moves the bubble forward inside due to the differences in liquid level at both sides of the bubble. These assumptions conflict with previous investigations of [49] and [22], who assumed $v_d^h = 0$ in 90 a closed horizontal pipe. [74] developed an ample experimental study covering $Eo \in [4.9 - 490]$ and $Mo \in [2.2 \cdot 10^{-11}, 1.5 \cdot 10^4]$. Furthermore, they proposed a correlation with a correction term Q which is a function of $\Delta Fr_d = Fr_d^v - Fr_d^h$. In their article, Fr_d^v and Fr_h^v are obtained by interpolation of the experimental 95 data, and they give a graphical general dimensionless correlation for horizontal tubes. [28] performed an experimental study for $\theta \in [58^\circ, 90^\circ]$ and proposed a new correlation for bubble velocity in stagnant liquid. Equation 5b is there justified for systems with large N_f and Eo values (e.g., $N_f > 300$ and $Eo > 100$) where Fr_d^v becomes constant. Furthermore, they assumed $v_d^h = 0$. [63] and 100 [1] studied experimentally and analytically the surface tension effects on the velocity of Taylor bubbles in inclined pipes, for which they used water and kerosene. [15] derived a semi-theoretical expression for the rise velocity of air bubbles in inclined pipes of stagnant water, and performed experiments with non-Newtonian fluids. [57] used the correlations of [73] for the horizontal drift velocity (equation 6a), and a modification of their vertical drift velocity. [62]

studied experimentally the motion of long bubbles in inclined tubes for 5° to 90° inclination angles, of Newtonian and non-Newtonian fluids. [26] investigated experimentally the effect of high oil viscosity on drift velocity for horizontal and inclined pipes using water and viscous oil. They proposed a new correlation for the horizontal drift velocity extending the analysis of [9] to include viscosity, and used the expression of [32] for the vertical drift velocity. [31] analyzed experimentally the Taylor bubble terminal velocity for high-viscosity oil, proposing a new horizontal drift velocity. They also used the expression of [32] for the vertical drift velocity. [48] conducted experiments with medium viscosity oils ($Eo = 804$, $Mo \in [1.25 \cdot 10^{-3}, 0.41]$) for inclination angles between 0° and 90° . Moreover, they proposed a unified dimensionless closure relationship for drift velocity using data from the literature as well as theirs. Similar to the correlation of [74] (equations 4), they used a correction factor Q dependent on $\Delta Fr_d = Fr_d^v - Fr_d^h$. Furthermore, they introduced four parameters, $a = 1.2391$, $b = 1.2315$, $c = 2.1589$, and $d = 0.70412$, in order to fit the data. Other experimental studies of slug flow in slightly deviated from horizontal tubes have been carried out by [10] and [64]. CFD simulations of Taylor bubbles in inclined pipes are computationally expensive, because axisymmetry cannot be assumed; as a result, there is no extensive study on the matter in the literature, and only [67] reported one inclined pipe case in their work.

As reviewed above, most multiphase models and correlations were developed with and for low viscosity fluids. For example, [7] and [28] used water, whose $Mo = 2.63 \cdot 10^{-11}$, a value which is within one order of magnitude of that for low viscosity oils. However, the oil and gas industry is currently moving towards the production of heavier oils. High density and high viscosity oils currently constitute nearly 70% of the available reserves in the world, increasing the need to gain and improve the knowledge of the flow behavior of these fluids. When $\mu \in [0.150, 1]$ Pa·s, oils are considered to be high viscous; medium viscosity oils when $\mu \in [0.030, 0.150]$ Pa·s; and low viscosity oils when $\mu \in [0.001, 0.030]$ Pa·s, corresponding to a Mo range of $[1 \cdot 10^{-10}, 5 \cdot 10^3]$. Furthermore, the range of Eo relevant to Taylor bubbles is $Eo \in [10, 700]$. Note that for $Eo \lesssim 4$ in

Table 2: Experimental studies of Taylor bubbles in inclined pipes with a stagnant fluid

	θ [°]	Eu	Mo
[77]	0 – 90	3.48 – 4,000	$2.59 \cdot 10^{-11} - 19.2$
[63]	0 – 90	50 – 10,000	$\sim 2.59 \cdot 10^{-11}$
[7]	0 – 90	50 – 340	$\sim 2.63 \cdot 10^{-11}$
[74]	0 – 90	4.9 – 490	$2.2 \cdot 10^{-11} - 1.5 \cdot 10^4$
[28]	58 – 90	2,200	$\sim 2.63 \cdot 10^{-11}$
[1]	0 – 90	800	$3.66 \cdot 10^{-6}$
[62]	5 – 90	21.9 – 629	$2.17 \cdot 10^{-11} - 6.11 \cdot 10^4$
[26]	5 – 90	349; 776	$2.63 \cdot 10^{-11}; 5.30 \cdot 10^{-1} - 1.24 \cdot 10^3$
[31]	0 – 90	765 – 6,970	0.258 – 49.2
[48]	0 – 90	804	$1.25 \cdot 10^{-3} - 0.41$
Present study	0 – 90	10 – 700	$1 \cdot 10^{-6} - 5 \cdot 10^3$

Table 3: Terminal velocity correlations for Taylor bubbles in inclined pipes with a stagnant

fluid Model	Correlation
[7]	$v_d = v_d^h \cos \theta + v_d^v \sin \theta, \quad (3a)$ $v_d^v = 0.351\sqrt{gd}, \quad (3b)$ $v_d^h = 0.542\sqrt{gd}. \quad (3c)$
[74]	$Fr_d = Fr_d^h \cos \theta + Fr_d^v \sin \theta + Q, \quad (4a)$ $Q = \begin{cases} 1.37(\Delta Fr_d)^{2/3} \sin \theta (1 - \sin \theta), & \text{if } \Delta Fr_d > 0, \\ 0, & \text{if } \Delta Fr_d \leq 0. \end{cases} \quad (4b)$
[28]	$v_d = v_d^v \sqrt{\sin \theta} (1 + \cos \theta)^{1.2}, \quad (5a)$ $v_d^v = 0.35\sqrt{gd}, \quad (5b)$
[57]	$v_d^h = \left(0.54 - \frac{1.76}{Eo^{0.56}}\right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (6a)$ $v_d^v = 0.345 \left(1 - e^{-Eo \cdot \exp(3.278 - 1.424 \ln Eo)}\right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (6b)$ $v_d = \min \left(0.316 \sqrt{\frac{\rho_L v_{d\infty} d}{2\mu_L}}, 1\right) \cdot (v_d^h \cos \theta + v_d^v \sin \theta), \quad (6c)$
[26]	$h/d = 0.1038 \ln \mu_L + 0.9684, \quad (7a)$ $S/d = \sqrt{1 - (2h/d - 1)^2}, \quad (7b)$ $\gamma_1 = \begin{cases} \pi - \sin^{-1}(S/d), & \text{if } h/d < 0.5, \\ \sin^{-1}(S/d), & \text{if } h/d \geq 0.5, \end{cases} \quad (7c)$ $\gamma = \min(\gamma_1, 1.444784), \quad (7d)$ $\zeta = (\gamma - 0.5 \sin 2\gamma)/\pi, \quad (7e)$ $\Delta = \frac{1 + \zeta}{\zeta} \left(\frac{d}{2} (1 - \cos \gamma) - \left(\frac{\frac{d}{2} (1 - (1 - \zeta) \cos \gamma - 2(\sin \gamma)^3 / 3\pi)}{1 - \zeta^2} \right) \right) \cdot 2.2, \quad (7f)$ $v_2 = \sqrt{2g \left(\frac{d}{2} (1 - \cos \gamma) - \Delta \right)}, \quad (7g)$ $v_d^h = (1 - \zeta)v_2, \quad (7h)$ $v_d^v = -\frac{8}{3} \frac{\mu_L}{\rho_L d} + \sqrt{\frac{2}{9}gd + \frac{64}{9} \left(\frac{\mu_L}{\rho_L d} \right)^2}, \quad (7i)$ $v_d = v_d^h (\cos \theta)^{1.5} + v_d^v (\sin \theta)^{0.7}. \quad (7j)$

Table 4: Terminal velocity correlations for Taylor bubbles in inclined pipes with a stagnant fluid (continuation)

Model	Correlation
[31]	$Fr_d = Fr_d^h \cos \theta + Fr_d^v \sin \theta, \quad (8a)$ $Fr_d^v = -\frac{8}{3}N_f^{-1} + \sqrt{\frac{2}{9}\frac{\rho_L}{\rho_L - \rho_g} + \frac{64}{9}N_f^{-2}} \quad (8b)$ $Fr_d^h = 0.53 \exp\left(-13.7N_f^{-0.46}Eo^{-0.1}\right). \quad (8c)$
[48]	$Fr_d = Fr_d^h \cos^{1.2391} \theta + Fr_d^v \sin^{1.2315} \theta + Q, \quad (9a)$ $Fr_d^v = -\frac{8}{3}N_f^{-1} + \sqrt{\frac{2}{9}\frac{\rho_L}{\rho_L - \rho_g} + \frac{64}{9}N_f^{-2}} - \left(\frac{\sqrt{2}}{3} - 0.35\right) \sqrt{\frac{\rho_L}{\rho_L - \rho_g}} \quad (9b)$ $Fr_d^h = 0.54 - \frac{N_f^{-1}}{1.886 + 0.01443N_f^{-1}}, \quad (9c)$ $Q = \begin{cases} 2.1589 \cdot (\Delta Fr_d)^{0.70412} \sin \theta (1 - \sin \theta), & \text{if } \Delta Fr_d \geq 0, \\ 0, & \text{if } \Delta Fr_d < 0. \end{cases} \quad (9d)$

vertical pipes, the bubble occupies the entire pipe cross section and basically does not move [75]. On the other hand, [35] proposed that the maximum stable cap bubble size for vertical pipes occurs at approximately $Eo \approx 900$, similar to what [36] predicted based on a two-dimensional Kelvin-Helmholtz instability analysis, and the experimental values reported by [19]. The implication is that the maximum pipe diameter for which Taylor bubbles and thus slug flow can exist corresponds to $Eo \approx 900$. In such pipes, bubbly flow transitions to either cap flow or churn-turbulent flow as the gas velocity increases [16, 52, 58, 56]. It should be noted that this limit increases with increasing inclination angle, i.e. slug flow can exist in inclined pipes at larger diameters than in vertical pipes [30, 51]. However, the critical values of the Eo number at which this transition occurs are not available in the literature.

3. CFD simulations

3.1. Mathematical model

3-D CFD Direct Numerical Simulations (DNS) are performed with the CMFD code [70], a finite-volume software developed at ASCOMP. The code uses structured meshes and MPI parallel-based algorithm to solve multi-fluid Navier-Stokes equations. Computer resources for this work include the supercomputers Titan and Eos of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory.

The code uses the one-fluid formulation approach, where the flow is described by one fluid with variable material properties, which vary according to a color function, which is advected by the flow. In the absence of phase change phenomena, the mass and momentum conservation equations are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (10a)$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \bar{\bar{\sigma}} + \rho \mathbf{g} + \mathbf{F}_s, \quad (10b)$$

where t is the time, $\mathbf{v}$ is the velocity vector, p is the pressure, $\bar{\bar{\sigma}} = \mu(\nabla \mathbf{v} + \nabla^T \mathbf{v})$ is the viscous stress tensor, $\mathbf{g}$ is the gravity vector, and $\mathbf{F}_s = \sigma \kappa \mathbf{n} \delta(\phi)$ is the surface tension term where $\kappa = \nabla \cdot (\nabla \phi / |\nabla \phi|)$ is the surface curvature, $\mathbf{n}$ is the vector normal to the interface, and δ is a smoothed delta function centered at the interface. In this work, the color function used is based on the Level Set (LS) method [54, 66], where the interface is represented by a continuous and monotonous function ϕ that represents the distance to the interface at which $\phi = 0$. The LS advection equation is given by

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0, \quad (11)$$

and material properties such as density and viscosity are updated locally based on ϕ , and smoothed across the interface using a smooth Heaviside function. Furthermore, the pipe is modeled as an embedded surface and represented in the fluid by the so-called Solid Level Set function where $\phi_s = 0$ is the fluid-solid

165 interface, i.e. the Immersed Surfaces Technology (IST) technique [17, 38]. The mesh is locally refined next to the pipe walls.

Simulations are carried out using the 2nd-order *Hybrid Linear/Parabolic Approximation* (HLP) scheme [76] for the discretization of the convective fluxes. An implicit 1st-order scheme is used for the time marching, where the time-step
 170 is adaptive and bounded by a Courant number fixed between 0.5 and 0.9 to guarantee stability of the simulations. The *SIMPLEC* (Semi-Implicit Method for Pressure Linked Equations-Consistent) algorithm is used for the pressure-velocity coupling [21]. For the level-set, a 3rd-order WENO scheme is used for re-distancing, and mass conservation is enforced using global and local mass
 175 conservation schemes [39]. Finally, the solvers used depend on the simulation. For high viscosity cases where the Navier-Stokes equations tend to elliptic, the R-cycle adaptive *Algebraic Multigrid* (AMG) method is used [59]. Otherwise, either the incomplete lower-upper decomposition method *Strongly Implicit Procedure* (SIP) [65] or the *Generalized Minimum Residual* method (GMRES) [61]
 180 are used, the latter with *hypr* AMG preconditioning [25] of the parallel PETSc (Portable, Extensible Toolkit for Scientific Computation) library [5].

3.2. CFD simulations

The test matrix explored in this study covers the ranges $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$ and $Eo \in [10, 700]$, and consists of the 25 logarithmically spaced cases shown in
 185 figure 1 and summarized in table 2. It can be observed that there are more points for lower Eo as there is a sharp transition in the velocity behavior for $Eo \approx 20$, as shown later. For each case, up to seven inclination angles ($5^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ, 90^\circ$) are simulated for a total of 147. This test matrix constitutes a substantial expansion of the ranges of parameters explored in
 190 previous studies.

The simulations start with a single bubble in still liquid and finish when the bubble reaches its terminal velocity. The initial bubble shape is a cylinder closed at the ends by two semi-spherical caps, and is placed inside a closed pipe embedded in the numerical domain. It should be emphasized that the

Figure 1: The map of [75] with the location of the numbered numerical database generated to obtain the Fr correlation of equations 16 (●), numerical cases used to validate the CMFD code (○, where ◻ are the experiments performed in this study), and experimental cases gathered from the literature [77, 74, 62, 26, 48] to test the proposed correlation (×).

195 initial bubble shape, size, and position within the pipe do not affect the results,
as we extract the data after the bubble has reached its terminal velocity and
shape. We have verified it through direct simulation of a few cases for evaluation
of these sensitivities. Bubble volume ranges from $\lambda = 1$ to 1.35, where
the parameter λ is the ratio of the sphere-volume equivalent bub-
200 ble diameter to the pipe diameter, $\lambda = d_e/d$. The pipe is the reference
frame, thus its velocity is set to zero, and its length is case dependent so that
boundary effects do not affect the results, with typical values around $10d$. The
boundary conditions of the numerical domain are symmetry planes where the
normal velocity and pressure gradient components are set to zero. The no-slip
205 condition at the wall is imposed through a relaxation term which acts as a
distributed momentum sink reducing the fluid velocity as the indicator function
goes to zero [6]. The structured mesh size is dependent on the case study and is
refined until the terminal velocity converges, capturing the Kolmogorov scale,
 η , estimated as $\eta \sim d \cdot Re^{-3/4}$, where $Re = Fr \cdot N_f$. Re ranges between 0.01
210 and 1000, and the Kolmogorov scale, η , between 0.6 and 0.0001 m. Number of
cells ranges from 1 million up to 8.5 million cells, with mesh refinement at
the pipe wall and a maximum cell aspect ratio of 3.

Figure 2: Snapshot of the Taylor bubble and the streamlines for $Eo = 29$, $Mo = 0.07$, and $\theta = 30^\circ$.

Furthermore, two results are analyzed based on two verified assumptions:
the Taylor bubble length does not affect its rising velocity in inclined pipes
and there exists a lubricating film between the Taylor bubble and the pipe
wall at all inclinations. The first assumption is justified in AppendixC. The

second assumption is verified by application of the film drainage and breakup criterion proposed in [43]. This criterion states that film breakup does not occur if the non-dimensional bubble passage time, $\bar{t}_{bubble} = t_{bubble}/\tau < 0.01$, where τ is the characteristic drainage time. The bubble passage time can be calculated as $t_{bubble} = L/v_{TB}$, where L is the bubble length, and v_{TB} is the bubble velocity. The characteristic time is $\tau = 3\mu_L R/(2\rho g \cos \theta h_c^2)$, where h_c is the critical thickness. The critical thickness order-of-magnitude estimate for the cases studied in steel pipe is $h_c \sim 1\mu\text{m}$, using the expressions of [72]. The most critical case we simulate is that for $\theta = 5^\circ$. At that point, the critical length below which the film does not break is calculated based on the aforementioned criterion as

$$(L/d)_c = 0.01v_{TB}\tau/d. \quad (12)$$

The results from equation 12 are reported in the last column of table A.7 of AppendixA. The lowest value of $(L/d)_c$ is three hundred, that is, the length of
215 the Taylor bubble simulated is much lower than the critical length calculated. Thus, the lubricating film is indeed present above the Taylor bubble in all cases simulated.

Representative snapshots of the shape and streamlines of a Taylor bubble with $Eu = 29$, $Mo = 0.07$, and $\theta = 30^\circ$ are shown in figure 2. We validated
220 the code using data from the literature for the Taylor bubble terminal velocity in vertical and inclined pipes. The calculated bubble shape was compared with experimental data from [50] for a case with $Eu = 192$ and $Mo = 4.75 \cdot 10^{-2}$, and the calculated velocity vectors were compared to experimental Particle Image Velocimetry (PIV) data from [14] for a case with $Eu = 98.4$ and $Mo = 1.52 \cdot$
225 10^{-2} . Details are reported in AppendixB and more can be found in [40, 42, 41].

4. Results

For vertical pipes, the Fr obtained numerically is compared with the results obtained using the correlations of [71] and [37]. The average terminal error of the simulations is 3.9% and 7.4%, with a standard deviation of 1.1% and

230 1.5%, respectively (see figure 3). Based on these results, the correlation of
 [71] appears to be an accurate tool to ~~predict~~calculate the terminal velocity
 of Taylor bubbles in vertical pipes, although the correlation of [37] pre-
dicts more accurately for air-water systems with $Eu < 30$. Furthermore,
 the dimensionless film thickness, $\bar{h} = h/d$, is compared with the correlation of
 235 [44]. Although the authors developed the correlation using experimental data
 where interfacial tension can be neglected, they proposed a generalization of the
 model to the cases where interfacial tension cannot be neglected. According to
 our data, this works well: the average error is $3.1\% \pm 1.3\%$.

Figure 3: Taylor bubble terminal Fr numerical results compared with the values obtained from literature correlations for vertical pipes

As far as inclined pipes are concerned, figure 4 shows the results from a few
 240 representative simulations of ours and the predictions of the correlations of [7],
 [28], [57], [26], [31], and [48] (see tables 3 and 4). Note the agreement of the
 correlations with each other and the numerical data is rather poor, which further
 motivates the need for a new broadly-applicable and accurate correlation. The
 maxima results from the competing effects of drag coefficient (lower at lower
 245 angles, where most of the liquid bypasses the bubble through a larger flow
 area), and buoyancy (higher at higher angles). Figure 5 shows this behavior
 for case 16 ($Eu = 83.7$ and $Mo = 7.07 \cdot 10^{-2}$) and three inclination angles: at
 $\theta = 90^\circ$, the bubble is axisymmetric and the drag coefficient is maximum. As

Figure 4: Fr as a function of θ for $Eo = 31.2$ and $Mo = 19.2$ (a) and $Eo = 38.6$ and $Mo = 1.17 \cdot 10^{-4}$ (b) compared with experimental correlations from the literature

the pipe inclines, the bubble front area is reduced as it approaches the pipe wall, and axisymmetry no longer applies. It should be noted that the longitudinal and radial directions, z and r , respectively, are normalized by the pipe radius, R , so that the dimensionless longitudinal and radial directions, z^* and r^* , respectively, are used.

Our complete numerical database is shown in figure 6. The plots are superimposed over the $Eo - Mo$ map, and then within each plot the dependence of Fr/Fr_v on the inclination angle is shown, where Fr_v is the vertical pipe Fr . The continuous lines in the plots are from the models explained in the next section. For each case, the maximum value occurs at around $\theta = 45^\circ$. Furthermore, two distinct regions are observed regarding the maximum value of the normalized Fr , (Fr/Fr_v): for $Eo > 20$, the amplitude of Fr/Fr_v is small for low Mo and high Eo , and slightly higher for high Mo –low Eo cases. However, for $Eo < 20$, this amplitude is significantly bigger. At this Eo range and vertical pipes, the bubble presents a bulge of higher radius in its bottom, making the liquid film effectively thinner and increasing the form drag. For example, the bulge can only be observed for the cases with $Eo = 10$ and 17 of figure 7, where the bubble bottom shape is shown for the cases with $\theta = 90^\circ$, and $Mo = 7.1 \cdot 10^{-2}$ and 19, respectively. As the pipe inclines, the bubble moves to the wall and the flow area increases in higher proportion than for the cases with

Figure 5: Bubble shape and velocity vectors at a cross sectional cut for case 16 ($Eo = 83.7$ and $Mo = 7.07 \cdot 10^{-2}$), at $\theta = 90^\circ$ (a), $\theta = 45^\circ$ (b), and $\theta = 5^\circ$ (c)

270 $Eo > 20$, as the disappearance of the bulge also contributes to this increment. Another feature observed in the map is the flat profile for low Mo and high Eo cases, where the velocity drops rapidly for low inclination angles.

Figure 6: Normalized Taylor bubble terminal Fr (Fr/Fr_v), for the values of $Eo-Mo$ shown in figure 1: numerical results ($\circ$), correlation of equation 14 ($-\cdot-$), and correlation of equations 16 ($-$).

5. Proposed new correlation for Taylor bubble velocity

We will now use the numerical database to generate a correlation that can serve as closure relation for Taylor bubble velocity in mechanistic models of slug flow. Following the procedure of [28], we can start by considering the balance of buoyancy and drag force that determines the terminal velocity of a Taylor bubble; after the pi -groups are introduced, the force balance yields an expression

Figure 7: Taylor bubble bottom shape for the cases with $\theta = 90^\circ$, and $Mo = 7.1 \cdot 10^{-2}$ (a) and 19 (b). The bulge at the bottom decreases with Eo and disappears for $Eo > 20$.

for Fr as follows:

$$Fr = Fr_v(\sin \theta)^{1/2}g(Eo, Mo, \theta), \quad (13)$$

where the function $g(Eo, Mo, \theta)$ is assumed to be $(1 + \cos \theta)^{Eo^a Mo^b}$ so that

$$Fr = Fr_v(\sin \theta)^{1/2}(1 + \cos \theta)^{Eo^a Mo^b}, \quad (14)$$

and the exponents a and b are then fitted to maximize the accuracy of equation 14 in reproducing the numerical database. The fit is performed using the nonlinear optimization algorithms built in [47]. However, the results are not satisfactory at low inclination angles for high Mo and low Eo values (see figure 6). Thus, a new function is proposed:

$$Fr = Fr_v(1 - \exp(-b(Eo, Mo)\theta))(1 + c(Eo, Mo) \sin(2\theta)), \quad (15)$$

where the exponential function reproduces the rapid velocity decay observed at low inclination angles, and the sinusoidal function reproduces the maximum velocity at $\theta = 45^\circ$. The coefficients $b(Eo, Mo)$ and $c(Eo, Mo)$ are chosen to yield the most accurate fit:

$$Fr = Fr_v(1 - \exp(-b(Eo, Mo)\theta))(1 + c(Eo, Mo) \sin(2\theta)), \quad (16a)$$

$$b(Eo, Mo) = 47.06Fr_v + 4, \quad (16b)$$

$$c(Eo, Mo) = -0.9118Fr_v + 0.67 + \frac{-0.0148(\log_{10} Mo)^2 + 0.125 \log_{10} Mo + 0.9118Fr_v + 1.118}{(1 + (Eo/20)^8)^8}. \quad (16c)$$

The coefficient $c(Eo, Mo)$ is predicted with a logistic dose-response curve that connects the two differentiated regions described above [55, 33]. In order to use this **this** new correlation for any values of Eo , Mo (or N_f) and θ , first calculate Fr_v from the correlation of [71], equations 2. Then, calculate the coefficients b and c from equations 16b and 16c, respectively, and finally, calculate Fr from equation 16a. Note that equation 16 is a continuous and smooth function of all the relevant variables and thus suitable for use as a closure relation in codes that implement the mechanistic model.

6. Performance of the new correlation

In this section, the performance of the proposed correlation (equations 16) is compared with the performance of the other correlations and models in the literature: [7], [28], [57], [26], [31], and [48] (see tables 3 and 4). Two databases are used for the comparison: the numerical database (section 6.1) and the experimental database (section 6.2). In the comparison we shall use several statistical parameters that characterize the performance of the models and are explained in AppendixD.

6.1. Numerical database

Table 5 summarizes the error statistics. Figure 8a reports the values of Fr from the numerical simulations versus the predictions of equations 16. On its right, figure 8b shows the cumulative plot of the relative error, E_2 (equation D.2), for the numerical database. It can be seen that the proposed correlation outperforms the other ones: using the proposed correlation, up to 70% of the cases show a relative error, E_2 , of less than 10%. On the other hand, the other literature models predict less than 10% of the cases with a relative error, E_2 , of less than 10%.

Of course the excellent performance of our correlation in reproducing the numerical database is not surprising since it was developed as a best fit of the numerical database, and the functions proposed are able to capture the velocity trends.

Figure 8: Fr numerical values versus the predictions of the proposed correlation, equations 16 (a), and cumulative plot of the relative error, E_2 , for the numerical database using the proposed and literature correlations (b).

Table 5: Statistical parameters of the models analyzed using the numerical database generated

Model	E_1	E_2	E_3	E_4	E_5	E_6	R^2
[7]	860	860	2400	0.34	0.34	0.16	-5.79
[48]	430	450	1400	0.22	0.22	0.14	-2.22
[28]	530	540	1300	0.22	0.23	0.16	-2.55
[31]	120	130	250	0.10	0.11	0.092	0.086
[57]	120	120	190	0.096	0.097	0.060	0.40
[26]	220	220	310	0.21	0.21	0.10	-1.63
Proposed (equations 16)	1.4	8.6	12.1	0.0041	0.017	0.026	0.976

6.2. Experimental database

We have also tested the models against the experimental data shown in figure 9a, and reported in AppendixA. It is worth mentioning that these experimental data were not used in fitting the coefficients of equations 16. The 178 experimental datapoints, gathered from the literature [77, 74, 62, 26, 48], cover the whole range of inclination angles and an ample region in the $EO - Mo$ map. Figure 9b depicts the results of Fr/Fr_v for both the experimental values and the predicted ones with equations 16. In general, the model predicts well the behavior except for cases 6 and 7, which were performed with an air/water mixture with $Mo = 2.63 \cdot 10^{-11}$ outside the ranges of our numerical database, as seen in figure 9a.

Figure 9: Numbered experimental cases gathered from the literature [77, 74, 62, 26, 48] to test our model ($\times$) located in the map of [75] together with the numerical database developed in this study ($\bullet$) and the cases to validate the CMFD code ($\circ, \square$) (a), and the Taylor bubble terminal Fr over the vertical Fr_v , Fr/Fr_v , for the experimental database: experimental results ($\circ$), and predictions of equations 16 ($-$) (b).

Figure 10a depicts the experimental values of Fr versus the proposed correlation. Furthermore, the cumulative error plot of the relative error, E_2 , for the experimental database is shown in figure 10b. It can be seen that the proposed correlation again outperforms the other ones: using the proposed model, up to 70% of the cases show a relative error, E_2 , of less than 10%. On the other hand,

around 20% of the cases show a relative error, E_2 , of less than 10% using the literature models. The three datapoints of figure 10a that are well below the 30% prediction error correspond to $\theta = 5^\circ$ of [62] (cases 18, 19 and 22 of figure 9b) where the velocity is remarkably low.

Figure 10: Fr experimental values versus the predictions of the proposed correlation, equations 16 (a), and cumulative plot of the relative error, E_2 , for the experimental database using the proposed and literature correlations (b).

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Finally, table 6 shows the statistical parameters that characterize the performance of the models. It is worth noting that our proposed correlation reports a coefficient of determination $R^2 = 0.84$, while without the cases 6 and 7 $R^2 = 0.87$. The second best model is that of [31] with $R^2 = 0.17$. Moreover, both E_2 and E_3 are 13% and 39% using our proposed model, respectively, while they are 37% and 56%, respectively, using the model of [31].

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7. Conclusions

In this work, a new unified correlation for the terminal velocity of Taylor bubbles in pipes with a stagnant liquid for an ample range of fluid properties and pipe inclination angles was presented (equations 16). The correlation was developed based on a CFD-generated database covering $Eu \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$, $\theta \in [0^\circ, 90^\circ]$, and within those ranges it clearly outperforms current correlations when tested against both the numerical database and experimental data: the absolute average relative error is 8.6% and 13%, while the coefficient

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Table 6: Statistical parameters of the models analyzed using the experimental database shown in figure 9a

Model	E_1	E_2	E_3	E_4	E_5	E_6	R^2
[7]	110	110	190	0.20	0.20	0.13	-2.90
[48]	63	64	130	0.12	0.13	0.10	-0.81
[28]	66	69	130	0.11	0.12	0.12	-0.79
[31]	34	37	56	0.087	0.095	0.068	0.17
[57]	35	39	65	0.080	0.093	0.087	0.052
[26]	51	52	94	0.12	0.13	0.083	-0.50
Proposed (equations 16)	0.32	13	39	-0.104	0.032	0.048	0.84

of determination R^2 coefficient is 0.97 and 0.84, respectively. The second best correlation reports an absolute average relative error of 120% and 37%, and a coefficient of determination R^2 equal to 0.40 and 0.17, respectively. The new correlation is recommended for use as a slug flow closure relation in codes that implement the mechanistic model.

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Table A.7: Numerical database for the vertical pipe simulations							
Case	Eu	Mo	N_f	Fr		Re	$(L/d)_c$
				Simulated	[71]		
1	10	$1 \cdot 10^{-6}$	180	0.13	0.14	23	$1.4 \cdot 10^3$
2	10	$2.7 \cdot 10^{-4}$	44	0.063	0.066	2.8	$2.3 \cdot 10^3$
3	10	$7.1 \cdot 10^{-2}$	11	0.019	0.16	0.20	$2.8 \cdot 10^3$
4	10	19	2.7	0.0038	0.0038	0.010	$2.8 \cdot 10^3$
5	17	$1 \cdot 10^{-6}$	260	0.23	0.25	62	$2.0 \cdot 10^3$
6	17	$2.7 \cdot 10^{-4}$	66	0.17	0.19	11	$4.1 \cdot 10^3$
7	17	$7.1 \cdot 10^{-2}$	16	0.063	0.063	1.03	$4.6 \cdot 10^3$
8	17	19	4.0	0.016	0.015	0.066	$5.1 \cdot 10^3$
9	29	$1 \cdot 10^{-6}$	390	0.30	0.31	120	$2.1 \cdot 10^3$
10	29	$2.7 \cdot 10^{-4}$	98	0.25	0.26	24	$5.7 \cdot 10^3$
11	29	$7.1 \cdot 10^{-2}$	24	0.13	0.13	3.2	$8.8 \cdot 10^3$
12	31	19	6.3	0.042	0.043	0.26	$8.7 \cdot 10^3$
13	29	$5 \cdot 10^3$	1.5	0.0095	0.0095	0.014	$8.6 \cdot 10^3$
14	84	$1 \cdot 10^{-6}$	870	0.34	0.34	290	$1.3 \cdot 10^3$
15	84	$2.7 \cdot 10^{-4}$	220	0.30	0.32	64	$4.7 \cdot 10^3$
16	84	$7.1 \cdot 10^{-2}$	54	0.25	0.25	14	$1.2 \cdot 10^4$
17	84	19	13	0.11	0.11	1.5	$1.5 \cdot 10^4$
18	84	$5 \cdot 10^3$	3.3	0.030	0.031	0.099	$1.4 \cdot 10^4$
19	240	$1 \cdot 10^{-6}$	1900	0.36	0.34	700	$2.8 \cdot 10^2$
20	240	$2.7 \cdot 10^{-4}$	480	0.34	0.34	160	$2.5 \cdot 10^3$
21	240	$7.1 \cdot 10^{-2}$	120	0.31	0.31	37	$8.3 \cdot 10^3$
22	240	19	30	0.21	0.20	3.2	$1.8 \cdot 10^4$
23	240	$5 \cdot 10^3$	7.3	0.071	0.070	0.52	$1.8 \cdot 10^4$
24	700	19	65	0.28	0.28	18	$1.3 \cdot 10^4$
25	700	$5 \cdot 10^3$	16	0.15	0.14	2.4	$1.8 \cdot 10^4$

Figure B.11: The Taylor bubble shape of case with $Eo = 192$ and $Mo = 4.75 \cdot 10^{-2}$ obtained numerically is compared with the experimental results from [50].

Appendix B. Code validation

In this section, the bubble shape calculated by the CFD code is compared with experimental data from [50] for a case with $Eo = 192$ and $Mo = 4.75 \cdot 10^{-2}$ (figure B.11), and in-house experiments generated with the experimental setup described later in Appendix C for $Eo = 57$ and $Mo = 3.1 \cdot 10^{-9}$ (figures B.12). Moreover, and the calculated velocity vectors are compared to experimental PIV data from [14] for a case with $Eo = 98.4$ and $Mo = 1.52 \cdot 10^{-2}$ (figures B.13 to B.15). Further validation results of the numerical method used in this study can be found in [40, 42, 41], e.g. the average error of the numerically obtained Taylor bubble velocity with respect to inclined in-house experiments is $-1.4\% \pm 3.3\%$.

In figure B.11, the bubble profile in the yz -plane (where the z -axis is the vertical) overlaps with the bubble profile in the perpendicular xz -plane, confirming an axisymmetric profile. On the other hand, figure B.12 depicts the tip bubble shape comparison for two inclined pipes ($\theta = 30^\circ$ and 5°) with 25% DI water and 75% methanol in volume ($Eo = 57$, $Mo = 3.1 \cdot 10^{-9}$), ensuring that the numerical method employed can be applied to Taylor bubbles in inclined pipes.

Figure B.13a shows the axial velocity component along the tube axis above

Figure B.12: Tip bubble shape comparison between experimental and numerical results for the mixture of 25% DI water and 75% methanol in volume and two different inclination angles.

the tip of the bubble: note that the presence of the bubble does not affect the flow beyond one diameter ahead of its tip. The axial and radial velocity components at $z/R = 0.222$ above the bubble tip are shown on figure B.13b. The axial velocity is positive in the center region of the pipe, and becomes negative in the periphery due to the suction of the film around the Taylor bubble. The radial velocity is zero at the tube axis due to symmetry and at $z/R = 1$ due to the tube wall, and is positive elsewhere since liquid is moving from the center region towards the pipe wall where it is suctioned by the liquid film. Figure B.14a shows the axial and radial velocity components in the film transition region at $z/R = 1.008$ below the bubble nose. The film is still developing since the radial velocity is not zero there. The axial velocity is negative in the whole film region. PIV particles are only observed in the liquid region, and the absence of them indicates the presence of the gas phase. Figure B.14b shows the axial velocity profile in the fully developed falling film at a distance $z/R = 4.64$ from the bubble nose. In this fully developed region, the radial velocity is zero as expected. Finally, figure B.15 depicts the axial and radial velocity components in the wake of the bubble at a distance $z/R = 0.4$ below the bubble tail. The radial velocity is negative since the liquid coming from the falling film at the pipe wall moves towards the pipe inner core. Furthermore, the axial velocity is positive in the inner core, and negative in the outer core due to the falling film, a characteristic of the recirculation taking place in this case's bubble wake. The comparison between simulations and experiments is successful and provides confidence in the use of the commercial code in this study.

²Note that error bars were not provided in their article

Figure B.13: The velocity profile of case with $Eo = 98.4$ and $Mo = 1.52 \cdot 10^{-2}$ ahead of the bubble in the pipe centerline (a) and across the radial axis (b) obtained numerically is compared with the experimental data of [14]².

Figure B.14: The velocity profile of case with $Eo = 98.4$ and $Mo = 1.52 \cdot 10^{-2}$ in the developing region of the falling film (a) and in the developed film (b) obtained numerically is compared with the experimental data of [14].

Figure B.15: The velocity profile of case with $Eo = 98.4$ and $Mo = 1.52 \cdot 10^{-2}$ in the wake of the bubble along the radial axis obtained numerically is compared with the experimental data of [14].

Appendix C. Effect of Taylor bubble length on its terminal velocity and shape in inclined pipes

It is well known that the dynamics of Taylor bubbles in vertical pipes are independent of their length [27, 44, 45, 69]. However, the effect of bubble length in inclined pipes has only been mentioned by [77], who stated that, in his experiments, “the propagation velocity is independent of length as long as the volume of the bubble corresponds to a cylinder with the tube radius and a length of three tube radii”. Here, we present both experiments and simulations showing that not only the terminal velocity but also the Taylor bubble shape are independent of its length in inclined pipes.

We measure the terminal velocity of Taylor bubbles with different volumes in inclined pipes. We analyze four liquids (methanol, ethanol, DI water, and a mixture of 50% DI water and 50% methanol in volume) at five inclination angles ($\theta = 5^\circ, 15^\circ, 30^\circ, 37.5^\circ, 45^\circ$). The experimental setup used [43], shown in figure C.16, consists of a High Speed Camera (HSC), a compressor, a polycarbonate tube of diameter $d = 0.0127$ m, and three valves. The experimental procedure is as following: first, air at atmospheric pressure is introduced and held between the closed valves at “b” and “c”. Then, valve “c” is opened and the Taylor

Figure C.16: Experimental setup (not drawn to scale)

bubble advances up through the tube due to buoyancy. The HSC records the bubble movement once it has reached its terminal velocity. The experiment finishes when the bubble reaches point “d”.

For each liquid and inclination angle, several measurements are taken. In the first five measurements, $i = 1, \dots, 5$, valve “c” is maintained open and the compartment “b”-“c” fills up completely with liquid. In the following measurements, $i > 5$, valve “c” is closed progressively earlier in time so that air remains in the compartment “b”-“c” and the volume of the experimental bubble rising the tube is progressively smaller, $V_i \geq V_{i+1}$. For all four fluids and five inclination angles, the measured terminal velocity was found to vary by no more than 1% when the bubble volume was varied up to 85% with respect to V_1 , corresponding to approximately the same bubble length variation. This indicates that the bubble volume and length do not affect significantly the terminal velocity.

Numerical simulations also confirm that the terminal velocity and bubble shape do not depend on the bubble volume/length. Here we analyze a fluid with $Mo = 19$ and $Eo = 31$ at two inclination angles ($\theta = 60^\circ, 45^\circ$). Bubble volumes are characterized by $\lambda = 1.05, 1.17$, ~~where the parameter λ is calculated as $\lambda = d_e/d$, where d_e is the sphere-volume equivalent diameter~~

435 **of the bubble.** The differences between the terminal velocities of both volumes are 0.07% and 0.2% for $\theta = 60^\circ$ and $\theta = 45^\circ$, respectively. Furthermore, figure C.17 shows that the bubble tip shapes overlap for both inclination angles.

Figure C.17: Taylor bubble shapes in a liquid with $Mo = 19$ and $Eo = 31$ overlap for two different bubble volumes ($\lambda = 1.17, 1.05$) for $\theta = 60^\circ$ (a) and $\theta = 45^\circ$ (b)

Thus, it is concluded that the Taylor bubble length does not affect its dynamics in inclined pipes, which is an important assumption made in the analysis described in section 3.2.

Appendix D. Statistical parameters

E_1 is the average relative error in percentage points,

$$E_1 = \left(\frac{1}{N} \sum_i \frac{Fr_{pred,i} - Fr_{sim,i}}{Fr_{sim,i}} \right) \cdot 100, \quad (D.1)$$

where N is the number of points, $Fr_{pred,i}$ is the predicted Fr value of case i using a correlation, and $Fr_{sim,i}$ is the numerically obtained Fr value of case i .

E_2 is the absolute average relative error in percentage points,

$$E_2 = \left(\frac{1}{N} \sum_i \frac{|Fr_{pred,i} - Fr_{sim,i}|}{Fr_{sim,i}} \right) \cdot 100, \quad (D.2)$$

E_3 is the standard deviation of the relative error in percentage points,

$$E_3 = \sqrt{\frac{1}{N-1} \sum_i \left(\frac{Fr_{pred,i} - Fr_{sim,i}}{Fr_{sim,i}} - \frac{E_1}{100} \right)^2} \cdot 100, \quad (D.3)$$

E_4 is the average error in basis points,

$$E_4 = \frac{1}{N} \sum_i^N (Fr_{pred,i} - Fr_{sim,i}), \quad (D.4)$$

E_5 is the absolute average error in basis points,

$$E_5 = \frac{1}{N} \sum_i^N |Fr_{pred,i} - Fr_{sim,i}|, \quad (D.5)$$

E_6 is the standard deviation of the absolute error in basis points,

$$E_6 = \sqrt{\frac{1}{N-1} \sum_i^N (Fr_{pred,i} - Fr_{sim,i} - E_4)^2}, \quad (D.6)$$

and finally, R^2 is the coefficient of determination, a number that indicates how well data fit a model,

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}, \quad (D.7)$$

where SS_{res} is the sum of squares of the residuals, also called the residual sum of squares, and SS_{tot} is the total sum of squares which is proportional to the variance of the data:

$$SS_{res} = \sum_i^N (Fr_{sim,i} - Fr_{pred,i})^2, \quad (D.8a)$$

$$SS_{tot} = \sum_i^N (Fr_{sim,i} - \bar{Fr}_{sim})^2, \quad (D.8b)$$

445 where $\bar{Fr}_{sim}$ is the mean of the observed data, $\bar{Fr}_{sim} = \sum_i^N Fr_{sim,i}/N$.

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