Karlsruhe Institute of Technology

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A correlation for the characteristic velocity ratio to predict hydrodynamics of capillary gas-liquid Taylor flow

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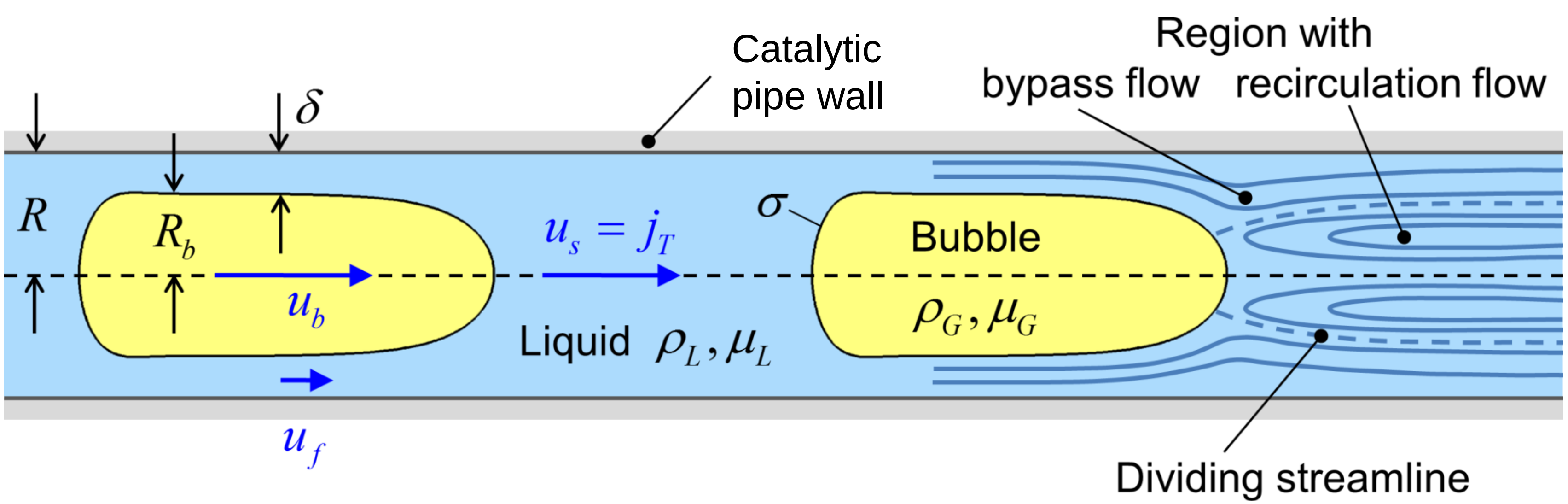
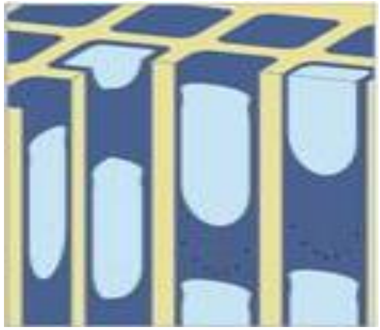


Outline

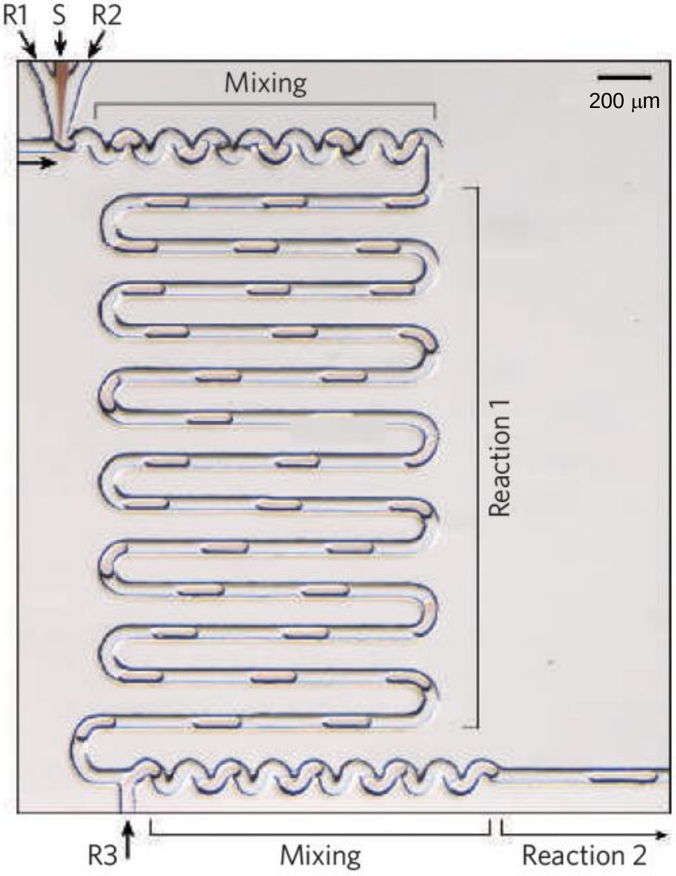
- Introduction
  - Two-phase flows in microchannels
  - Motivation and goal
- Characteristic velocity ratio of Taylor flow
  - Relations from mass balance
  - State-of-the-art information from literature
- Development of correlation
  - Identifying a master curve
  - Determining free parameters
  - Test against literature data
- Conclusions and outlook

Taylor flow in microchannels

- Advantages
  - Large interfacial area per unit volume and thin liquid film
    $\Rightarrow$ Efficient heat/mass transfer
  - Axial segmentation of continuous liquid phase
    $\Rightarrow$ Reduced axial dispersion
- Applications
  - Monolith reactors
  - Micro reactors
  - Lab-on-a chip
  - Heat exchangers
  - Fuel cells
  - ...



Kreutzer, Kapteijn, Moulijn, …



📖 Shestopalov et al., *Lab Chip* **4** (2004) 316-321

Problem statement and goal

- Of special interest for Taylor flow are two quantities
  - Bubble velocity $u_b \rightarrow$ residence time in microchannel
  - Liquid film thickness $\delta = \delta(u_b) \rightarrow$ heat and mass transfer with wall
- Problem
  - Bubble velocity u_b, δ and void fraction α are <u>not</u> prior known in general
  - Prior known are volumetric flow rates Q_G, Q_L and superficial velocities

$$j_G = Q_G / A = \alpha u_b, \quad j_L = Q_L / A = (1-\alpha) u_L \;, \quad j_T = j_L + j_G, \quad \beta = j_G / j_T$$

  - Useful would be a relation for the **characteristic velocity ratio** η which is formulated in terms of prior known parameters only, as this will allow to estimate u_b and $\delta(u_b)$ from prior known quantities

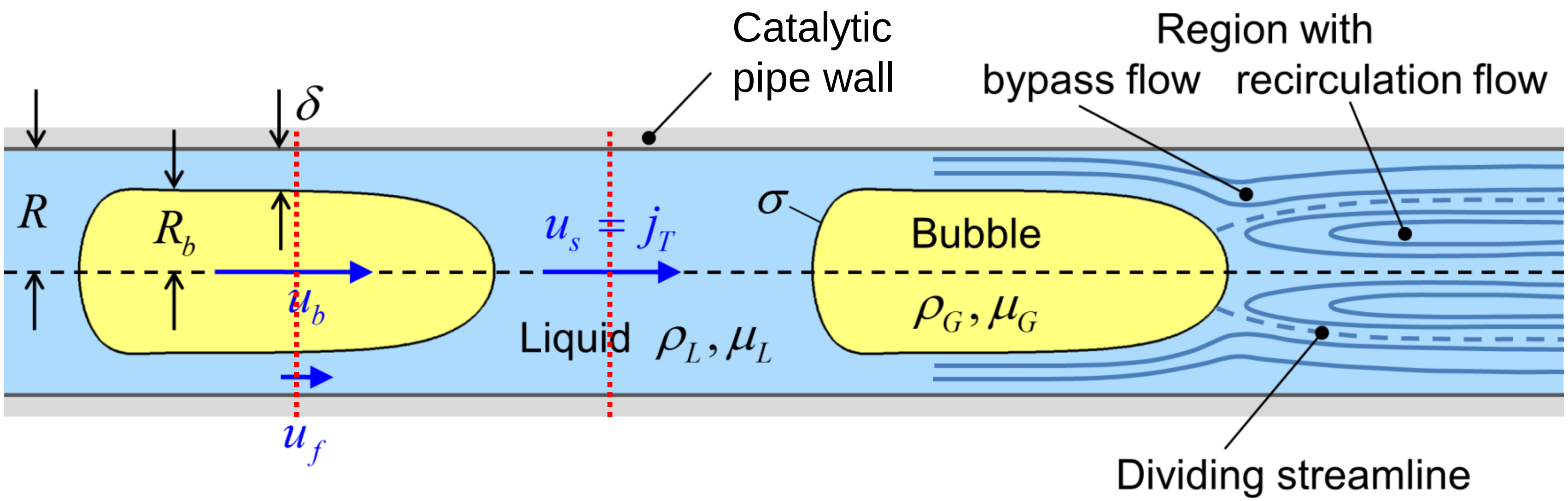
$$\eta := \frac{u_b}{j_T} = f_\eta(j_T, \beta, \rho_L, \mu_L, \sigma, \ldots)$$

- <u>Goal</u>: develop such a correlation using information from literature

Procedure

- Collect information from literature for η
  - Mass conservation principle, theoretical results
  - Empirical relations, DNS data
- Development of correlation
  - Identify suitable functional relationship ($\rightarrow$ logistic curve)
  - Determine free parameters by regression analysis
  - Test performance by comparison with experimental data
  - *Restriction to laminar gas-liquid Taylor flow in small circular pipes*
- Non-dimensional numbers based on velocity scales u_b, j_T
  - Bubble velocity $Ca_b = u_b \mu_L / \sigma$ $Re_b = 2\rho_L u_b R / \mu_L$
  - Total superficial velocity $Ca = j_T \mu_L / \sigma$ $Re = 2\rho_L j_T R / \mu_L$
  - Relations $Ca_b = \eta Ca$ $Re_b = \eta Re$

Taylor flow – continuity relation



$$\underbrace{u_f \underbrace{\pi(R^2 - R_b^2)}_{=A_f}}_{=Q_f} + \underbrace{u_b \underbrace{\pi R_b^2}_{=A_b}}_{=Q_b} = \underbrace{j_T \underbrace{\pi R^2}_{=A}}_{=Q_s}$$

Wetting fraction w

$$w := \frac{A_f}{A} = 1 - \frac{R_b^2}{R^2} = \frac{2\delta}{R}\left(1 - \frac{\delta}{2R}\right)$$

Subscripts
b = bubble
f = film
s = slug

continuity

$$\eta = \frac{u_b}{j_T} = \frac{1}{1-w}\,\frac{1}{1 + Q_f / Q_b}$$

Characteristic velocity ratio η

- Theoretical study (lubrication theory) by Bretherton (1961)

$$\eta_{\mathrm{Breth}} = 1 + 1.29 \times (3Ca_b)^{2/3} \quad Ca_b \le 10^{-3}$$

- Empirical correlations based on experimental data
  - Liu et al. (2005)

$$\eta_{\mathrm{Liu}} = \frac{1}{1 - 0.61 Ca^{0.33}} \quad 2\times 10^{-4} \le Ca \le 0.39$$

  - Abiev (2013)

$$\eta_{\mathrm{Abiev}} = 1 + 1.716\left[1 - \exp\left(-f_{\mathrm{Abiev}}(Ca_b)\right)\right] \quad 10^{-4} \le Ca_b \le 50$$

$$f_{\mathrm{Abiev}}(Ca_b) = \exp\left[-0.0204 + 0.4714 \ln Ca_b - 0.0211(\ln Ca_b)^2\right]$$

📖 F.P. Bretherton, *J. Fluid Mech.* **10** (1961) 166-188

📖 H. Liu, C.O. Vandu, R. Krishna, *Ind. Eng. Chem. Res.* **44** (2005) 4884-4897

📖 R.S. Abiev, *Chem. Eng. J.* **227** (2013) 66-79

Liquid film thickness δ

- Aussilious & Quere (2000), theoretical ($Ca_b \leq 1.4$, negligible inertia)

$$\frac{\delta_{\mathrm{AQ}}}{R} = \frac{P \cdot Ca_b^{2/3}}{1 + \underbrace{2.5 \times P}_{=F} \cdot Ca_b^{2/3}} = \frac{1.3375 Ca_b^{2/3}}{1 + 3.344 Ca_b^{2/3}}$$

P = 1.3375 from Bretherton theory
F = 2.5 from experiments by Taylor

- Han & Shikazono (2009), experiments ($Ca_b \leq 1.4$, $Re_b \leq 2000$)

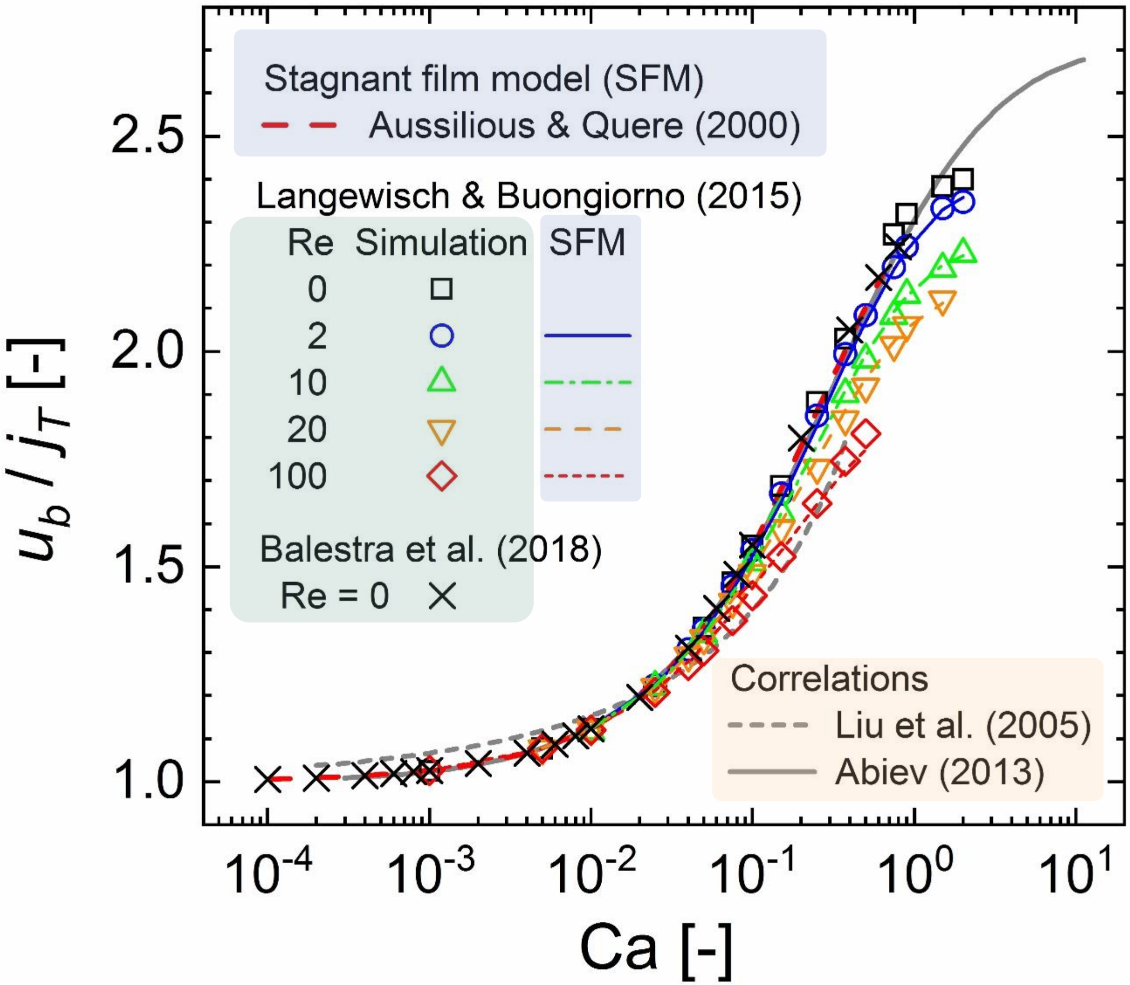
$$\frac{\delta_{\mathrm{HS}}}{R} = \frac{0.643 (3 Ca_b)^{2/3}}{1 + 3.13 Ca_b^{2/3} + 0.504 Ca_b^{0.672} Re_b^{0.589} - 0.352 We_b^{0.629}}$$

- Langewisch & Buongiorno (2015), DNS ($Ca \leq 0.2$, $Re \leq 900$)

$$\frac{\delta_{\mathrm{LB}}}{R} = \frac{1.3375 \mathrm{Ca}^{2/3}}{1 + 2.86 \left[1 + \Phi(Re)\right] Ca^{0.764}} \qquad \Phi(Re) = \left(\frac{32.05}{Re^{0.593}} + 4.564 \times 10^{-5} Re^{1.909} \right)^{-1}$$

- P. Aussillous, D. Quere, *Phys. Fluids* **12** (2000)
- G.I. Taylor, *J. Fluid Mech.* **10** (1961) 161-165
- Y. Han, N. Shikazono, *Int. J. Heat Fluid Flow* **30** (2009) 842-853
- D.R. Langewisch, J. Buongiorno, *Int. J. Heat Fluid Flow* **54** (2015) 250-257

Summary of literature information



Continuity relation

$$\eta = \frac{1}{1-w}\frac{1}{1+Q_f/Q_b}$$

$$w = \frac{2\delta}{R}\left(1-\frac{\delta}{2R}\right)$$

Stagnant film model (SFM)

$$\mu_G \ll \mu_L \rightarrow Q_f/Q_b \ll 1$$

$$\rightarrow \quad \eta_{AQ} \approx \frac{1}{1-w_{AQ}}$$

Symbols = DNS data for different Reynolds numbers

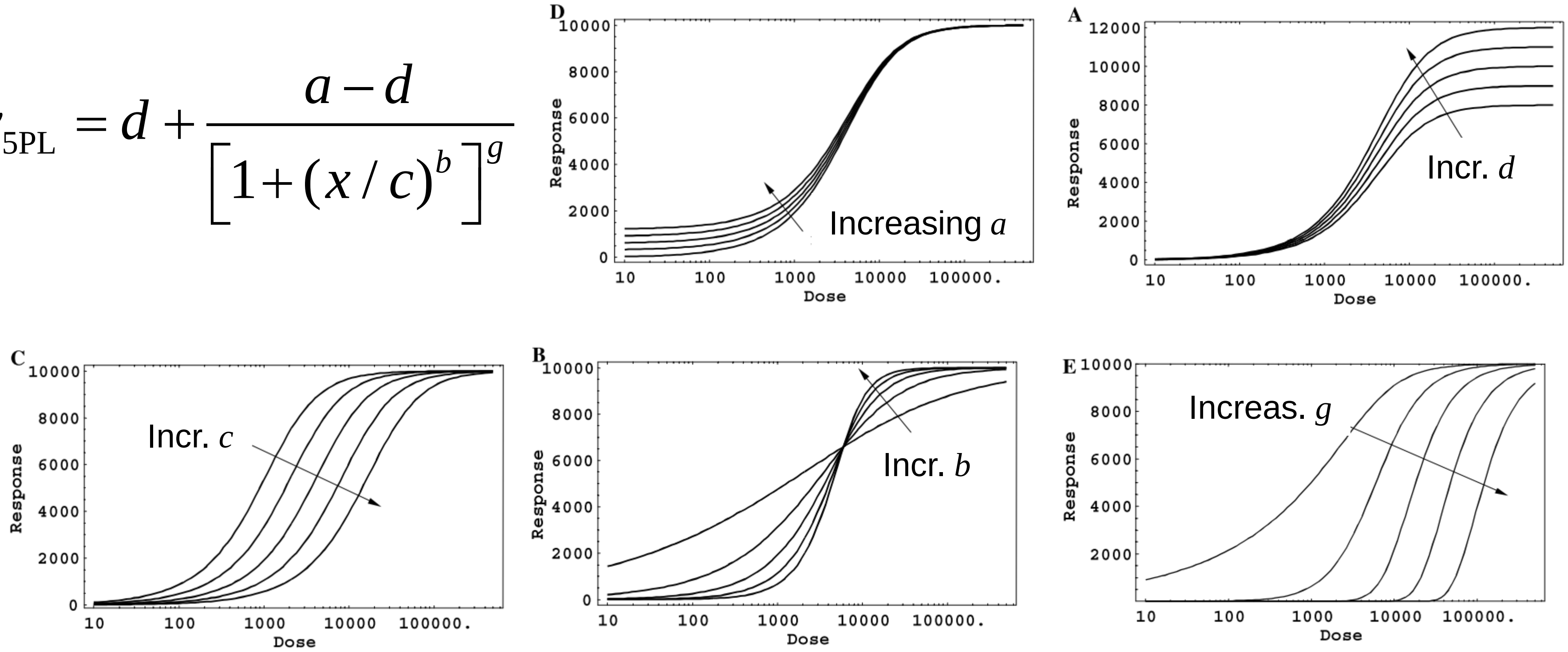
📖 D.R. Langewisch, J. Buongiorno, *Int. J. Heat Fluid Flow* **54** (2015) 250-257
📖 G. Balestra, L. Zhu, F. Gallaire, *Microfluidics and Nanofluidics* **22** (2018) 67

Sigmoidal master curve

Sigmoidal master function

- Asymmetric five parameter logistic (5PL) function

$$y_{5PL} = d + \frac{a-d}{\left[1+(x/c)^b\right]^g}$$



*“The **inability of standard algorithms to reliably fit the 5PL curve** has undoubtedly limited the use of the 5PL curve for modeling data”*

📖 P.G. Gottschalk, J.R. Dunn, *Analytical Biochemistry* **343** (2005) 54-65

Reducing no. of free parameters

- Slightly different 5PL for present case

$$y_{\mathrm{5PL}} = a + \frac{d-a}{\left[1+(x/c)^{-h}\right]^{s}} \xrightarrow[a=1]{y=\eta,\, x=Ca} \eta_{\mathrm{4PL}} = 1 + \frac{d-1}{\left[1+(Ca/c)^{-h}\right]^{s}}$$

- Idea for further reducing the free parameters of the 4PL
  - The limit of η_{4PL} for $Ca \to 0$ shall agree with Bretherton limit

$$Ca \to 0 \overset{h>0}{\Rightarrow} (Ca/c)^{-h} \gg 1 \Rightarrow \eta_{\mathrm{4PL}} \approx 1 + (d-1)c^{-h\cdot s} Ca^{h\cdot s}$$

$$\eta_{\mathrm{Breth}} = 1 + 1.29 \times (3Ca_b)^{2/3} \approx 1 + 1.29 \cdot 3^{2/3} Ca^{2/3}$$

  - Keeping d and s as free parameters, h and c follow from relations

$$h = \frac{2}{3s}, \quad c = \frac{1}{3}\left(\frac{d-1}{1.29}\right)^{3/2}$$

Key step in model development!

📖 F.P. Bretherton, *J. Fluid Mech.* **10** (1961) 166-188

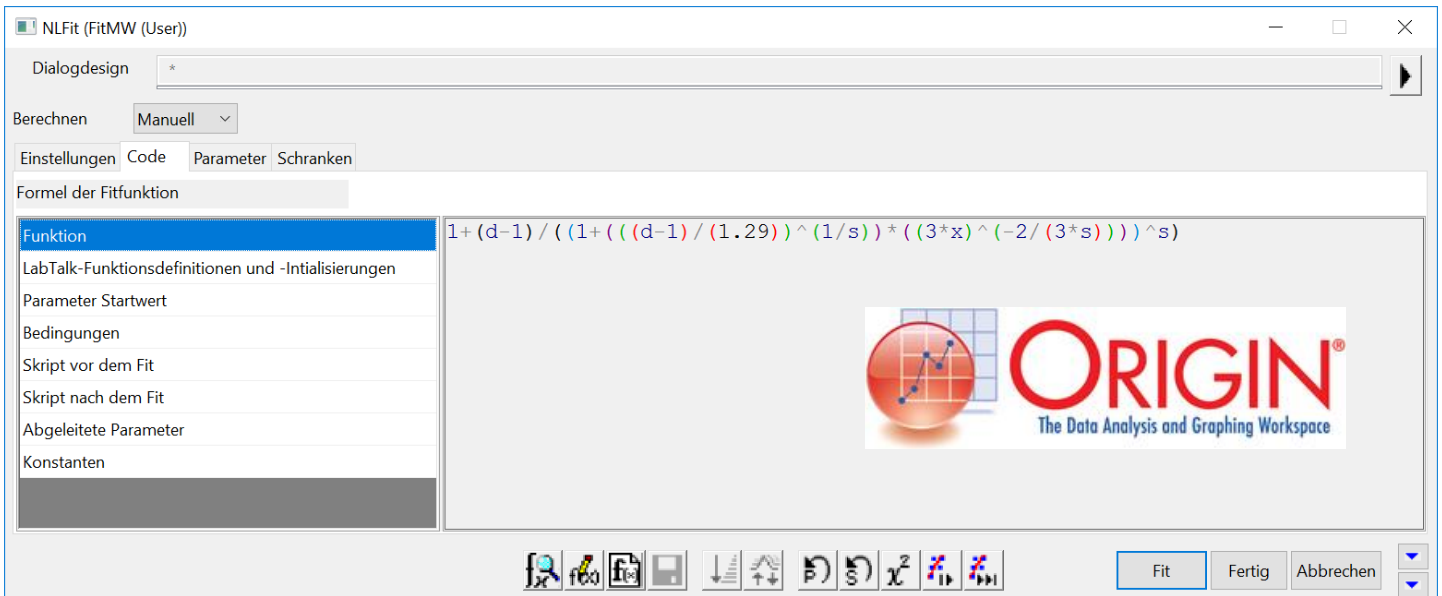
2PL with Bretherton limit

- Only two free parameters remain (d, s)

$$\eta_{2PL} = 1 + \frac{d-1}{\left[1+\left(\frac{d-1}{1.29}\right)^{1/s}(3Ca)^{-2/3s}\right]^{s}}$$

Two-parameter logistic curve with Bretherton limit as $Ca \to 0$

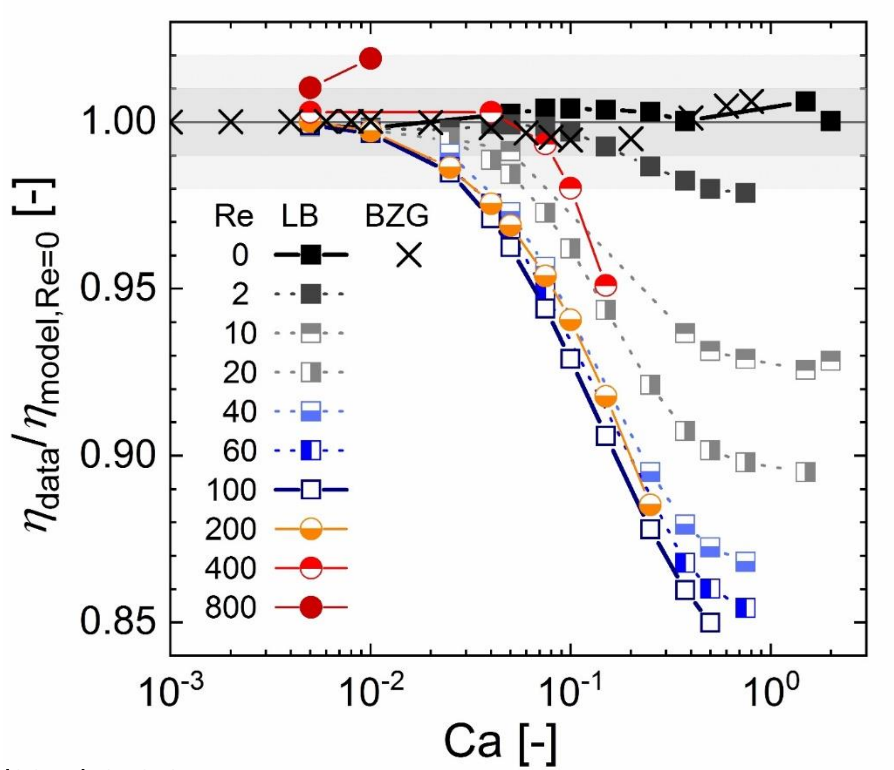
- Regression analysis using ORIGIN



Model for <u>negligible inertia</u> ($Re \to 0$)

- Determine d and s by regression analysis using DNS data
  - Langewisch & Buongiorno (2015), Balestra et al. (2018)
  - Regression gives $s(Re{=}0) = 0.474$ and $d(Re{=}0) = 2.467$

$$\eta_{Re=0} = 1 + \frac{1.467}{\left(1 + 0.28\,Ca^{-1.408}\right)^{0.474}}$$

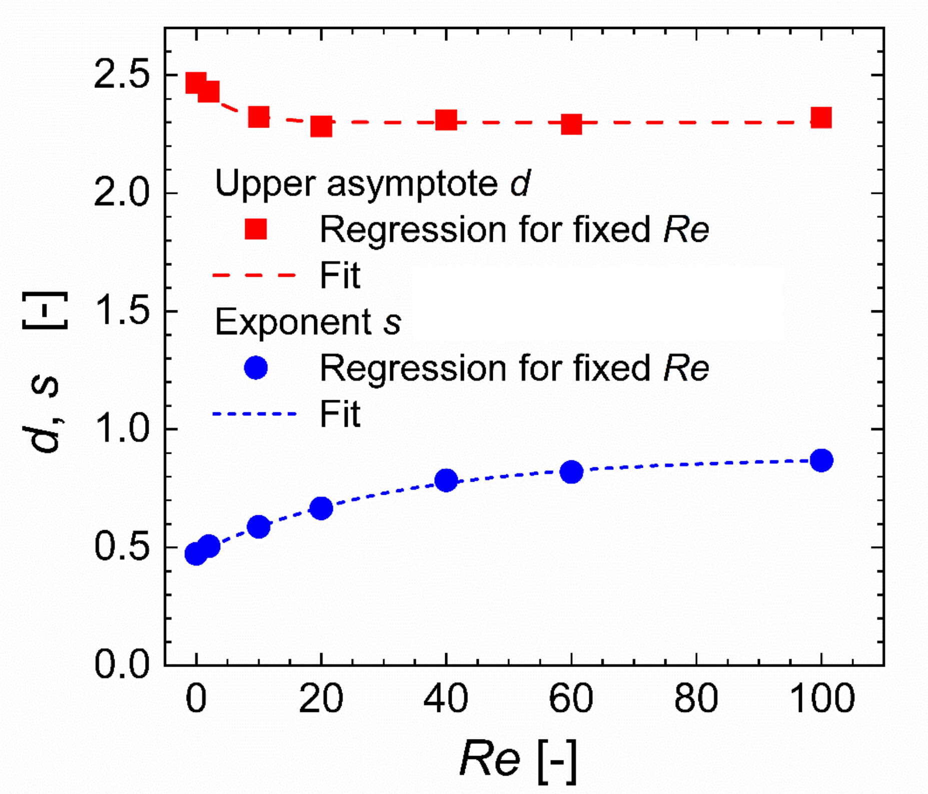


- Comp. model $\leftrightarrow$ DNS data
  - $Re = 0 \rightarrow$ deviation < 1%
  - $Re = 2 \rightarrow$ deviation < 2%
  - Significant deviations for larger values of Re especially at large capillary numbers

📖 D.R. Langewisch, J. Buongiorno, *Int. J. Heat Fluid Flow* **54** (2015) 250-257
📖 G. Balestra, L. Zhu, F. Gallaire, *Microfluidics and Nanofluidics* **22** (2018) 67

Model for finite inertia ($Re \leq 100$)

- Determine d and s by regression analysis using DNS data
  - Langewisch & Buongiorno (2015) data for $Re = 2, 10, 20, 40, 60, 100$
  - For higher values of Re, only few DNS data in small range of Ca



$$d = 2.3 + 0.167 \times 0.83^{Re}$$

$$s = 0.884 - 0.41 \times 0.968^{Re}$$

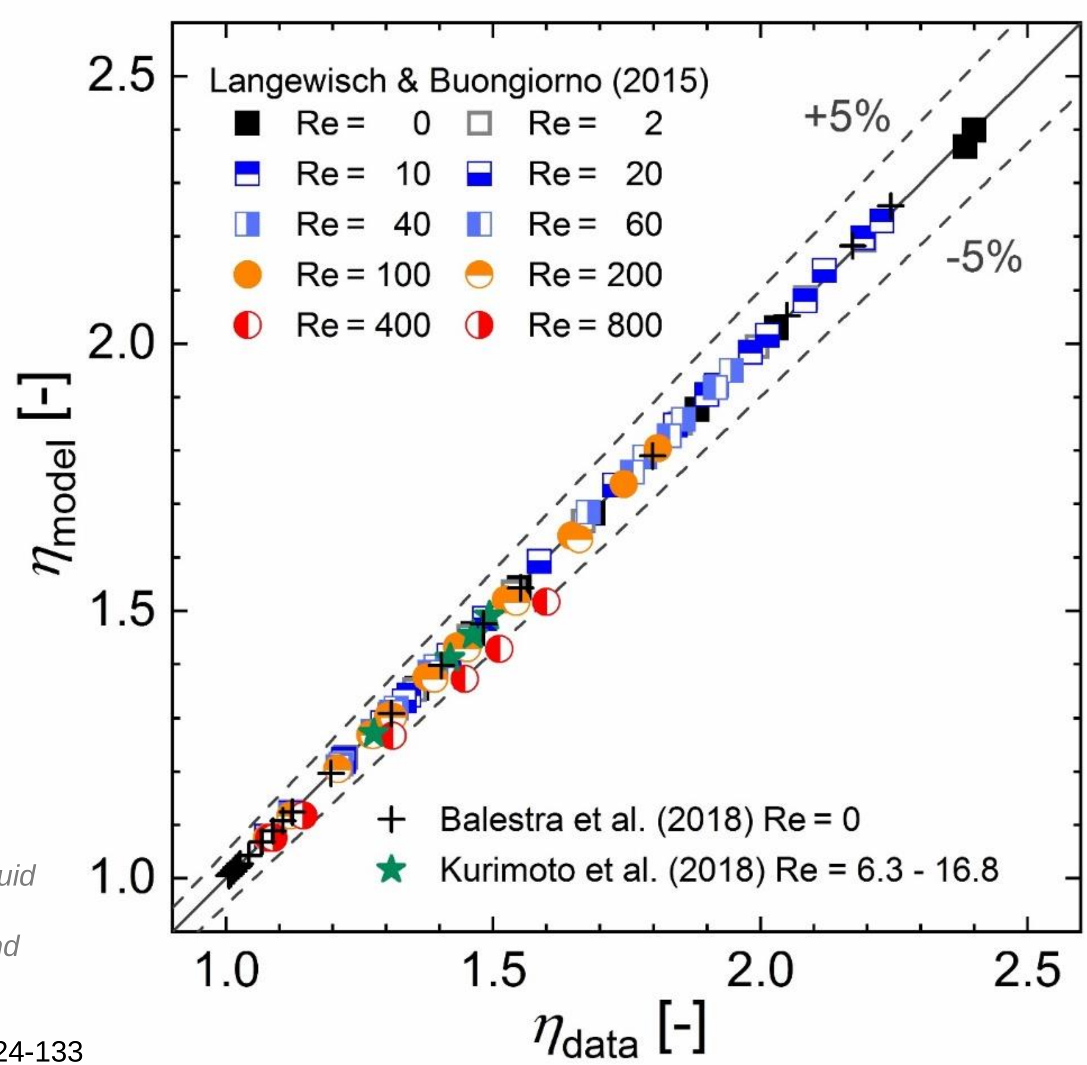
$$\eta_{2\mathrm{PL}} = 1 + \frac{d-1}{\left[1 + \left(\frac{d-1}{1.29}\right)^{1/s} (3Ca)^{-2/3s}\right]^{s}}$$

$$Ca = \mu_L j_T / \sigma, \quad Re = 2\rho_L j_T R / \mu_L$$

New model

Model performance vs. DNS data

- Additional DNS data of Kurimoto et al. (2017) included for comparison
- Excellent agreement over entire range of Ca
  - $Re \leq 2 \quad \rightarrow$ dev. < 1%
  - $Re \leq 100 \rightarrow$ dev. < 2%
  - $Re \leq 800 \rightarrow$ dev. < 5%



📖 D.R. Langewisch, J. Buongiorno, *Int. J. Heat Fluid Flow* **54** (2015) 250-257

📖 G. Balestra, L. Zhu, F. Gallaire, *Microfluidics and Nanofluidics* **22** (2018) 67

📖 R. Kurimoto, K. Nakazawa, H. Minagawa, T. Yasuda, *Exp. Therm. Fluid Sci.* **88** (2017) 124-133

Model performance vs. exp. data

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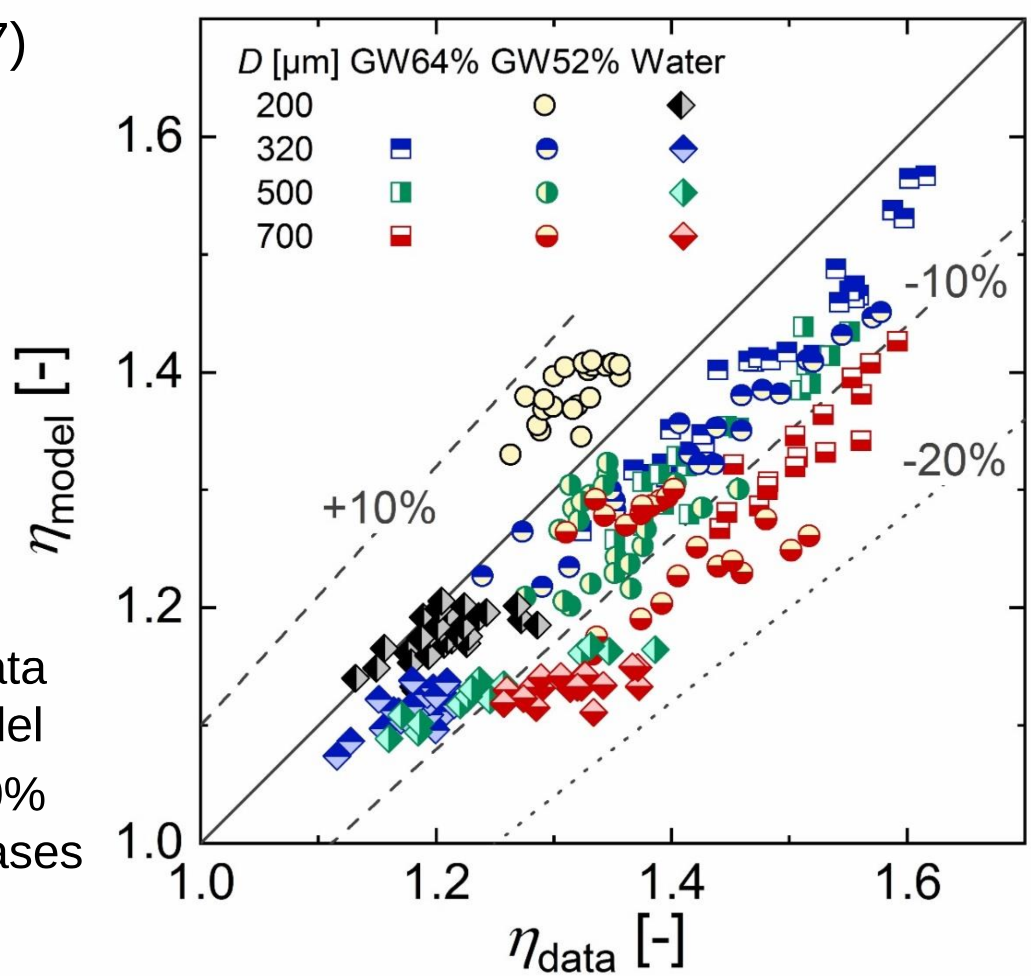
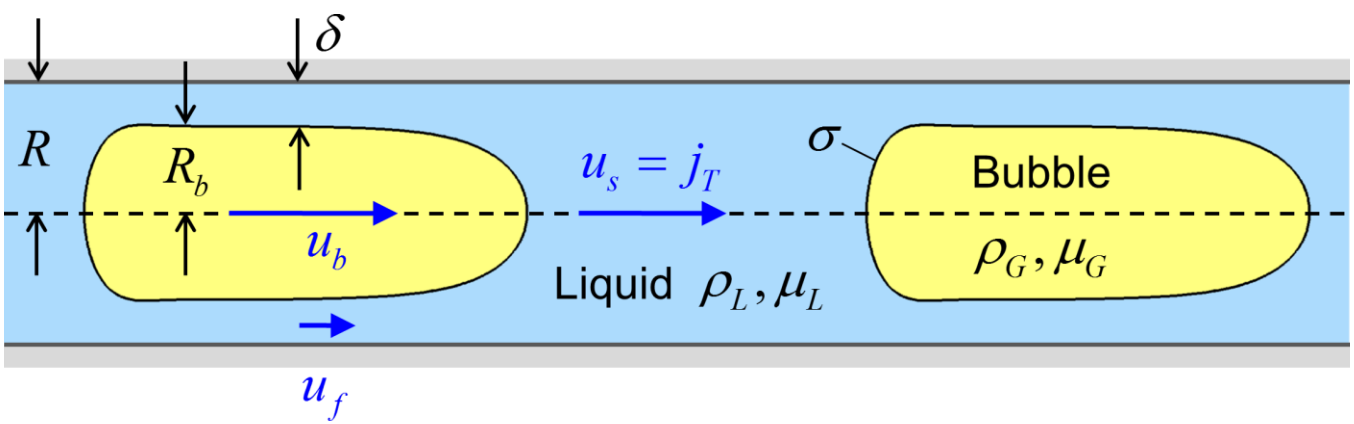
- Exp. by Kurimoto et al. (2017)
- Pipe diameters
  - D = 200, 320, 500, 700 µm
- Liquids
  - Glycerol-water mixture (52 and 64 wt% glycerol)
  - Water
- Reasonable agreement
  - With exception of case GW52%–200µm all exp. data are underestimated by model
  - Deviation mostly within ±10% but up to ±18% for some cases



📖 R. Kurimoto, K. Nakazawa, H. Minagawa, T. Yasuda, *Exp. Therm. Fluid Sci.* **88** (2017) 124-133

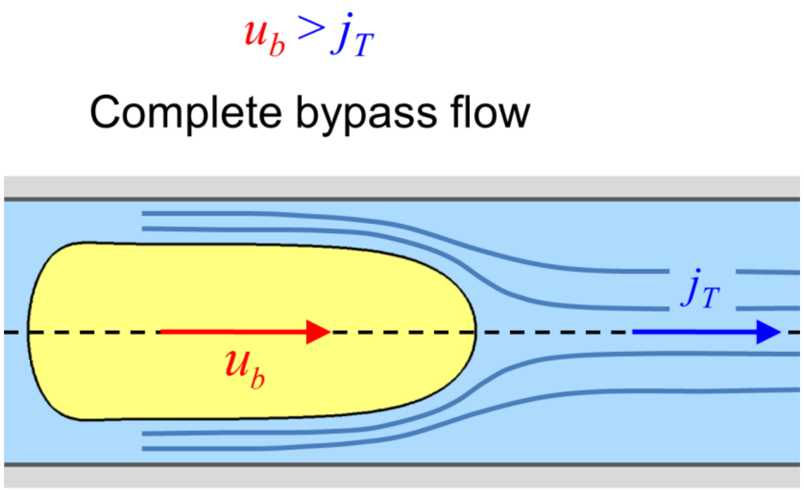
Predicting Taylor flow hydrodynamics

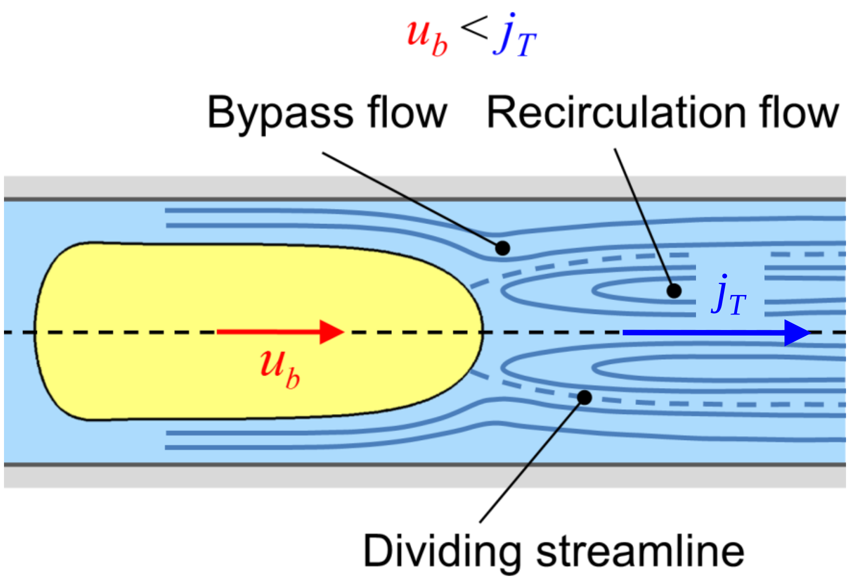
Unknown parameter	Relation with η and β	Condition
Void fraction	$\alpha = \beta / \eta$	
Bubble velocity	$u_b / j_T = \eta$	
Mean liquid velocity	$u_L / j_T = (1-\beta)/(1-\beta/\eta)$	
Slip ratio	$u_b / u_L = (\eta-\beta)/(1-\beta)$	
Relative drift velocity	$m = 1 - \eta^{-1}$	
Bubble radius	$R_b / R = \eta^{-1/2}$	Stagnant liquid film
Liquid film thickness	$\delta / R = 1 - \eta^{-1/2}$	"
Wetting fraction	$w = 1 - \eta^{-1}$	"



Streamline patterns in liquid slug

Unknown parameter	Relation with η
Condition for complete bypass flow	$\eta > 2$
Condition for recirculation region to occur	$\eta < 2$
– Radius of dividing streamline	$R_{ds} / R = (2 - \eta)^{1/2}$
– Radius zero velocity in moving reference frame	$R_0 / R = (1 - \eta /2)^{1/2}$
– Non-dimensional recirculation time	$\tau = (\eta^{-1} - 0.5)^{-1}$





Conclusions and outlook

- The ratio between bubble velocity (u_b) and total superficial velocity of the two-phase flow (j_T) is a key parameter in Taylor flow
- Correlations for this characteristic velocity ratio (η) being valid over the entire range of capillary numbers have been missing so far
- Proposal of a new correlation for η
  - Based on asymmetric sigmoidal curve (5 parameter logistic function)
  - Approaches theoretical relation of Bretherton for low capillary number
  - Correlation relies on prior known parameters only (j_T as velocity scale)
  - Correlation is accurate to about ±5% and ±18% in comparison with numerical (DNS) and experimental data, respectively
  - Should be useful to estimate/predict various hydrodynamic features of Taylor flow such as bubble velocity, liquid film thickness, ...
- Developed 2PL may serve as prototype for similar correlations with larger and/or non-circular channels and liquid-liquid Taylor flow

Thank you for your attention

📖 M. Wörner, *Theoretical Foundations of Chemical Engineering*, accepted

Table 1
Summary of film thickness, bubble velocity, and pressure drop ($\Delta P_b = \frac{\sigma}{R}\Delta P_b^*$) data from Gerris simulations.

Ca	*Re*	δ/D	$U_b/\overline{U}$	ΔP_b^*	*Ca*	*Re*	δ/D	$U_b/\overline{U}$	ΔP_b^*	*Ca*	*Re*	δ/D	$U_b/\overline{U}$	ΔP_b^*
0.005	0	0.0182	1.0771	0.207	0.040	300	0.0601	1.2922	1.742	0.150	0	0.1151	1.6876	2.006
0.005	20	0.0181	1.0766	0.212	0.040	400	0.0634	1.3116	1.883	0.150	2	0.1130	1.6692	1.975
0.005	50	0.0181	1.0767	0.217	0.050	0	0.0710	1.3583	0.791	0.150	20	0.1031	1.5868	2.032
0.005	100	0.0182	1.0771	0.230	0.050	2	0.0703	1.3539	0.789	0.150	100	0.0949	1.5233	1.571
0.005	160	0.0184	1.0778	0.247	0.050	4	0.0698	1.3505	0.771	0.150	200	0.0975	1.5434	1.627
0.005	200	0.0185	1.0783	0.258	0.050	6	0.0694	1.3484	0.776	0.150	300	0.1013	1.5729	2.080
0.005	300	0.0188	1.0797	0.285	0.050	8	0.0690	1.3459	0.786	0.150	400	0.1046	1.5993	1.644
0.005	400	0.0192	1.0814	0.315	0.050	10	0.0685	1.3430	0.793	0.250	0	0.1355	1.8821	3.597
0.005	800	0.0209	1.0893	0.477	0.050	20	0.0670	1.3337	0.867	0.250	2	0.1325	1.8510	3.499
0.010	0	0.0279	1.1219	0.304	0.050	40	0.0645	1.3181	0.932	0.250	20	0.1197	1.7282	3.346
0.010	2	0.0279	1.1218	0.306	0.050	60	0.0631	1.3100	1.037	0.250	40	0.1141	1.6789	3.103
0.010	20	0.0278	1.1214	0.315	0.050	80	0.0623	1.3049	1.151	0.250	100	0.1104	1.6469	3.364
0.010	60	0.0277	1.1206	0.336	0.050	100	0.0622	1.3041	1.267	0.250	200	0.1120	1.6608	3.008
0.010	100	0.0276	1.1202	0.360	0.050	120	0.0620	1.3033	1.392	0.375	0	0.1490	2.0297	5.905
0.010	120	0.0276	1.1201	0.373	0.050	140	0.0622	1.3046	1.487	0.375	2	0.1459	1.9937	5.714
0.010	140	0.0276	1.1202	0.387	0.050	160	0.0626	1.3065	1.554	0.375	10	0.1374	1.9010	5.428
0.010	160	0.0276	1.1204	0.403	0.050	180	0.0630	1.3092	1.592	0.375	20	0.1315	1.8412	5.317
0.010	180	0.0277	1.1205	0.418	0.050	200	0.0636	1.3129	1.662	0.375	40	0.1257	1.7845	5.373
0.010	200	0.0277	1.1209	0.434	0.050	220	0.0642	1.3166	1.681	0.375	60	0.1232	1.7611	5.322
0.010	300	0.0282	1.1233	0.520	0.050	240	0.0648	1.3200	1.658	0.375	80	0.1220	1.7498	5.140
0.010	600	0.0308	1.1354	0.930	0.050	260	0.0654	1.3238	1.849	0.375	100	0.1214	1.7445	5.402
0.010	800	0.0328	1.1454	1.209	0.050	280	0.0663	1.3291	1.845	0.500	2	0.1537	2.0849	8.076
0.010	900	0.0340	1.1511	1.318	0.050	300	0.0670	1.3332	1.767	0.500	10	0.1448	1.9818	7.731
0.025	2	0.0480	1.2239	0.499	0.075	0	0.0866	1.4626	1.061	0.500	20	0.1390	1.9183	7.578
0.025	5	0.0478	1.2229	0.505	0.075	2	0.0854	1.4547	1.058	0.500	40	0.1330	1.8565	7.600
0.025	10	0.0475	1.2211	0.514	0.075	20	0.0800	1.4172	1.172	0.500	60	0.1304	1.8299	7.472
0.025	20	0.0473	1.2199	0.545	0.075	40	0.0764	1.3935	1.264	0.500	80	0.1290	1.8159	7.308
0.025	40	0.0464	1.2151	0.582	0.075	60	0.0747	1.3821	1.416	0.500	100	0.1282	1.8084	6.918

📖 D.R. Langewisch, J. Buongiorno, *Int. J. Heat Fluid Flow* **54** (2015) 250-257

Master curve for correlation

- Sigmoid curve = a monotonic function $y(x)$ that is constrained by a pair of horizontal asymptotes as $x \to \pm\infty$
- Four parameter logistic function (4PL)
  - a = lower asymptote
  - d = upper asymptote ($d > a$)
  - b = slope factor ($b > 0$)
  - c = mid-range abscissa (inflection point, $c > 0$)

$$y_{4\mathrm{PL}} = d + \frac{a-d}{1+(x/c)^b}$$

https://www.biolegend.com/newsdetail/5468