Supplementary Information (SI) for Digital Discovery.

Supplementary Information for Opentrons for Automated and High-Throughput Viscometry

Beatrice W. Soh[1], Aniket Chitre[2], Shu Zheng Tan[3], Yuhan Wang[1], Yinqi Yi[1], Wendy Soh[3], Kedar Hippalgaonkar[1,3] and D. Ian Wilson[2]

*[1]Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A*STAR), Singapore 138634, Singapore*

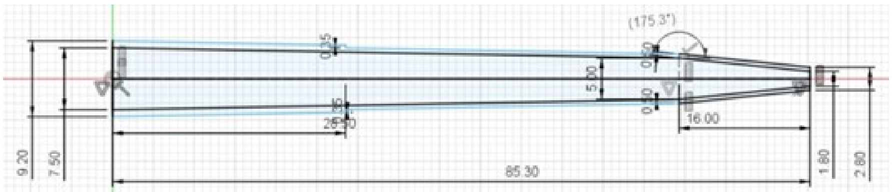
[2]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, United Kingdom

[3]Department of Materials Science and Engineering, Nanyang Technological University, Singapore 117575, Singapore

1. Pipette Tip Schematics

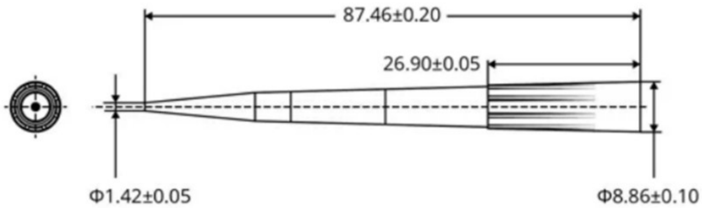
All dimensions in mm.

Fisher Scientific wide bore 1000 μL tip:



Opentrons 1000 μL pipette tip (reproduced from https://www.genfollower.com/1000ul-pipette-tip-for-opentrons/):

External geometry

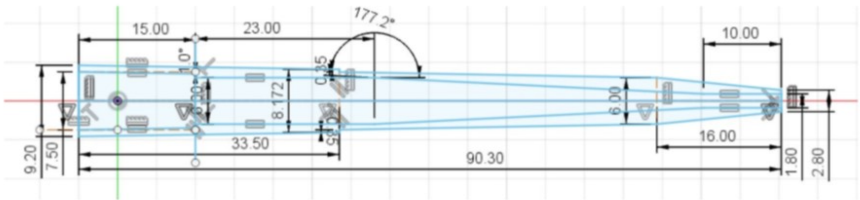


Internal geometry

Custom pipette design – reproduced from Soh *et al.*:

---

[1] Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A∗STAR), Singapore 138634, Singapore
[2] Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, United Kingdom


15.00
23.00
177.2°
10.00
1.0°
0.35
8.172
6.00
33.50
16.00
9.20
7.50
90.30
1.80
2.80

2. Viscosity Standards (Newtonian liquids)

Table S1. List of Newtonian viscosity standards used in experiments

Viscosity (cP)
28.5
99.8
204.8
398.4
505.4
817.4
1021
1275
1525
1925
2096
2375
2615
3032
3083
3405
3792
3941
4804
4928
5095
5291
5464
5882
5921
6033
6226
6695
6698
6813
7000
7782
7982
8254
9002
9884
11470
14020
15900
20960

3. Detailed method for training regression models

The datasets corresponding to different flow rates (10, 20, 50, 65, and 80 μL/s) were independently pre-processed and used to train separate models. Each flow rate dataset was standardized independently by removing the mean and scaling to unit variance. Within each flow rate dataset, the data was split into training and testing sets using stratified sampling to ensure a consistent distribution of viscosities across splits. Specifically, we binned the viscosities into 5 different bins and stratified the split according to the bin number.

A grid search was performed to tune hyperparameters for each model, trained on each individual flow rate dataset. For support vector regression (SVR), the parameters C and gamma were optimized over different kernels; for ridge regression, the alpha parameter was optimized; for Gaussian process regression (GPR), the parameters alpha and number of restarts of the optimizer were optimized over different kernels. Cross-validation (5-fold) was used within the grid search to evaluate model performance and the final models were trained using the optimal hyperparameters identified through the search.

4. Derivation of Newtonian result

The model is based on a statement of volume conservation

$$Q_p - \frac{V_0 P_0 dP_{in}}{P_{in}^2 \; dt} - \left(\frac{P_{in} - P_{atm}}{B}\right)^{\frac{1}{n}} = 0 \tag{8}$$

The pressure drop – flow rate result, Eqn. (6), for a Newtonian fluid takes the form

$$P_{in} - P_{atm} = \beta \mu Q_L \tag{S1}$$

with β the product of the geometrical factors. For the Thermo Scientific 1000 μL wide bore pipette tip β = 15×10^9. The linearity of Eqn. (S1) allows Eqn. (8) to be written as

$$Q_p - \frac{V_0 P_0}{P_{in}^2} \beta \mu \frac{dQ_L}{dt} - Q_L = 0 \tag{S2}$$

Setting $Q^* = Q_L / Q_P$ and rearranging

$$Q^* + \frac{dQ^*}{dt}\left[\frac{\beta \mu V_0 P_0}{P_{in}^2}\right] - 1 = 0 \tag{S3}$$

Substituting for P_{in} within the term in square brackets yields, after some manipulation

$$Q^* + \frac{dQ^*}{dt}\left[\frac{V_0 P_0}{\beta \mu Q_P^2}\right] \frac{1}{\left(Q^* + P_{atm}/\, \beta \mu Q_p\right)^2} - 1 = 0 \tag{S4}$$

This can be written in dimensionless form, *viz*.

$$\frac{dQ^*}{d\tau} \frac{1}{\left(Q^* + c\right)^2} = 1 - Q^* \tag{S5}$$

with $c = P_{atm}/\, \beta \mu Q_p$ and τ dimensionless time, with characteristic timescale $t_C = V_0 P_0 /\, \beta \mu Q_P^2$. Substituting for Q^* using $\theta = 1 - Q^*$ gives

$$-\frac{d\theta}{d\tau} = \theta(c + 1 - \theta)^2 = \theta(c' - \theta)^2 \tag{S6}$$

where $c' = c + 1$. This first order ordinary differential equation can be solved using partial fractions,

$$d\tau = \left\{ \frac{-1}{c'^2(c'-\theta)} - \frac{1}{c'(c'-\theta)^2} - \frac{1}{c'^2\theta} \right\} d\theta \tag{S7}$$

The solution is

$$\tau + k = \frac{1}{c'^2}\left\{ ln(c'-\theta) - \frac{c'}{(c'-\theta)} - ln\theta \right\} \tag{S8}$$

Setting initial condition $Q_L = 0$ at $t = 0$ $(\theta = 1, \tau = 0)$ gives the result

$$\tau = \frac{1}{c'^2}\left\{ ln\frac{(c'-\theta)}{\theta(c'-1)} - \frac{c'}{(c'-\theta)} - \frac{c'}{(c'-1)} \right\} \tag{S9}$$

Approximate result

Since $0 \le Q^* \le 1$, an approximate result can be obtained when $c' \gg 1$. Eqn. (S5) collapses to

$$\frac{dQ^*}{d\tau} \cong c^2(1 - Q^*) \tag{S10}$$

with solution, when $Q_L(0) = 0$, is

$$Q_L = Q_P\{1 - exp(-c^2\tau)\} \tag{S11}$$

Now

$$c^2\tau = \left(\frac{P_{atm}}{\beta\mu Q_p}\right)^2 \frac{t}{t_C} = \left(\frac{P_{atm}}{\beta\mu Q_p}\right)^2 \frac{\beta\mu Q_P^2}{V_0 P_0} t \tag{S12}$$

Assuming $P_0 \sim P_{atm}$

$$c^2\tau \approx \frac{P_{atm}}{\beta\mu V_0} t \equiv \varphi t \tag{S13}$$

The average volumetric flow rate in a test of duration t_E is given by

$$\bar{Q} = \frac{V(t_E)}{t_E} = \frac{Q_P}{t_E}\int_0^{t_E} \{1 - exp(-\varphi t')\} dt' \tag{S14}$$

with solution

$$\bar{Q} = \frac{Q_P}{\varphi t_E}\left\{ e^{-\varphi t_E} + \varphi t_E - 1 \right\} \tag{S15}$$

Substituting the truncated Taylor series $e^{-\varphi t_E} = 1 - \varphi t_E + \frac{1}{2}(\varphi t_E)^2 - \frac{1}{6}(\varphi t_E)^3$

$$\frac{\bar{Q}}{Q_P} = \left\{\frac{\varphi t_E}{2} - \frac{(\varphi t_E)^2}{6}\right\} \tag{S15}$$

For the example case, $\varphi = P_{atm}/\beta\mu V_0 = 10^5/(15 \times 10^9 \times 6 \times 2000 \times 10^{-9}) =$ 0.56 s^{-1}.