Modelling the fermentation process in the brewing industry

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The fermentation process in brewing is modelled using Langevin's equations. They are solved by an Euler-Mayruma scheme and the density is found to follow a normal distribution with increasing variance. An advection-diffusion equation is recovered and using pseudospectral methods it is solved on a brewing cylinder composed by three quadrilaterals. The sedimentation time is found to be 5 time units at which point 70 % has sedimented in the two bottom shapes.

In the brewery, one is interested in producing beer as quickly as possible with minimal contamination risks[9]. To fully model the fermentation process one would require to do experiments with ethanol rate, CO_2 concentration etc[10]. This project does not aim to propose such a full model but to use basic dynamical-density functional theory (DDFT) to study the concentration of yeast and sedimentation time on a realistic geometry.

In the fermentation process, yeast particles of size 1 mm[4] are suspended in water molecules of size 1 nm[11]. Larger particles suspended in smaller ones were already studied by Robert Brown in 1827 when he discovered that pollen travelled in water according to Brownian motion[5]. Einstein showed in 1905 that Brownian particles give rise to a diffusion equation for the density[1] whose exact solution is a normal distribution with variance $2Dt$, where D is a diffusion coefficient depending on measurable factors.

The difference in mass between the yeast particles and water molecules means the latter will move much faster. The difference in scale makes the problem practically impossible to solve exactly[7]. However, it allows us to approximate the collisions of yeast particles and water molecules as noise $\mathbf{f}$, a normally distributed random variable which is independent in time and space, and thereby obtain a model for only the yeast particles. The position $\mathbf{r} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$ and momentum $\mathbf{p} = (\mathbf{p}_1, \ldots, \mathbf{p}_N)$ of N yeast particles can be described by Langevin's equations[2],

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{m}, \quad \frac{d\mathbf{p}}{dt} = -\nabla_{\mathbf{r}} V(\mathbf{r}, t) - \gamma(\mathbf{r})\mathbf{p} + A(\mathbf{r})\mathbf{f}(t). \quad (1)$$

where m is the mass, γ is friction, V a potential (e.g electric charge) and $A = \sqrt{2mk_BT\gamma}$ where T is absolute temperature and k_B Boltzmann's constant. As no experiments have been done and to avoid a small scale, we set $m = k_BT = 1$.

Equation (1) has no analytic solution even for two particles and we thus turn to numerical methods. An Euler-Mayruma scheme is applied with 1000 timesteps and 30 particles with $\gamma = 3$ and $V(\mathbf{r}, t) = 2(0.045\mathbf{r}^4 - \mathbf{r}^2)$. For each particle, the initial position, momentum and random force are generated from the distribution $N(0, 1)$ and Equation (1) is solved for each time step. This is iterated

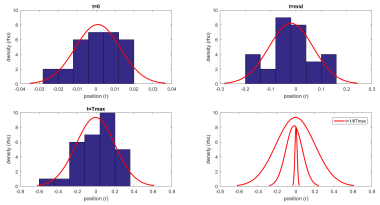


FIG. 1. Density of particles as function of position

100 times and an average of positions at the timesteps is taken. The distribution of the positions of the particles $\mathbf{r}$ (one of the space coordinates in fact) at $0.1, 0.3$ and 2 seconds is shown Figure 1. It seems to follow a normal distribution with increasing variance, which agrees with Einstein's solution of the Brownian motion problem[1].

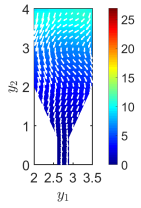
Even with a numerical method, Langevin's equations are computationally intensive[2]. For an overdamped system, that is $\gamma >> 1$, one can approximate Langevin's equations with an advection-diffusion equation for the particle density. To model a brewing process, we would like to solve it on a geometry as in Figure 2. Basic DDFT and pseudo-spectral methods allow us to do this. Using code base developed by Ben Goddard and Andreas Nold at Imperial College in 2013 and ideas in [3], the diffusion equation

$$\frac{\partial \rho}{dt} = D\frac{\partial^2 \rho}{\partial t^2}, \rho(\text{boundary}) = 0, \rho(0) = \exp\left(-\frac{y^2}{4Dt}\right) \quad (2)$$

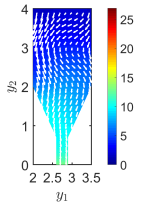
where y is position, is solved on an infinite line, semi-infinite line with different boundary conditions and a square. The equation is solved on $[-1, 1]$ ($[-1, 1] \times [-1, 1]$ in two dimensions) and a mapping is used to go to the physical space. 30 collocation points are used to approximate the solution. The solution is shown in Figure 3, 4, 5, 6, 7 and 8. It starts with a Delta distribution and the variance increases with time so that the density converges to zero. Note that this agrees with the stochastic analysis carried out in Figure 1. To model yeast sedimentation in a brewing cylinder, an advection-diffusion equation

$$\frac{\partial \rho}{dt} = \Delta\rho + \text{div}(-\rho v + g + \rho M\rho), \quad (3)$$

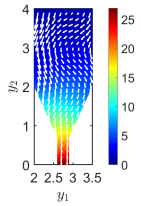
where M is a linear operator, was solved on three quadrilaterals glued together as in Figure 2. The density was forced to agree where the shapes are joined and no flux was applied on left, right, top and bottom. Different initial conditions, inflows, velocity flows and gravity strengths were tried to obtain a reasonable result.



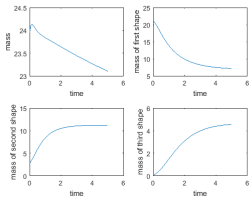
(a) $t = 0.1$



(b) $t = 0.15$



(c) $t = 2$



(d) Mass diagram for the subshapes

FIG. 2. Model of yeast sedimentation. Polynomial initial condition, velocity flow $v_1 = 0.2y_2 \sin(y_2\pi)$ in horizontal direction and $v_2 = 0.2y_2 \cos((y_1+1)\pi) - 1$ in vertical direction, gravity 0.2.

The evolution of density in space (shown by colour) and the mass at each of the three subshapes are shown in Fig 2. After around 5 time units, 70 % of the yeast had sedimented in the bottom two shapes and an equilibrium was attained. More complicated geometries such as a loop, hole, two joined squares and a U-formation were also considered and the result is shown in Figure 9. It was noted the density often builds up near a wall. The pseudo-spectral method is accurate but rather expensive. Figure 10 shows that the running time is linear and Figure 11 that the error converges to 0 exponentially. The drawback of this method is the instability which boundaries introduce. It was noted that 20 % of the mass seemed to disappear, due to no flux boundary conditions. The gluing technique was explored by cutting a 3×3 square into quadrilaterals in different ways as in 12(b). The computation time as function of number of boundaries is shown in Figure 12(a). For 3 boundaries or less, the problem is solved quickly but with more boundaries, the running time increases rapidly. The pseudo-spectral technique used here extends to other physical systems. By using a strip, one can model flows in blood vessels. With more complicated physical systems, e.g with a sophisticated potential in Equation (1), more interesting dynamics is likely to appear and equilibriums can be studied[2].

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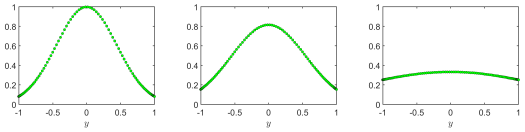
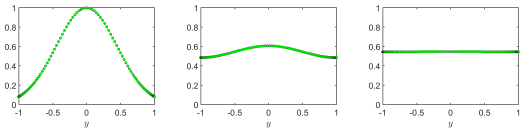
Appendix A: Solutions to the diffusion equation on different geometries and boundary conditions



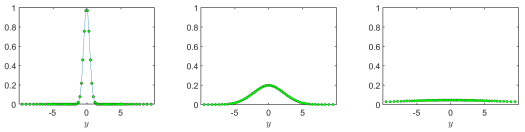
(a) $t = 0.1$ (b) $t = 0.15$ (c) $t = 2$

FIG. 3. $[-1, 1]$, Dirichlet boundary conditions, (density as a function of position)



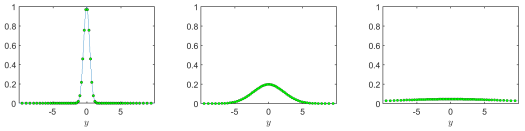
(a) $t = 0.1$ (b) $t = 0.15$ (c) $t = 2$

FIG. 4. $[-1, 1]$, no flux



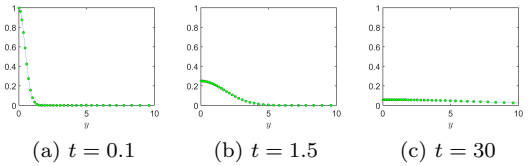
(a) $t = 0.1$ (b) $t = 0.15$ (c) $t = 2$

FIG. 5. real line, Dirichlet boundary conditions



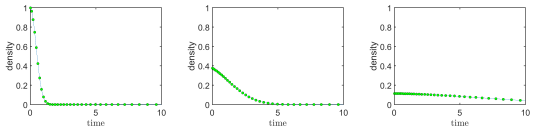
(a) $t = 0.1$ (b) $t = 2.5$ (c) $t = 50$

FIG. 6. real line, no flux



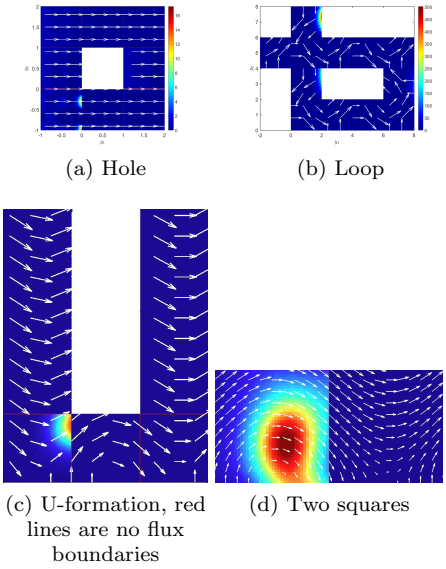
(a) $t = 0.1$ (b) $t = 1.5$ (c) $t = 30$

FIG. 7. $[0, \infty)$, Dirichlet boundary conditions



(a) $t = 0.1$ (b) $t = 1.5$ (c) $t = 30$

FIG. 8. $[0, \infty)$, no flux

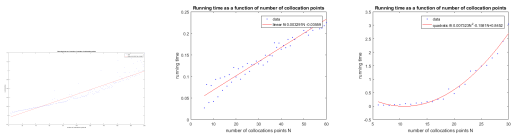


(a) Hole (b) Loop

(c) U-formation, red lines are no flux boundaries (d) Two squares

FIG. 9. The advection-diffusion equation solved on complicated geometries. The density profile shown for the final time $t = 3$. Matching boundary conditions and exponential initial condition used.

Appendix B: Running time and error for pseudo-spectral method



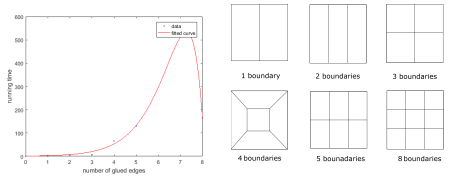
(a) interval, no flux (b) real line, no flux (c) box, no flux

FIG. 10. Running time as function of number of collocation points

(a) real line, Dirichlet (b) real line, no flux (c) $[0, \infty)$

FIG. 11. Error as function of number of collocation points

Appendix C: Cost of gluing technique



(a) Running time as a function of number of boundaries

(b) Gluing of shapes

FIG. 12. Cost of gluing shapes with matching boundary conditions