

Mathematical Modelling 2016

Group 9

Student numbers 741731, 750345, 701017, 740130, 759161

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Abstract

In this report a simplified diesel filter, the velocity field in the channel with the filter and the accumulation of soot particles in the filter is studied. The model is studied at different levels of simplifications, where at the end the flux is taken into consideration. When studying the accumulation of particles it was shown that a hexagon shaped channel will be the most efficient one.

Contents

0	Introduction	1
1	Filter Efficiency	1
2	Modeling Equation for Gas in Channels	1
3	Approximation of the Viscous Force in Channel	2
3.1	Poisson Equation	2
3.2	a for Specific Shapes	2
4	One Dimensional Approximation of the Channel	3
4.1	Relation Between One- and Three-Dimensional Model	3
4.2	Steady State	4
4.3	Perturbation Around the Stationary State	4
5	Mass Loss From the Wall	5
6	Porous Medium Layer	5
6.1	Incoming Flux	5
7	Accumulation of Particles Due To Diffusion	5
7.1	Model and Simplifications, The Two Dimensional Case	6
7.2	Examining the Two Dimensional Case and Expanding to Three Dimensions	6
7.3	Hexagon	6
7.4	Evaluation	7

0 Introduction

The combustion of fuel in a diesel motor happens at high pressure and temperature but is often incomplete. To avoid emitting the resulting soot particles to the environment, a filter that contains channels in a honeycomb structure is used. Throughout this paper the longitudinal direction of the channel is called direction 1 or x. Each channel is either open to the inlet of gas from the motor or to the outlet of gas to the environment, such that the gas must go into the inlet channel, through the filter wall to the outlet channel and out of the outlet channel. One option is that the inlet channel is a square such that the outlet channel is also a square. Another option is that the outlet channel is one big box with inlet channels with filter walls placed into the box. In the latter case the inlet channel can for instance have a circular or hexagonal shape. First off in this report our results of questions 1 through 6 are presented. In the last section accumulation of soot particles due to diffusion has been explored, and the results are presented and discussed.

1 Filter Efficiency

The velocity and the pressure of the gas before and after the filter can be measured, but this is not enough to compute the energy consumed by the filter. Buckingham's pi theorem gives that any physical relation between n objects is equivalent to a relation between $n - r$ dimensionless variables, where r is the number of dependent dimensions. The units of the parameters are $[E] = kgm^2s^{-2}$, $[u] = ms^{-1}$, $[p] = kgm^{-1}s^{-2}$. With three different SI units and the same number of parameters there are no independent dimensions. Energy can not be evaluated from only velocity and pressure as no physical relation can exist with only those three as parameters.

The parameters that play a role are pressure p , velocity u , energy E , channel diameter D , channel length L , channel roughness e , viscosity μ and fluid density ρ . The dimension matrix of the problem is

$$A = \begin{bmatrix} & E & p & u & D & L & e & \mu & \rho \\ kg & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ m & 2 & -1 & 1 & 1 & 1 & 1 & -1 & -3 \\ s & -2 & -2 & -1 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}$$

which has rank $r = 3$. This gives that there are $8 - 3 = 5$ dimensionless combinations. u , D and ρ are chosen as core variables as these are independent

columns. This gives the following dimensionless variables

$$\begin{aligned} \pi_1 &= \frac{E}{u^2 D^3 \rho} \\ \pi_2 &= \frac{p}{u^2 \rho} \\ \pi_3 &= \frac{L}{D} \\ \pi_4 &= \frac{e}{D} \\ \pi_5 &= \frac{\mu}{uD\rho} \end{aligned}$$

such that an expression for E will be on the form

$$E = u^2 D^3 \rho \psi\left(\frac{p}{u^2 \rho}, \frac{L}{D}, \frac{e}{D}, \frac{\mu}{uD\rho}\right).$$

2 Modeling Equation for Gas in Channels

To model the gas in the channel we turn to the equations for conservation of material variables. First we will derive the conservation equation for mass by considering what goes in and what comes out of an arbitrary volume V in the channel. The total mass inside this volume will be given by $\int_V \rho dV$. Assuming ρ is sufficiently smooth¹, the rate of decrease of mass can thus be expressed as

$$-\frac{d}{dt} \int_V \rho dV = - \int_V \frac{\partial \rho}{\partial t} dV.$$

For mass to be conserved, this equation has to equal the total rate of mass flux out of V , which can be expressed as $\int_{\partial V} \rho \mathbf{u} \cdot \mathbf{n} d\sigma$ or by Greens theorem, as $\int_V \nabla \cdot (\rho \mathbf{u}) dV$. Hence

$$- \int_V \frac{\partial \rho}{\partial t} dV = \int_V \nabla \cdot (\rho \mathbf{u}) dV,$$

or also

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

as we assume the integrands are sufficiently smooth.

¹Volumes with different number of soot particles might have different mass density if the densities of the fluid is different from that of the soot. In addition the fluid (air) might be compressible. If the soot particles are homogenously mixed in the fluid, and each soot particle is small compared to the scale of the channel, $\rho(t)$ will be sufficiently smooth.

Newtons second law states that the sum of the forces on an object equals the time derivative of its momentum; $F = \frac{d}{dt}(m\mathbf{u})$. The momentum is also a material variable, and will be conserved. Defining $R(t)$ to be a moving region in the channel that always contains the same gass and soot particles, Newtons second law can be written as

$$\mathbf{F} = \frac{d}{dt} \int_{R(t)} \rho \mathbf{u} dV .$$

$R(0) = V$ at $t = 0$, is an arbitrary continuous volume

$$\mathbf{F} = \frac{d}{dt} \int_V \rho \mathbf{u} dV + \int_{\partial V} (\rho \mathbf{u})(\mathbf{u} \cdot \mathbf{n}) d\sigma$$

by Reynolds theorem of transportation. Using Greens theorem and assuming sufficient smoothness, this can be expressed as a volumetric force

$$\mathbf{f} = (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u}^T \mathbf{u}) , \quad (2)$$

where $\mathbf{u}^T \mathbf{u}$ is a three by three matrix.

Again, considering an arbitrary volume in the channel, the forces on this object are due to viscosity, pressure and gravity. In addition the acceleration of the car will act as a force, as our coordinate system is accelerated along with the car. In this analysis we will only take pressure and viscosity into account. The viscous force is

$$\begin{aligned} & \int_{\partial V} (\lambda(\nabla \cdot \mathbf{u}) \cdot \mathbf{n} + 2\mu \epsilon(\mathbf{u}) \cdot \mathbf{n}) d\sigma \\ &= \int_V (\lambda \nabla \cdot (\nabla \mathbf{u}) d\Omega + 2\mu \nabla \cdot \epsilon(\mathbf{u})) dV , \end{aligned}$$

where $\epsilon(\mathbf{u})$ is

$$\epsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) . \quad (3)$$

Hence the sum of forces is

$$\mathbf{F} = \int_V (-\nabla p + \lambda \nabla(\nabla \cdot \mathbf{u}) + 2\mu \nabla \cdot \epsilon(\mathbf{u})) dV ,$$

which can be written as a volumetric force

$$\mathbf{f} = -\nabla p + \lambda \nabla(\nabla \cdot \mathbf{u}) + 2\mu \nabla \cdot \epsilon(\mathbf{u}) . \quad (4)$$

This is equal to the expression in equation (2). The channel has two boundaries; the end wall and the inlet point. Assuming the pressure is constant, then at the inlet point the boundary condition is $\frac{\partial p}{\partial x} = 0$, and the only force is due to viscosity. The end wall will stop the liquid and impose a no flux boundary condition such that the viscous forces are zero.

3 Approximation of the Viscous Force in Channel

Now consider a simplified model with incompressible gass flowing through an infinitely long channel with no flux through the walls, such that after steady state is reached the velocity \mathbf{u} does not vary in the longitudinal direction. For this to be true the transversal component of the velocity must be 0 and there is no acceleration of particles in the longitudinal direction through a slice of the channel. This means that the force on each particle is $\mathbf{f} = 0$, and that $\nabla \cdot \mathbf{u} = 0$.

3.1 Poisson Equation

By considering this infinite channel in one-dimesion equation (4) and (3) can be re-written as

$$0 = -\frac{\partial p}{\partial x} + \mu \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) , \quad (5)$$

where $u_2 = 0$ and $u_3 = 0$. Since $\frac{\partial \mathbf{u}}{\partial x} = 0$, the last term in (5) will be

$$\nabla \cdot (\nabla \mathbf{u})^T = \begin{bmatrix} \frac{\partial^2 u_1}{\partial x^2} + \frac{\partial^2 u_2}{\partial x \partial y} + \frac{\partial^2 u_3}{\partial x \partial z} \\ \frac{\partial^2 u_1}{\partial y \partial x} + \frac{\partial^2 u_2}{\partial y^2} + \frac{\partial^2 u_3}{\partial y \partial z} \\ \frac{\partial^2 u_1}{\partial z \partial x} + \frac{\partial^2 u_2}{\partial z \partial y} + \frac{\partial^2 u_3}{\partial z^2} \end{bmatrix} = \vec{0} .$$

Equation (5) is then reduced to

$$\mu \left(\frac{d^2 u}{dy^2} + \frac{d^2 u}{dz^2} \right) = \frac{\partial p}{\partial x} .$$

Since $\nabla f = 0$ it follows that $\nabla^2 p = 0$ and ∇p is a constant. We can write

$$\mu \nabla^2 u = -a \bar{u} \quad (6)$$

where the Laplace operator is in the two directions of the cross section we are studying and

$$\bar{u} = \frac{1}{|\Omega|} \int_{\Omega} u dA , \quad (7)$$

the average velocity on the surface. The number a will depend on the shape and area, and we can find it by solving the Poisson equation $\nabla^2 u = \frac{-\alpha}{\mu}$ with $\alpha = a\bar{u}$.

3.2 a for Specific Shapes

When the cross section Ω is a circle with radius R , the solution to the Poisson equation is

$$u = \frac{-\alpha}{4\mu} (y^2 + z^2 + R^2) .$$

To find the constant a in equation (6) in this case, we use (7) to find

$$\bar{u} = \frac{1}{\pi R^2} \int_{\theta=0}^{2\pi} \int_{r=0}^1 -\frac{\alpha}{4\mu} (r^2 - R^2) r \, dr \, d\theta$$

$$\bar{u} = \frac{\alpha R^2}{8\mu} = \frac{a R^2 \bar{u}}{8\mu}$$

so $a = \frac{8\mu}{R^2}$.

Table 1: Table of a/μ for different shapes

Shape	a/μ
Circle	25.14
Hexagon	27
Square	28.5
Triangle	36

For other cross sections, the ratio was found using finite element method in matlab. The results are in table 1, where each cross section has area 1. As expected, the ratio increases as the ratio of circumference to area increases. This is due to the fact that higher circumference and smaller area leads to the no-slip condition at the boundary having a bigger effect.

In figure 1 the solution to the Poisson equation on a hexagon shaped cross section is displayed. Figure

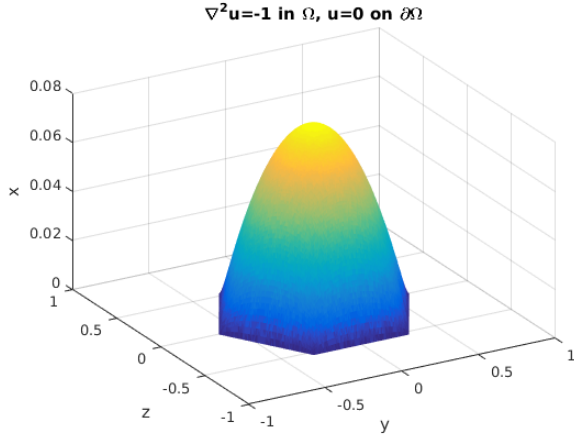


Figure 1: Hexagon

2 shows the results on a square channel. In both figures it is clear that the velocity is at the highest in the center of the channel, which is what one would expect. Homogeneous Dirichlet boundary conditions are used in both models, which corresponds to the no-slip condition.

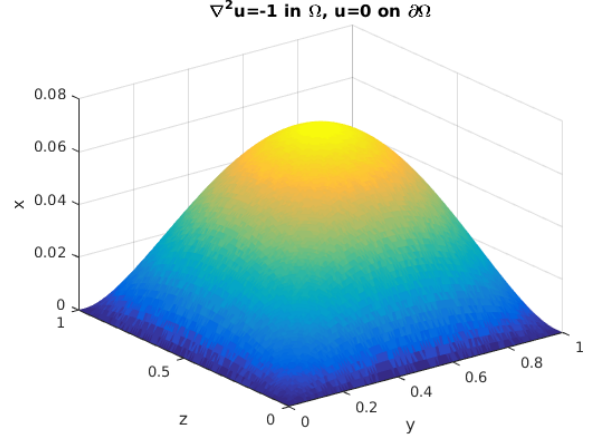


Figure 2: Square

4 One Dimensional Approximation of the Channel

The model of the channel from the last subsection yields flow only in the longitudinal direction as the mass loss through the filter is not accounted for. This motivates us to consider the one dimensional approximation where the channel is viewed as a line.

4.1 Relation Between One- and Three-Dimensional Model

Let ρ be the mass per line segment, and express the conservation of mass as

$$\frac{d}{dt} \int_B^{B+\epsilon} \rho(x, t) \, dx + j(B, t, \rho(B, t)) - j(B + \epsilon, t, \rho(B + \epsilon, t)) = 0, \quad (8)$$

where j is the mass flux. Assuming ρ to be sufficiently smooth we get for $B \leq \psi \leq B + \epsilon$ that

$$\frac{\partial \rho(\psi, t)}{\partial t} \epsilon + j(B, t, \rho(B, t)) - j(B + \epsilon, t, \rho(B + \epsilon, t)) = 0.$$

Dividing by ϵ and letting ϵ go to zero, conservation of mass is expressed as

$$\rho_t + (\rho u)_x = 0, \quad (9)$$

as the mass flux is $j = \rho u$ when u is the average velocity over the cross section. Since momentum is also a material variable we have analogously that

$$(\rho u)_t + (\rho u^2)_x = f,$$

where f is the sum of forces parallel to the channel per line segment. f has unit $[f] = Nm^{-1}$. The parallel pressure gradient is $-\frac{\partial}{\partial x}p$ and the viscous forces depend linearly on the pressure such that the analogue of equation (2) now becomes

$$(\rho u)_t + (\rho u^2)_x = -\frac{\partial}{\partial x}p - au. \quad (10)$$

The derivation of equations (9) and (10) is analogous to the corresponding equations (1) and (2), except from in the assumptions. Equations (9) and (10) only hold for a line segment under the assumptions that u is only in the longitudinal direction and that there is no flux through the porous medium, while equations (1) and (2) hold anywhere. It is also important to note that ρ represent different things in these equations, with for the ρ of section 2 $[\rho] = kg\,m^{-3}$ while in this section $[\rho] = kg\,m^{-2}$.

4.2 Steady State

By modeling the gass as an ideal gass such that $p = r\rho T$, equation (10) can be written

$$\rho u_t + \rho u u_x = -R\rho_x - au$$

where $R=rT$ is the universal gas constant times the temperature in Kelvin. When steady state is reached the time derivatives are zero, and the equations become

$$\begin{aligned} (\rho u)_x &= 0, \\ \rho u u_x &= -R\rho_x - au. \end{aligned}$$

The first equation gives that ρ and u are inversly proportional. By inserting $\rho = c/u$ for a constant c into the second equation, the relation $\frac{du}{dx} = \frac{-au}{c(u-R)}$ is found. This was solved in matlab using forward Euler method. The result is shown in figure 3. As the figure shows, the velocity of a segment of fluid decreases the further into the channel it gets, while the mass density increases. Note that this would not be possible in a finite pipe with a closed end, as this kind of flow would not be stationary. Also note that u will not reach 0, as u_x is singular when $u \approx R$. This solution is not physically correct.

4.3 Perturbation Around the Stationary State

The unscaled equations are

$$\begin{aligned} \rho_{t^*}^* + \rho^* u_{x^*}^* &= 0 \\ \rho^* u_{t^*}^* + \rho^* u^* u_{x^*}^* &= -R\rho_{x^*}^* - au^* \end{aligned} \quad (11)$$

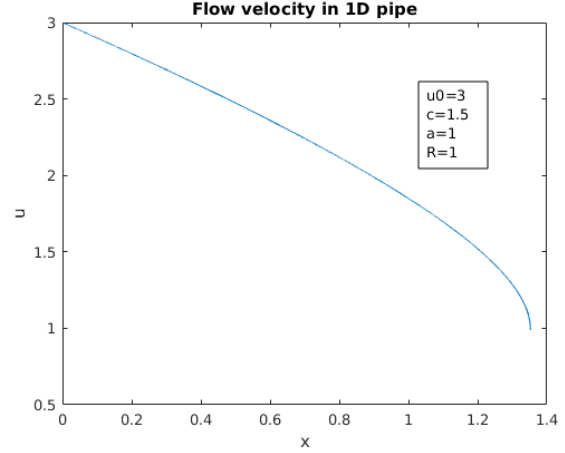


Figure 3: Example of a solution. Here flow into pipe is 3m/s, mass density is 0.5kg/m, $a=1$, and $R=1$

where $\rho^* = P\rho$, $u^* = Uu$, $t^* = Tt$, and $x^* = Xx$. Insterting this into the (11), they become

$$\begin{aligned} \frac{P}{T}\rho_t + \frac{PU}{X}(\rho u)_x &= 0 \\ \frac{PU}{T}\rho u_t + \frac{PU^2}{X}\rho u u_x &= -\frac{RP}{X}\rho_x - aUu. \end{aligned} \quad (12)$$

Since this is a perturbation around a stationary state, we want the time derivative terms to be small. For the first equation in (12), scaling the second term to one gives $X = PU$. Inserting this into the second equation gives

$$\frac{PU}{T}\rho u_t + U\rho u u_x = -\frac{R}{U}\rho_x - aUu$$

For the second equation in (12), one choice of balancing is between the second and third terms. This gives $U = \sqrt{R}$. Insterting these scales and dividing the second equation by \sqrt{R} , the system becomes

$$\begin{aligned} \epsilon\rho_t + (\rho u)_x &= 0 \\ \epsilon\rho u_t + \rho u u_x &= -\rho_x - au \end{aligned}$$

with $\epsilon = \frac{P}{T}$. We now insert $\rho = \rho^0 + \epsilon\rho^1$ and $u = u^0 + \epsilon u^1$ and collect the zero and first order of ϵ . The perturbations are

$$\begin{aligned} (\rho^0 u^0)_x &= 0 \\ \rho^0 u^0 u_x^0 &= -\rho_x^0 - au^0 \end{aligned}$$

and

$$\begin{aligned} \rho_t^0 + (\rho^1 u^0 + \rho^0 u^1)_x &= 0 \\ \rho^0 u_t^0 + \rho^1 u^0 u_x^0 + \rho^0 u^1 u_x^0 + \rho^0 u^0 u_x^1 &= -\rho_x^1 - au^1. \end{aligned}$$

5 Mass Loss From the Wall

Considering a constant mass loss ϕ from the wall per time and line segment such that it contributes with $\int_B^{B+\epsilon} \phi dx$ to the mass flux in equation (8), equation (9) becomes

$$\rho_t + (\rho u)_x + \phi = 0.$$

Assuming that the longitudinal component of the velocity of the fluid that goes through the porous medium is zero, the momentum equation in the longitudinal direction is the same as in equation (10). If we assume the opposite, that the speed in longitudinal direction of the gas that enters the porous medium is equal to the average velocity at that point in the pipe, we would get an additional flux term analogous to in the mass flux such that equation (10) becomes

$$(\rho u)_t + (\rho u^2)_x + \phi \rho u = -\frac{\partial}{\partial x} p - au.$$

6 Porous Medium Layer

For a porous medium layer a Darcy flow is given by $\mathbf{q} = -\frac{K}{\mu} \nabla \mathbf{p}$, where K is the permeability tensor. For an ideal gas one have that $pV = nrT \Rightarrow p = r\rho T$ for some constant r .

6.1 Incoming Flux

The total mass of the fluid is always conserved so that total mass flux into the the porous media minus total mass flux out of it is equals the amount of particles absorbed by it. This can be expressed as in (1). Assuming incompressible flow, i.e. $\nabla \cdot \mathbf{u} = \rho_t = 0$, (1) shows that $\nabla(\rho \mathbf{q}) = 0 \Rightarrow -\frac{K}{\mu} \nabla^2 p = 0$ when using the Darcy flow for \mathbf{u} . Solving $\nabla^2 p = 0$ will give the governing equation in a porous medium. This has not been solved in general in this paper, but in the case of a circular channel and a square channel.

For a circular channel the solution to the laplacian of p is solved with polar coordinates yielding the following

$$\begin{aligned} \nabla^2(p) &= \frac{1}{r} \frac{d}{dr} \left(r \frac{dp}{dr} \right) = 0 \\ \Rightarrow r \frac{dp}{dr} &= C_1 \Rightarrow \frac{dp}{dr} = \frac{C_1}{r} \\ \Rightarrow p &= C_1 \ln(r) + C_2. \end{aligned}$$

Since we only need the gradient of p , C_2 is not needed. To determine the constant C_1 we use the boundary conditions which are continuity of pressure:

$$\begin{aligned} p_i &= C_1 \ln(r_i) + C_2 \\ p_e &= C_1 \ln(r_e) + C_2. \end{aligned}$$

By subtracting the two we find that $p_i - p_e = C_1(\ln(r_i) - \ln(r_e)) = C_1 \ln\left(\frac{r_i}{r_e}\right) \Rightarrow C_1 = (p_i - p_e) / (\ln\left(\frac{r_i}{r_e}\right))$.

This gives that

$$\nabla p = C_1 \frac{\partial p}{\partial r} = \frac{p_i - p_e}{r \ln \frac{r_i}{r_e}}.$$

We use that q is Darcy flow in radial direction so that the flux can be written

$$\begin{aligned} U &= \int_{\Gamma} \mathbf{q} \cdot \mathbf{n} dA = 2\pi L R q \\ &= 2\pi R L \left(-\frac{K}{\mu} \frac{dp}{dr} \right) \Big|_{r=R} = -\frac{2\pi L R K}{\mu} \left(\frac{p_i - p_e}{\ln\left(\frac{r_i}{r_e}\right)} \right) \frac{1}{R} \\ &= -\frac{2\pi L K}{\mu \ln\left(\frac{r_i}{r_e}\right)} (p_i - p_e) \end{aligned}$$

where R is a radius (inner or outer or their mean) and L is the length of the channel. This shows that there is a constant $\kappa = -\frac{2\pi L K}{\mu \ln\left(\frac{r_i}{r_e}\right)}$ so that $U = \kappa(p_i - p_e)$.

Similarly we find for a quadratic channel that

$$U = -\frac{8r_i L K}{\mu(r_e - r_i)} (p_i - p_e)$$

where κ is now $-\frac{8r_i L K}{\mu(r_e - r_i)}$.

7 Accumulation of Particles Due To Diffusion

The particles will move both with the gas flow and due to diffusion, and both movement processes will result in soot particles accumulating at the wall of the filter. The diffusion is only expected to govern the behavior at low speeds. Here we will explore accumulation due to diffusion. Diffusion is a process by which collisions between particles cause particles to move around even in "still" fluids. We look at the effect of diffusion on the soot particles in the channel and attempt to model how it would contribute to particle clogging. We will assume the particle remains where it first makes contact with one of the walls. As soot particles accumulate the position of the channel

walls change, but we simplify and assume that the boundaries remain the same and don't factor in accumulation of soot in our model. We begin with the two dimensional case.

7.1 Model and Simplifications, The Two Dimensional Case

We model the two dimensional case for a cylinder with radius 1 in Matlab first by making the particle take a step in a random direction y , $-y$, z or $-z$ with step length $s \ll 1$. The result is a symmetric impact with the boundaries in z and y direction. The number of steps taken before impact is shown to be exponentially distributed.

We model the same case for a square with side length 1. The result is still symmetric, and the number of steps before impact still seems exponentially distributed. However, the impact points are no longer uniformly distributed along the boundaries, see figure 4. The two dimensional model was changed to

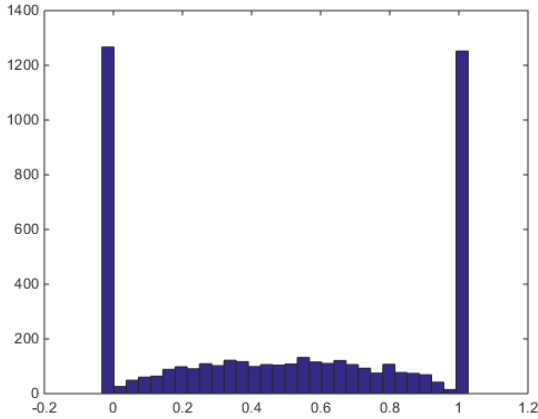


Figure 4: Impact points along the z axis in the case of a square channel. The two tall columns on either side show the number of particles that have been absorbed by the boundaries $z = 0$ and $z = 1$, which represent the two walls perpendicular to z .

allow for a uniformly distributed direction and a step length generated from a standard normal distribution multiplied by a small step length s . The results were indistinguishable from the simpler lattice case, both for the circle and the square.

7.2 Examining the Two Dimensional Case and Expanding to Three Dimensions

Literature on modelling particle dispersion by random walks reveals a wide and varied approach when it comes to the mathematical models utilised. Above we saw that the simple and more sophisticated model gave results that were indistinguishable. Consulting theory on modelling diffusion through random walks we find that by the central limit theorem, as long as sufficient number of steps is taken and the distribution of each step is sufficiently thin-tailed for the second moment to exist, the statistical properties of any random walk will tend toward universal distributions [1].

When extending to the three dimensional case in our models the next particle step is chosen by adding a normally distributed random number ($N(0,1)$) * s (where the step length $s \ll 1$) to the x -coordinate. Then the same is done for the z and y -coordinate. This gives a Rayleigh distributed step length and universally distributed step direction. The Rayleigh distribution is convenient to work with in the three dimensional case as the step lengths in the x , y and z direction are added independently, making it easy to add a velocity to each particle if we want to expand the model to include the velocity field of the gas to our dispersion model. The Rayleigh distribution has a defined and existing 2nd moment and the step length is chosen sufficiently small to ensure the terms of the central limit theorem are met. A constant velocity is added to the x -direction.

The results are shown in 6 and 5. As the model is symmetric the figures for the square case here shows the sum of impacts on all sides superimposed onto one axis. The distance seems exponentially distributed, the log plot for it looks linear. There is a significant accumulation of particles in the centre of the wall.

7.3 Hexagon

The next case models particle impact through dispersion in a channel with a hexagonal cross section. We use the assumption of symmetry and model the hexagon as one triangle with equal sides. By using polar coordinates the triangle is modeled with periodic boundaries. This means that a particle that has moved outside the triangle by a certain distance and angle comes back into the triangle on the opposite

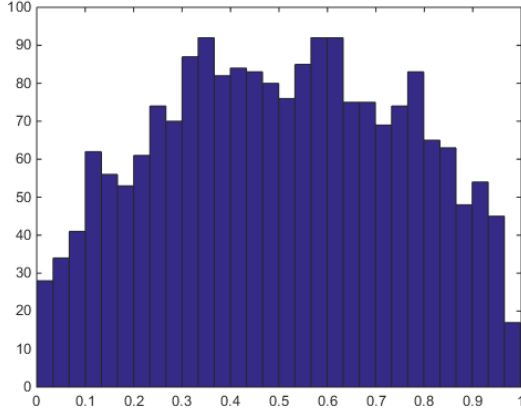


Figure 5: 5000 particles, step length 0.01

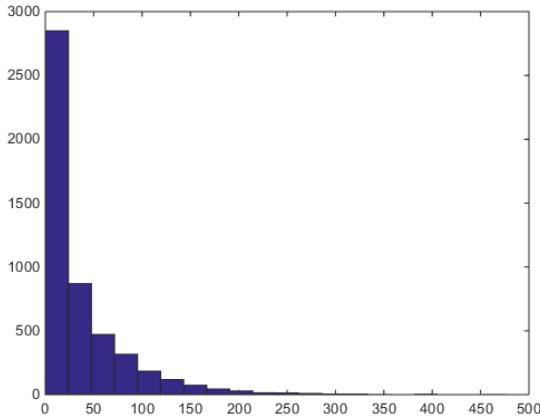


Figure 6: Velocity 0.05, steplength 0.01, 5000 particles

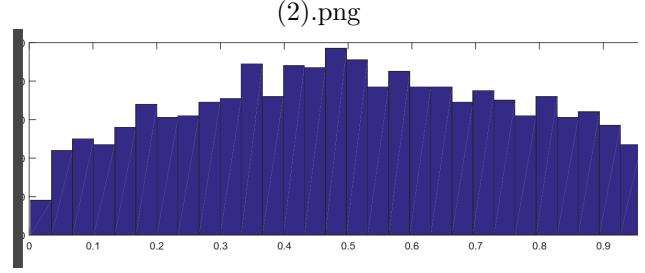


Figure 7: Velocity 0.05, steplength 0.01, 2000 particles

side by the same distance and angle. Thus our triangle represents all 6 triangles in the hexagon and when modelling 2000 particles our result is equivalent to the result expected for one side of a hexagon when 12000 particles are modelled. There is still significantly more impact in the centre, but less pronouncedly so than in the square case.

7.4 Evaluation

The Maxwell-Boltzman distribution describes the speed of particles moving in an ideal gas. The estimate for the most probable speed is given by the maximum likelihood estimator for the mean:

$$v_p = \sqrt{\frac{2kT}{m}}.$$

Soot particles vary in size and density[2] typically ranging from 10-100nm. Using the diameter 50nm at $1.819g\,cm^{-3}$ [2] we estimate that a soot particle travels at speed $0.008ms^{-1}$ at room temperature (300K).

To determine whether diffusion at this low speed would have any impact on the total accumulation of soot Δt time per step in the stochastic model can be set equal to $\frac{s}{v}$ where s in meters is the step length of the particle. It would then be possible to add the velocity of the gas in the channel and read out of the model how big the effect of diffusion might be. It could be significant if the speed of the gas in the system is low.

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