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Polishing lead crystal glass

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1 Introduction

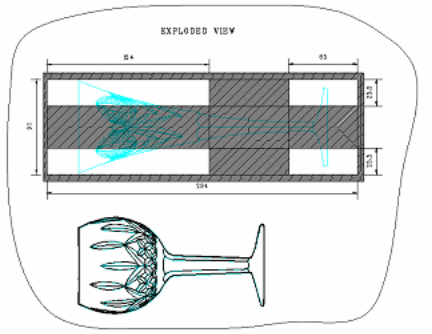
1.1 Crystal industry

The glass making process is very interesting. Traditionally, artisans are engaged in groups around a furnace where the glass is melted thanks to graceful movements of their craft.

A ball of melted glass is gathered from the pot to the end of a blow-iron (a steel tube). It is continuously rotated in order to distribute it so the glass worker blows through the tube and the hot glass becomes a hollow sphere, the blow-iron is turned, tilted and swung in a way which almost magically influences the shape which is developing. Afterwards it goes to an oven and then, once it is cool enough, the cutting process starts.

Holding the glass against the edge of a revolving wheel, the artisans decorate the piece making several specific cuts. It sounds like a very simple process, but it actually calls for a very high degree of skill. The glass is then ready for polishing.

Our Irish manufacturer produces high quality lead crystal glasses (containing lead, potassium and silicate). The glasses have designs cut into them, but these cuts damage the surface below and are optically opaque. In order to restore transparency and smoothness, the glass is polished by immersion in a solution of hydrofluoric and sulphuric acid, rinsing it in a tank containing water. Finally solid reaction products settle out of the acid solution in a settlement tank.



The glasses are introduced in inserts like the one we can see in the picture.

Those inserts belong to a basket which is immersed in the acid solution.

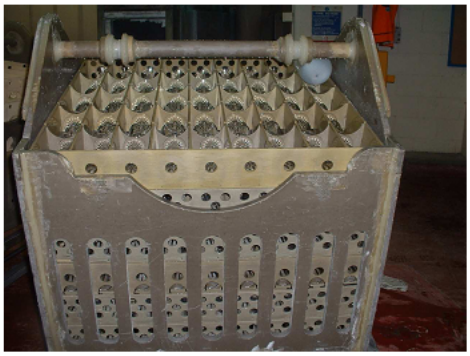


Figure 1: Crystal process

1.2 Polishing process

The crystals contain lead, potassium and silica (oxids); they react with the acids becoming soluble and insoluble salts as follows:

$$\begin{aligned} SiO_2 + 4HF &\longrightarrow SiF_4 + 2H_2O \\ PbO + H_2SO_4 &\longrightarrow PbSO_4 + H_2O \\ K_2O + 2HF &\longrightarrow 2KF + H_2O \\ SiF_4 + 2HF &\longrightarrow H_2SiF_6 \end{aligned}$$

The soluble salts disappear in the rinsing process and the insoluble ones precipitate once the glasses are allowed to settle down.

The acids first react with the crystal cuts due to the fact that the molecules are more separated in there, without initially attacking the smooth parts.

1.3 What is the problem?

The Irish Crystal company needs to know how the chemical and physical process works. Their first concern is the time the glass should be immersed in the acid, in order to make roughness disappear without damaging the already smooth parts, as well as maintaining the sharpness of the cut edges while still polishing to an acceptable degree of transparency. It could as well be interesting to know the concentration rate from the reactions, in order to suggest several experiments they could make.

2 General assumptions

- **One dimension:** We will consider our glass as a line with different shapes, we will work with the idea that the acid attacks our glass from its surface vertically, from the top to the bottom.
- **Sinus form:** We have decided to make the assumption that our initial shape will be similar to the sinus one, (simulating the roughness). This fact does not affect neither our models or results. If we had empirical values from the crystal shape in time 0, we could adjust a distribution function and use it for the initial value.
- **Boundary Conditions:** As our extremes are points we will not take into account the conditions for them, then we will assume homogeneous Neumann conditions, being aware of the fact that the behaviour from the inside is what matters.

3 Model 1. Constant velocity

We have started with a first model where $s(x,t)$ describes the profile of the lead crystal glass surface after the cutting process, as we can see in the Fig 2. We have defined a new function F as follows

$$F(x,z,t) = z - s(x,t), \tag{1}$$

where z is the vertical axis. In this way, the glass surface is given by

$$F(x,z,t) = 0 \tag{2}$$

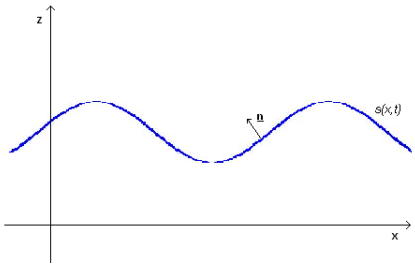


Figure 2: Surface

We consider $\underline{n}$ as the unit normal vector that points outwards. In this case, $\underline{n}$ is

$$\underline{n} = \frac{\nabla F}{\|\nabla F\|}. \tag{3}$$

Making easy calculations, the gradient of F becames $\nabla F = (-s_x, 1)$, so the unit normal vector would be:

$$\underline{n} = \frac{(-s_x, 1)}{\sqrt{1 + s_x^2}}. \tag{4}$$

From now on we will use the simbol $\frac{d}{dt}$ to denote the material derivative.
In our case $\frac{dF}{dt} = 0$, as $\frac{dF}{dt} = \frac{\partial F}{\partial t} + \underline{v} \cdot \nabla F$ we obtain

$$\frac{\partial F}{\partial t} + \underline{v} \cdot \nabla F = 0, \tag{5}$$

where $\underline{v}$ is the rate removal surface (our reaction velocity). **In this model we suppose that this velocity is constant**. According to (5) we obtain

$$\frac{\partial F}{\partial t} + v_n \|\nabla F\| = 0, \tag{6}$$

where v_n is the component of $\underline{v}$ in the normal direction. Then the final equation that describes the problem is

$$s_t = -v\sqrt{1 + s_x^2}, \tag{7}$$

using v instead of v_n.

3.1 Non-dimensionalisation

In this part we deal with the non-dimensionalisation of our equation by a suitable substitution of variables.In others words, we will make a scaling in order to simplify the form of the equation. According to this goal, let's consider the following transformations:

$$\begin{cases} x = lX \\ s = lS \\ t = \tau T \end{cases} \tag{8}$$

where l is the wave length of the system (of the roughness) and τ is the time factor scaling. If we apply the previous substitutions we get

$$\begin{cases} s_t = \frac{\partial s}{\partial t} = \frac{l}{\tau}\frac{\partial S}{\partial T} \\ s_x = \frac{\partial s}{\partial x} = \frac{l}{l}\frac{\partial S}{\partial X} = \frac{\partial S}{\partial X}, \end{cases} \tag{9}$$

and the equation (7) becomes

$$S_T = -\frac{v\tau}{l}\sqrt{1+S_X^2}. \tag{10}$$

So, if we set

$$\frac{v\tau}{l} = 1, \tag{11}$$

we will have

$$\tau = \frac{l}{v}. \tag{12}$$

Finally, the non-dimensionalised equation is

$$S_T = -\sqrt{1+S_X^2}. \tag{13}$$

To solve this equation we have used the characteristics method,also called The Lagrange-Charpit method (see Evan [2]). If we see the equation as a function

$$F(x,t,s,p,q) = q + \sqrt{1+p^2} = 0, \tag{14}$$

where $s = S$, $p = S_x$ and $q = S_t$, the characteristic equations of our PDE are

$$\begin{cases} \dot{x} = F_p = \frac{p}{\sqrt{1+p^2}} \\ \dot{t} = F_q = 1 \\ \dot{s} = pF_p + qF_q = \frac{p^2}{\sqrt{1+p^2}} + q = -\frac{1}{\sqrt{1+p^2}} \\ \dot{p} = -F_x - pF_s = 0 \\ \dot{q} = -F_t - qF_s = 0 \end{cases} \tag{15}$$

with initial conditions

$$\begin{cases} x = \xi \\ t = 0 \\ s = S_0(\xi) = A\sin(\xi) \\ p = S_0'(\xi) \\ q = -\sqrt{(1+S_0'(\xi)^2)}. \end{cases} \tag{16}$$

In this case we choose the sinus because it simulates a rough surface, where $A = \frac{a}{l}$ with $a = weight$ wave and $l = length$ wave.

Solving the system we found an expression for the characteristics $X(\xi,t)$ and the solution for the PDE $S(X(\xi,t),t)$ along them.

$$S(X(\xi,t),t) = S_0(\xi) - \frac{1}{\sqrt{1+S_0'^2}}t, \tag{17}$$

with

$$X(\xi,t) = \xi + \frac{S_0'}{\sqrt{1+S_0'^2}}t. \tag{18}$$

3.2 Solving with matlab

We have plotted the solution and the characteristics from the non-dimensionalised model using a matlab script. In the following graphics we will show their time evolution.

We have tried with different values for the parameter $A = \frac{a}{l}$:

time $[0, 3]$**, space** $[-15, 15]$ **time step 1**, **space step 0.1**

In Figure 3 we see our characteristics as straight lines with different shapes. As the shapes depend on the initial conditions, they are bounded to cross and our solution will be devalued so it will go wrong.

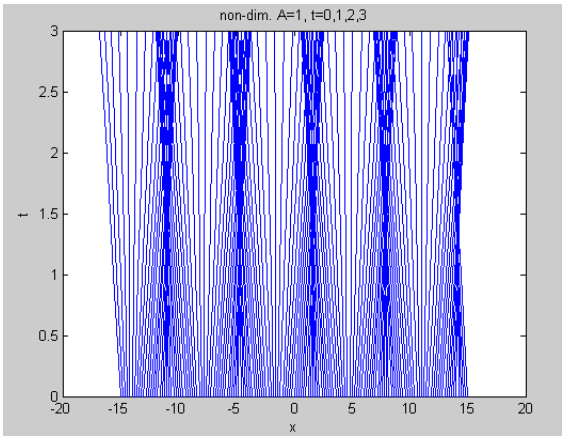


Figure 3: Characteristics; A=1

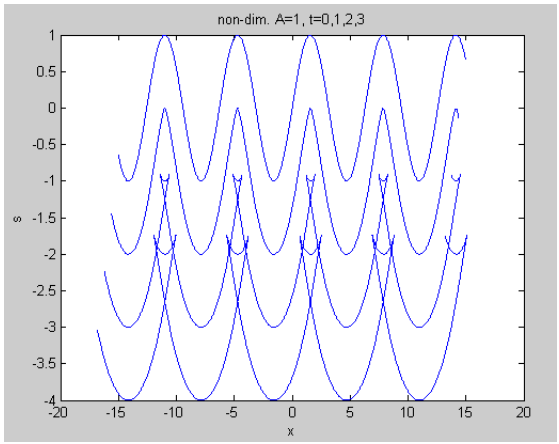


Figure 4: Solution; A=1

In the figure above we see our solution development, starting with the known sinus form. We observe how it clearly forms corners and how the peaks get sharper. It shows the mathematical solution, but when the characteristics intersect, it is multivalued and we should not continue plotting.

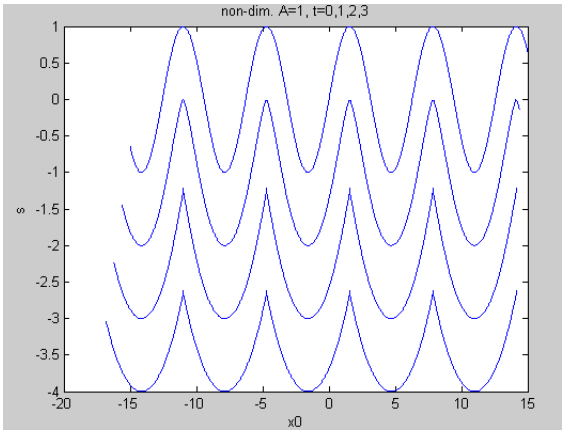


Figure 5: Physical solution; A=1

What happens if the solution goes on longer? We see how it gets smaller and eventualy it becames flat. We observe that approximately at time $t = 30$ it becomes totally flat (Figure 6).

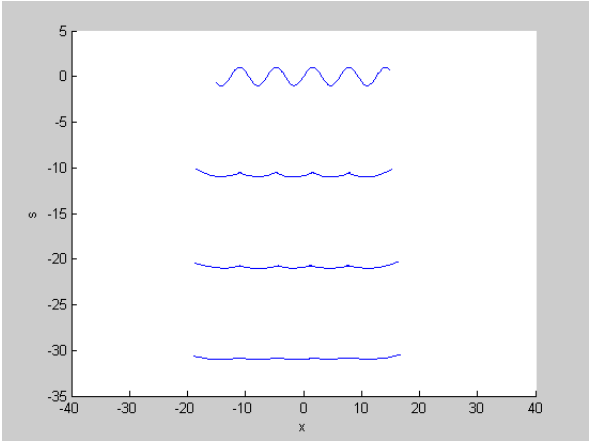


Figure 6: Solution became flat. Time $t \in [0, 30]$; time step= 10

time $[0,3]$**, space** $[0,2\pi]$ **, time step 1, space step 0.1**

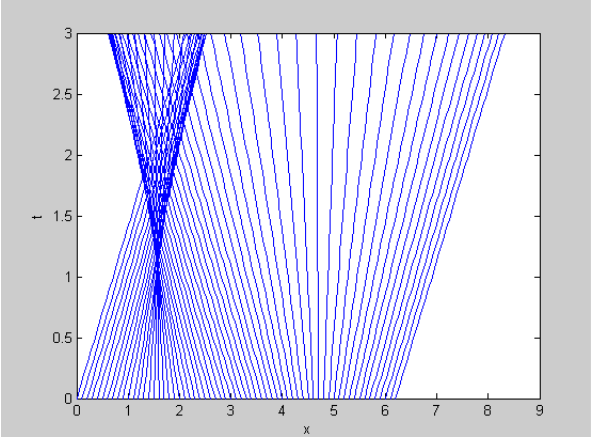


Figure 7: Characteristics shocks at time $t = 1$

We can observe that the crossing area corresponds to the maximum curvatrure and that the minimum curvature corresponds to the moment when the characteristics form an open figure (at the right).

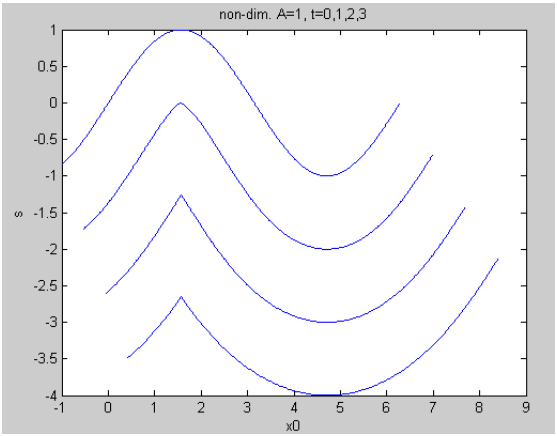


Figure 8: Solution details

In the Figure 8 we see how our solution goes down, getting smoother from time to time. The peaks we see belong to the discontinuities produced by the characteristics. This is due to that we have considered our velocity as a constant in every single point. The velocity pushes our surface down, so the balance from all the strenghts is our result. We can see this behaviour in the Figure 9:

This bad behaviour makes us think that the reaction velocity might depend on the surface curvature. From now on, we will change the values for A to see that $t_c^*(A) = \frac{1}{A}$ in the non-dimensionalised problem ($t^* = \frac{l}{v} t_c^*(A)$ in the original problem).

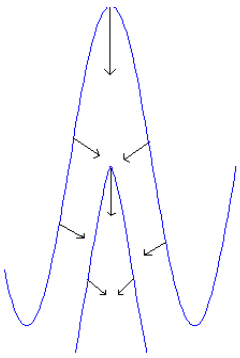


Figure 9: Velocity balance

Now we show the behaviours of different values from the parameter A:

$$A = 2$$

time $[0, 2]$**, space** $[-2, 2\pi]$ **, time step 0.5, space step 0.1**

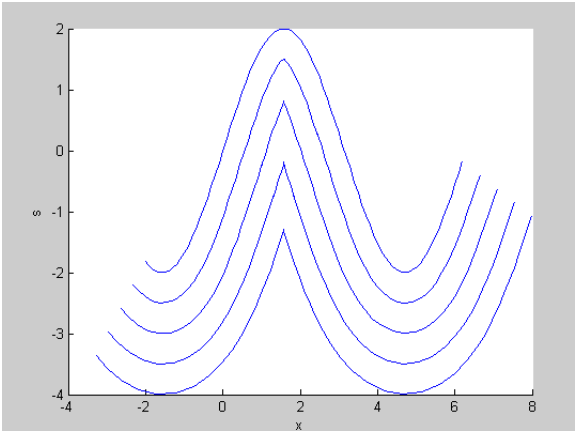


Figure 10: Solution; A=2

In Figure 10 and Figure 11 we see again the correspondance between the crossing characteristics and our surface getting smoother.

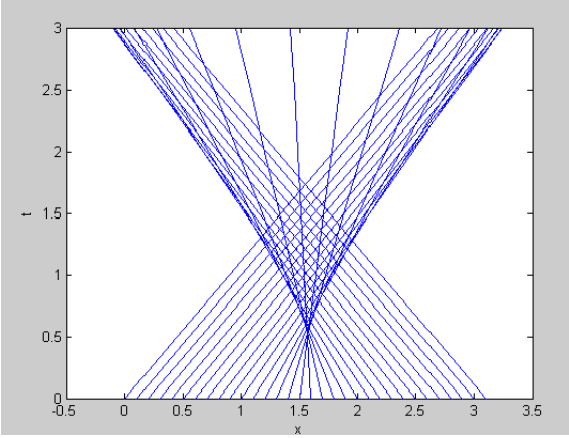


Figure 11: Characteristics shosck at time $t = 0.5$

$A = \frac{1}{2}$

time $[0, 3]$**, space** $[-2, 2\pi]$ **, time step 0.5, space step 0.3**

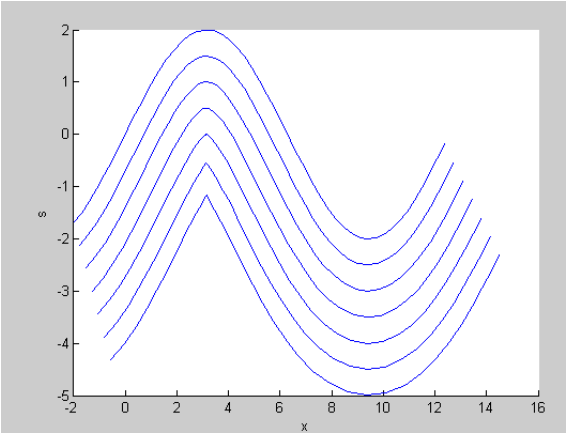


Figure 12: Solution; $A = \frac{1}{2}$

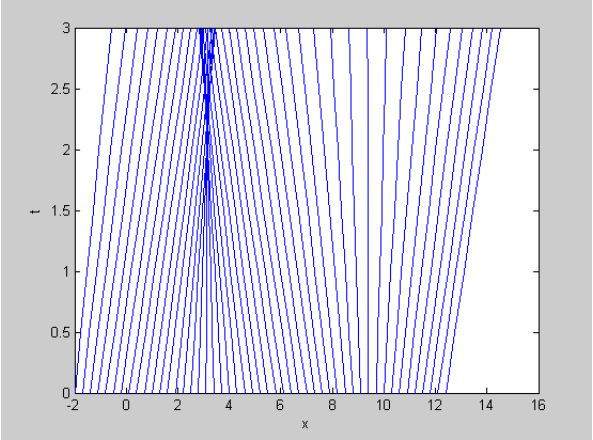


Figure 13: Characteristics shock at time $t = 2$

3.3 Solving with comsol

We decided to solve the equation directly using the finite element solver comsol offers us, just to confirm the process. In Figure 14 we can see the comsol output for time 0.5 and space $[-10, 10]$:

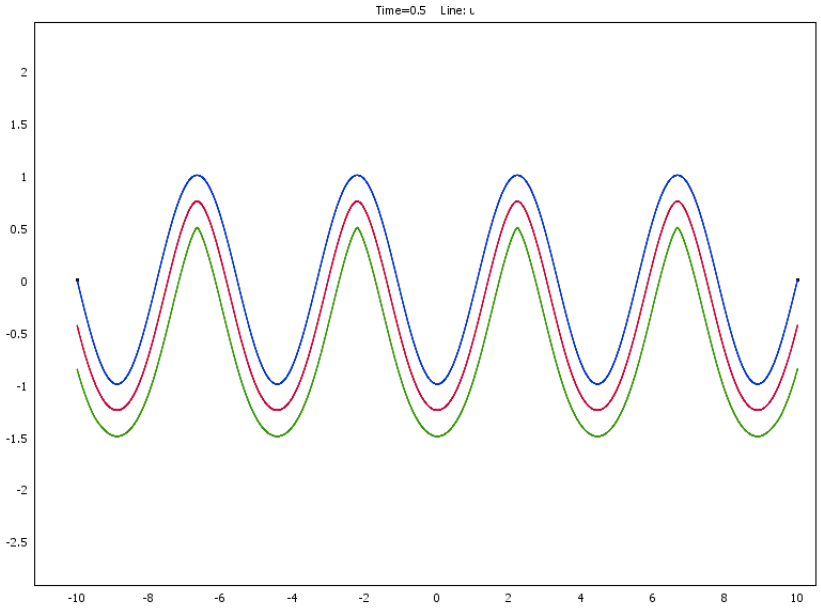


Figure 14: COMSOL solution graphic

If we look at the figure we can see the same initial sharpness we have seen before. Unfortunately we could not carry on the plotting because it could cause the same discontinuities we had with matlab. This leads us to the conclusion that we might have forgotten to include a physical process. In reality, we would not have a constant rate surface removal.

4 Model 2. Linear relationship between normal velocity and surface curvature

The reference [4] about the propagation rates in liquids, gives us the idea of establishing a linear ralationship between v and κ, such as $v = v_0 + v_1\kappa$ ($v_0 > 0$, $v_1 > 0$ constants).

If we apply this fact to the equation in (7)and that the curvature formula is:

$$\kappa = -\frac{s_{xx}}{(1+s_x^2)^{3/2}}. \tag{19}$$

we get

$$s_t = -(v_0 + v_1\kappa)\sqrt{1+s_x^2}. \tag{20}$$

$$s_t = -v_0\sqrt{1+s_x^2} + v_1\frac{s_{xx}}{1+s_x^2} \tag{21}$$

4.1 Non-dimensionalisation

The initial equation is

$$s_t = -v_0(1+s_x^2)^{\frac{1}{2}} + v_1\frac{s_{xx}}{1+s_x^2} \tag{22}$$

Doing the non-dimensionalisation, we choose the following transformation

$$\begin{cases} x = lX \\ s = lS \\ t = \tau T \end{cases} \tag{23}$$

With very easy calculations, we obtain

$$s_t = \frac{\partial s}{\partial t} = \frac{l}{\tau}\frac{\partial S}{\partial T} \tag{24}$$

$$s_x = \frac{\partial s}{\partial x} = \frac{l}{l}\frac{\partial S}{\partial X} = \frac{\partial S}{\partial X} \tag{25}$$

$$\frac{\partial^2 s}{\partial x^2} = \frac{\partial^2 (lS)}{\partial (lX)^2} = \frac{1}{l}\frac{\partial^2 S}{\partial X^2} \tag{26}$$

So, we have

$$S_T = -\frac{\tau v_0}{l}\left(1+S_X^2\right)^{\frac{1}{2}} + \frac{\tau v_1}{l^2}\frac{S_{XX}}{1+S_X^2}, \tag{27}$$

and, if we set

$$\frac{\tau v_0}{l} = 1 \qquad \Rightarrow \qquad \tau = \frac{l}{v_0} \tag{28}$$

$$\Rightarrow \qquad \frac{\tau v_1}{l^2} = \frac{l v_1}{l^2 v_0} = \frac{v_1}{l v_0}. \tag{29}$$

Now, if we define

$$\epsilon = \frac{v_1}{l v_0}, \tag{30}$$

we obtain the final equation for the second model

$$S_T = -\left(1 + S_X^2\right)^{\frac{1}{2}} + \epsilon \frac{S_{XX}}{1 + S_X^2}. \tag{31}$$

Be aware that when $\epsilon = 0$, we come back to the first model.

4.2 Solving with comsol

The goal of this section is to describe the numerical simulation of our second model. To solve the problem we chose the finite elements method, that the Comsol Multiphysics software offers us. The problem is given by

- The differential equation

$$s_t = -\left(1 + s_x^2\right)^{\frac{1}{2}} + \epsilon \frac{s_{xx}}{1 + s_x^2}. \tag{32}$$

- The One-dimensional spatial domain $[-10, 10]$ discretized in 3841 elements.
- The time range $[0, T]$.
- The boundary condition at the extreme points : homogeneous Neumann conditions

$$s_x \cdot \underline{n} = 0. \tag{33}$$

- The initial condition

$$s(x, 0) = A \sin(\alpha x + \beta), \tag{34}$$

where α and β are constants.

In the first case the input data are

Parameters	**Value**
A	1
ϵ	1
T	1
α	$9\pi/10$
β	$7\pi/2$

In Figure 15 the solutions for these values are shown. We can remark that, at the beginning, for $\epsilon = 1$ the glass surface goes up. However, this fact is not physically correct. It can be explained thanks to the assumption of a linear relationship between v and κ, $\epsilon = \frac{v1}{v0*l}$ so the relationship between v_1 and v_0 is essential. If $\kappa < 0$, the surface going up implies that $v_1\kappa$ is more important than v_0, and then, the velocity becomes negative.

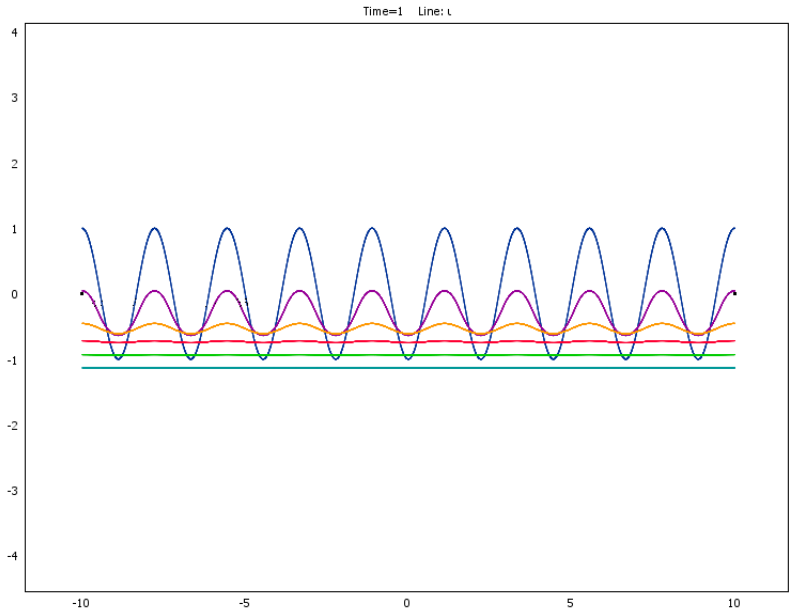


Figure 15: Solution; $A = 1$; $\epsilon = 1$

In Figure 16 we see how the surface has gone up when k is negative

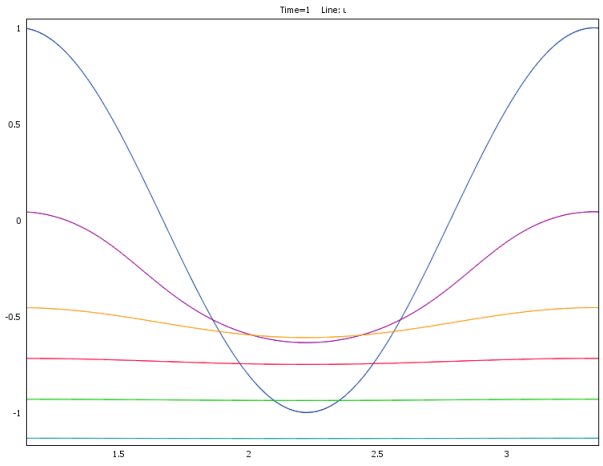


Figure 16: Detail of the solution in Figure 15

So, we changed the input values

Parameters	**Value**
A	1
ϵ	0.141
T	4
α	$9\pi/10$
β	$7\pi/2$

obtaining the Figure 17

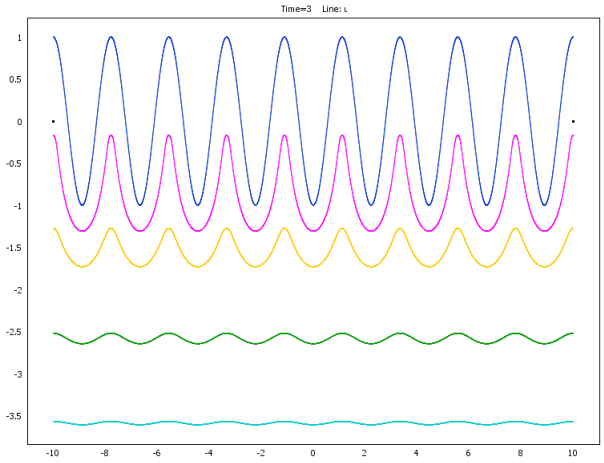


Figure 17: Solution; $A = 1$; $\epsilon = 0.141$

We observed that for smaller values of ϵ the glass surface at the beginning did not go up. To check this, we compared the initial condition (black line) with the solution at time $t = 0.05$ (red line). After several tries we found that the critical value for ϵ is $\epsilon^* = 0.141$. When ϵ is bigger than that everything goes fine, on the other hand, if it is smaller it does not work well.

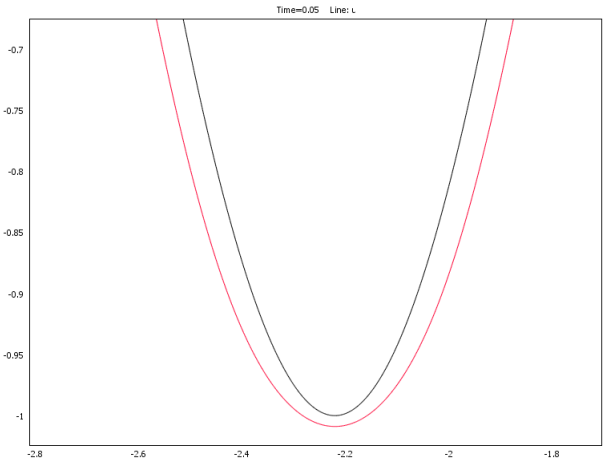


Figure 18: Detail of the solution in Figure 17 (red line) at $t = 0.05$

In this case, the time range is bigger than the one of the previous case. In fact, ϵ is associated to the rate of surface removal.

We considered important to point out the following consideration: The critical value of ϵ depends on the initial conditions, if we take smaller values for the parameter A the critical value of ϵ increases. For example, if $A = 0.1$, $\epsilon^* = 1.75$.

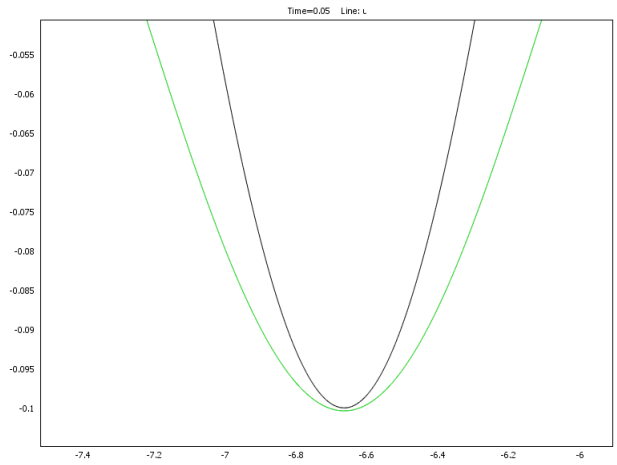


Figure 19: Detail of the solution (green line) al time $t = 0.05$; $A = 0.1$; $\epsilon = 1.75$

4.3 Solving with matlab

We have decided to solve the second model using finite differences with matlab, too. So we can check if our conclusions are right.

Althought the model is a non-linear model, the non-linear part appears in the term S_x and the term S_{xx} appears in linear form, then we can use an explicit-implicit model, explicit for the non-linear terms and implicit for the linear term. The next numerical discretization has been used:

$$S_t = \frac{S_{n+1} - S_n}{\tau} \tag{35}$$

$$S_x = \frac{S_n(x+h) - S_n(x-h)}{2h} \tag{36}$$

$$S_{xx} = \frac{S_{n+1}(x-h) - 2S_{n+1}(x) + S_{n+1}(x+h)}{h^2} \tag{37}$$

$$h = space \;\; step$$
$$\tau = time \;\; step$$

We have taken 1000 space steps and 100 time steps, which is enough for seeing the general behaviour. In fact, we only want to see what happens inside the curve, that is, without the boundaries. Then, we have forgotten the extremes, we only show the middle part of the curve.

We have fixed the initial condition as $\sin(x)$ with $x \in (-6\pi, 6\pi)$ and $t = 3$, so we could compare what happens for different values of ϵ.

- If you tried 0.1, you would get that the curve goes down slowly, and for smaller values than 0.1, it seems that the curve does not change, because we should wait longer.

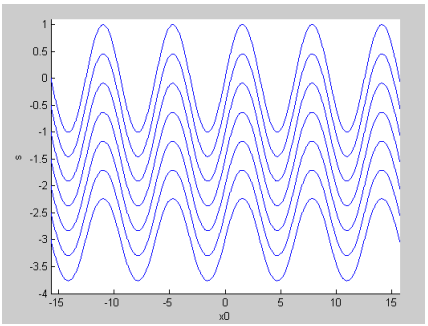


Figure 20: Solution $A = 1$; $\epsilon = 0.1$; $t = 3$

Here, we can see that at t=3 the crystal has changed only a little bit.

- If you tried with bigger values, you would get that the curve goes down faster.

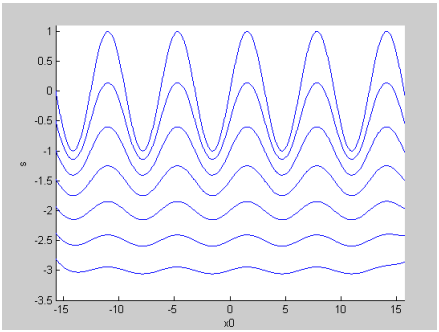


Figure 21: Solution $A = 1$; $\epsilon = 1$; $t = 3$

At $t = 3$ the curve is almost a straight line.

- But if you took values bigger than 1, you would get that the curve goes up, which is not possible. The bigger ϵ is, the higher the solution goes at first.

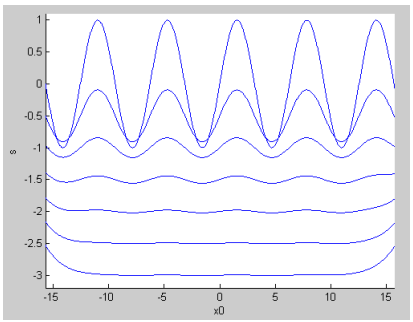


Figure 22: Solution $A = 1$; $\epsilon = 2$; $t = 3$

We can see that the curve changes quickly but in Figure 23 we see that the curve goes up.

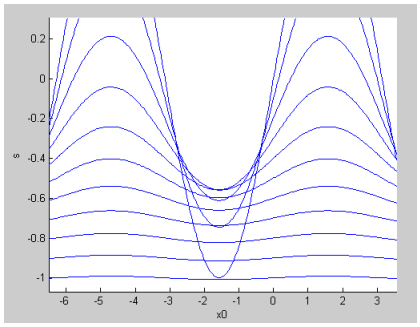


Figure 23: Detail showing the curve goes up $A = 1$; $\epsilon = 5$; $t = 3$

These methods are numerical methods and the critical values are different depending on the mesh you choose, but the important thing is that there is a critical value.

Another result we have confirmed is that the bigger ϵ is, the faster the rate of velocity goes.

To check the last conclusion about the influence of the parameter A, in this case we have fixed $t = 3$ and ϵ=1, we have taken different values for the parameter A ($A = 1$ and $A = 0.5$). We can show that the bigger A is, the slowlier rate of velocity goes.

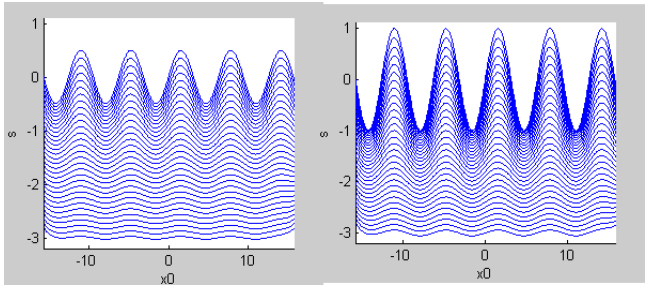


Figure 24: Comparation between $A = 1$ and $A = 0.5$. Final time $t = 3$

In this picture we can see that if A is smaller (A=0.5), at the same time ($t = 3$) the curve is flatter than with big A ($A = 1$).

5 Model 3.Exponential relationship between normal velocity and surface curvature

A solution to avoid the problem previously exposed of the negative velocity is to introduce a new hypothesis. Using the Taylor expansion we get

$$v = v_0 + v_1 k = v_0 \left(1 + \frac{v_1}{v_0} k\right) \cong v_0 \exp\left(\frac{-v_1 s_{xx}}{v_0 \left(1 + s_x^2\right)^{\frac{3}{2}}}\right) \tag{38}$$

We were not able to develop this argument due to our strict time schedule, but it could be a great starting point for new researchs.

6 Conclusions

We have tried different models and methods to analyse the problem. After studying the equations and the mathematics behind the process, we reach to the following conclusions:

- Assuming v as a constant is not possible because the model does not represent the real process. The rate of removal surface depends on its curvature.
- Maybe, the relationship between v and k can be linear but there is a problem when v appears to be negative. This situation is impossible because it would mean that the crystal would go up.
- One possibility would be to find an optimal value for ε, in order to have $v = v_0 + v_1 k$ always positive for $t > 0$. We have shown that v depends on ε, when ε is big enough, v increases and the curve becomes flat quickly. Although there are values for ε which make the curve to go up, if you take ε small enough, the rate of removal will be positive. The industry could take the linear model with ε in a certain range.
- Another point to remark is the relationship between the parameters: $t^* = \frac{l^2}{av}$. We have concluded that the bigger A is, the slowlier rate of velocity goes.
- Solving this problem has been a really challenging work, but there is much more to be done, taking an exponential model might be a good direction for a future research.

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