

Mathematical Model of Agate Band Formation

Julia Goldbaum¹

Sami Shamoon College of Engineering

Charles Howard²

Hadassah Medical Center

Avinoam Rabinovitch³

`avinoam@bgu.ac.il`

Ben-Gurion University of the Negev

Article

Keywords:

Posted Date: October 16th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-11154741/v1>

License:   This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Additional Declarations: No competing interests reported.

Mathematical Model of Agate Band Formation

AUTHOR NAMES

Julia Goldbaum¹, Charles Howard², and Avinoam Rabinovitch^{3*}

AUTHOR ADDRESSES

¹ Physics Department, Sami Shamoon College of Engineering, Beer-Sheva, Israel

² Macabee Health Fund, Orthopedic Department, Beer Sheva 8489312, Israel

³ Physics Department, 84105, Israel

*Corresponding Author: avinoam@bgu.ac.il

KEYWORDS Agate formation; reaction–diffusion; advection; pattern formation; cellular automata

ABSTRACT

To understand the band formation of agates, two sets of results were compared: accurate experimental evaluations of agate bands and advection–reaction–diffusion model calculations of the chemical process. Results show good agreement of coefficient of variance (CV) values and highlight the importance of model parameters controlling band formation mechanisms. A laboratory experiment provides experimental proof that such banding can be achieved under appropriate conditions.

1. Introduction

Agate geodes, exquisitely beautiful and fascinating rocks, are found worldwide within mostly volcanic and metamorphic rock strata. Agate is a variety of chalcedony [microcrystalline form of silica (silicon dioxide)]. Translucency, patterns of color, or moss-like inclusions may distinguish this stone from other forms of chalcedony, such as flint. Agates can show a wide variety of vivid, multiple colours. When cut, they are distinguished by their intricate patterns made up of layers (bands) of delicate colours (Figure 1).



Figure 1: Cut and polished agates from various parts of the world (Australia, Botswana, USA), Although varied in shape and colours, they all show the banded pattern.

They have been used as gems and carved ornaments due to their beauty since the Bronze Age and for grinding due to their hardness (6–7 on the Mohs scale). Yet despite their simple chemical formula and structure, it has not been possible to manufacture them in the laboratory. In addition, or perhaps because of, an accurate exposition of their genesis has not yet been illuminated. Howard and Rabinovitch¹ suggested that the chemical reaction of hydrogen ions entering a gel of silicate ions by advection and diffusion was a possible mechanism for band formation. This was supported by a series of qualitative experiments of placing an acid such as hydrochloric or sulphuric acid adjacent to a solution of sodium silicate, which resulted in the precipitation of silica in a banded, agate-like formation (Figure 2) To further investigate this, a mathematical model is presented showing the creation of this pattern

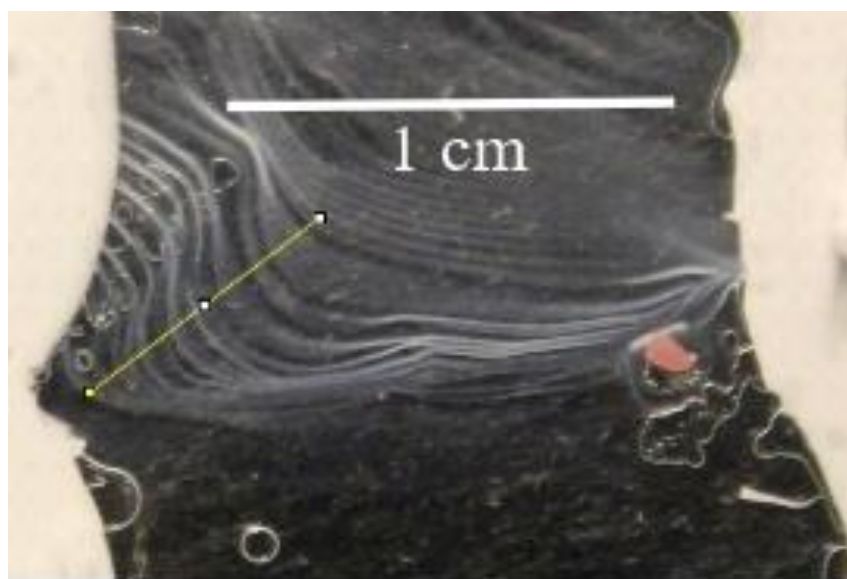
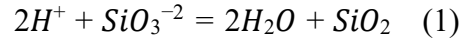


Figure 2: Photograph of a glass cell in which layers of sodium silicate and hydrochloric acid were placed next to each other without mixing. The resultant diffusion reaction/advection produced bands similar to those of agates. The yellow line is the profile used to compare similarity to our model (and by inference, agates)

According to our assumption¹, agates formation is related to the chemical reaction of hydrogen ions and SiO_3^{-2} ions.



The H^+ ions are interjected by an acid infiltrating into the agate geode (Silicate gel) from the acid-filled magma by *advection and diffusion*. The acid penetrates through the medium of silicon-oxygen tetrahedral radicals in the geode, reacting with them, according to the reaction above, to create the silica bands.

The model should therefore deal with three processes that take place consequently: diffusion, advection, and chemical reaction. Such models are usually built by a system of nonlinear differential equations. As is well known, over extended parameters' ranges, this system can have Turing (banded) patterns as its solutions^{2,3}. According to the discussion of Dai and Zhao² these patterns are obtained only when the advection term is non-zero.

Next, we present the experimental procedure to extract the structure of the agate bands and the theoretical three processes model with the results of their comparison.

2. Materials and Methods

We analyzed a high resolution (5184x3456) photograph of the glass cell experiment (Figure 2) and cut and polished agates, (3 from Madagascar and 4 from Botswana, Figs. 4a ,5a). These images were loaded into ImageJ software. A line was drawn as close as possible at right angles to the bands. ImageJ converts each RGB pixel to a single brightness, the grey value (0-255), then plots that value vs position on the line. These data were then saved as a .csv file for analysis in our model. These plots of the grey value of the bands were compared with the plots obtained from our model.

For the hydrochloric acid/sodium silicate experiment (Figure 2), a glass-cell 2mm width was half filled with a sodium silicate solution and a layer of hydrochloric acid laid on top of this being as careful as possible to avoid mixing of these layers.

3. Theory / Model

We developed a model that on the one hand would be as simple as possible while on the other hand would give a clear understanding of the agate band formation. We therefore chose to use a 1D numerical cellular-automata model incorporating the whole gamut of advection, diffusion, and reaction attributes. Although it is one dimensional while for agates the process is radially directed, the obtained qualitative similarity is clear.

Length is divided into discrete cells and time is also discrete and is measured by time units (TUs). The entire process stops at some moment so that it simulates an agate as a “frozen” picture.

In the following, we describe the generation process of the model and try to define the role of each parameter and its relation to the physical and chemical conditions.

3.1. Initial conditions

The initial condition (Figure 3) depicts the situation when the participating ions are separated:

The total number of cells is denoted by n . Their part occupying the left-hand side of a 1D line, is denoted by n_u , initially containing hydrogen ions (whose number in each cell is denoted by u), while the right-hand side cells (whose number is $n-n_u$) initially contain SiO_3^{-2} ions (whose number in each cell is denoted by v). Ion numbers in each cell change during the process. Initial values are given by ru and rv (input parameters), and have the form given in Figure 3. The maximum values of u and v are given by $n*ru$ and $n*rv$. The distribution of u is step-like (see Figure 3), with step length n_u . The distribution of v is 0 on the left-hand side, growing linearly, from n_u to n_u+sl . Both n_u and sl are also input parameters. From n_u+sl on, the number of SiO_3^{-2} ions, v , per cell takes its maximum value, $n*rv$. The linear slope is included to avoid the large peak that would immediately appear at the boundary (near cell No. n_u+sl) under the reaction process if no slope existed.

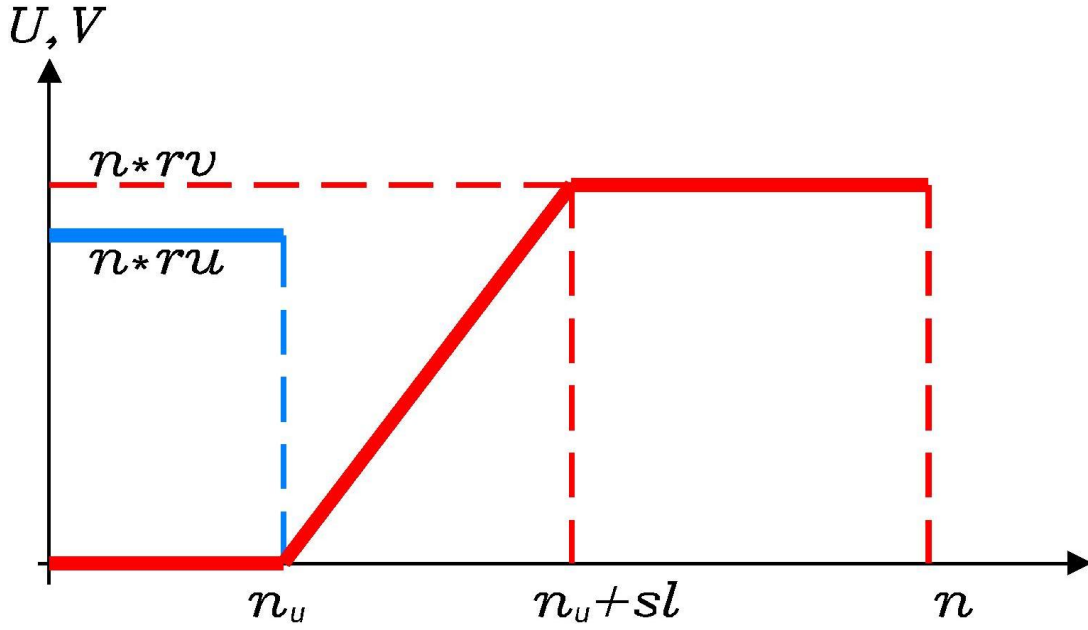


Figure 3: Initial numbers of hydrogen ions (u) and SiO_3^{-2} ions (v) distributions in the cells whose total number is n . Between 0 and n_u there is only a constant concentration $n*ru$ of hydrogen ions in the cells. An intermittent zone sized sl of a linearly growing concentrations of silica ions separates between the former region and the last one which contains a constant concentration $n*rv$ of silica ions

3.2. The advection-diffusion-reaction process

Since the natural formation process is limited in time (Ions are used up) so is the model process. The time duration of the whole process is given by the total number of time steps t . Once the time count starts, hydrogen ions enter the region of SiO_3^{-2} ions. This penetration is given by the advection rate A , which is equal to the number of $H^+(u)$ particles that move by one cell to the right at each time step. Advection may either last till the end of the process or be terminated at some time ts ($< t$). The u and v values, as functions of the cell number i , are calculated after every time-step.

As soon as particles of both types exist in a given cell, a chemical reaction is possible, the products of which are SiO_2 molecules, whose number per cell is denoted by w , and water molecules (not considered in the model, since their number is negligible relative to the quantity of the surrounding water).

The number of w particles in the cells is counted as a function of distance from the left-hand end. *The peaks in this function express the banded structure.*

3.3. The process

At the beginning, the ionic concentration profile is depicted in Figure 3. To pass from each time step to the next one, three processes are executed in the following order (though in the agate formation natural process the three activities occur simultaneously). The values of u and v (numbers of hydrogen ions and of SiO_3^{-2} ions for every cell) are updated after each time step. The entire process continues until time equals t and thus contains t time units. As a result we consider the w -profile, the number of product molecules, w , as a function of the cell number i at time t , the final time of the simulation. The process continues according to the following procedures:

(1) Advection is the movement of the hydrogen ions rightwards. Initial advection rate is given as A (input parameter). If hydrogen ions number u in cell i exceeds A , then A ions pass from cell i to cell $i+1$, that is $u(i)$ diminishes by A and $u(i+1)$ grows by A . If the number of hydrogen ions in cell i is less than A , all of them move to cell $i+1$. There is an option to stop the advection at some time $ts < t$ (ts is an input parameter), which can be useful to model the agate center formation (not presented in this paper). In the simulations presented herein, ts is taken equal to t .

(2) The model considers the **diffusion** of the two reacting materials (hydrogen ions H^+ and SiO_3^{-2} ions), and of the reaction product. The corresponding diffusion coefficients are denoted by du , dv , and dw which are input parameters. Hydrogen ions diffusion is fastest, while the diffusion coefficient of the SiO_3^{-2} ions, dv , is significantly lower, mainly because their size is much greater than that of the hydrogen ions. The lowest diffusion coefficient belongs to the product, silica, which precipitates out in chains/lattices. Its diffusion coefficient dw is small, almost zero.

The diffusion process itself is as follows: The difference between the number of particles of the given type in two neighboring cells is multiplied by the diffusion

coefficient, and the resulting number is passed from the cell with the bigger number to the cell with the smaller number. Then a similar operation is done for the next nearest neighbors, but the number of passing particles is half of the difference multiplied by the diffusion coefficient.

Consider for example the diffusion of the hydrogen ions, u . The diffusion coefficient du is an input parameter. Diffusion changes the numbers of particles in nearest neighbor (nn) cells and in the next nearest neighbor (nnn) cells, which are: for cell number i , the nn's are $i-1$ and $i+1$, and the nnn's are $i-2$ and $i+2$. Diffusion progresses according to:

$$u(i, t) = u(i, t-1) \pm du [u(i+/-1, t) - u(i, t)] \pm du [u(i+/-2, t) - u(i, t)] / 2. \quad (2)$$

The $\pm$ sign ensures that diffusion occurs from the cell with the higher u to the one with the lower u .

(3) Chemical reaction. Reaction probability in each cell is calculated for all cells from the numbers of the hydrogen ions and SiO_3^{-2} ions in this cell. Since the ratio of ions taking part in the reaction is 2:1 (See Eq.1), the probability is proportional to the product of the 2nd power of hydrogen ions number and the SiO_3^{-2} ions number:

$$p = ku^2v \quad (3)$$

Here, k is a constant input parameter. Note that if it is too low, the reaction is poor, if it is too high, the reaction leads to a SiO_2 plateau and not to bands.

The reaction occurs randomly according to the probability p . In case the reaction occurs in a cell, the number of hydrogen ions (u) in the cell diminishes by 2, the number of SiO_3^{-2} ions (v) diminishes by 1, and the number of the product molecules SiO_2 (w) grows by 1.

(4) The boundary conditions (BC) model a flow (advection) of hydrogen ions, namely, for each time step, a number A of u -ions is added to the first cell and subtracted from the last one.

In order to smooth the profiles of both types of ions boundaries, Danckwerts BC (zero derivative at the ends) are also applied for u and v , by simply equating the numbers of hydrogen ions and SiO_3^{-2} ions in the two first and the two last cells.

(5) Moving Average. To mitigate short-term, random fluctuations and identify trends in the formation of the bands, a simple moving average process of 3 or 5 cells was performed. For example, consider the array of w 's: $w_i, w_{i+1}, w_{i+2} \dots$. The average over 3, $(w_i + w_{i+1} + w_{i+2})/3$, is denoted as the new w_{i+1} and the process moves along the i index.

3.4. CV comparisons and the similarity parameter

This method was used for both the agates' structure and experimental bands comparisons with the model.

Agates' measured band shapes and our (dimensionless units) model results, obviously do not have the same units for length (coordinate) nor pulse amplitudes (strengths of “whiteness” of the bright parts of the agate bands, and SiO_2 concentrations w , respectively), therefore a direct comparison between these two values is impossible. We can only compare overall *forms* (how they appear to the eye) and, more analytically, use the coefficients of variation (CVs) similarity comparisons as our guides. Since the actual value of the CV is independent of the unit in which the measurement has been taken ($CV = \text{standard deviation} / \text{average}$), it is also dimensionless and hence is the right comparison measure between the measurements and our model results. We therefore compare CVs of peak heights (amplitudes), peak widths, area under peaks, and inter-peak intervals between agate experimental measurements, and our model results. Since the “best” parameter is the CV of the inter-peak intervals, its weight in the following defining difference parameter is highest.

We define an overall statistical parameter which we call “difference”, and another one called “similarity”. The relative weights used for the different CVs were chosen to achieve the best fit. Difference is defined as:

$$D = \frac{|CV_{sim,amp} - CV_{real,amp}| * 0.2 + |CV_{sim,int} - CV_{real,int}|}{CV_{real,amp} \quad CV_{real,int}}$$

$$* 0.5 + \frac{|CV_{sim,width} - CV_{real,width}|}{CV_{real,width}} * 0.2$$

$$+ \frac{|CV_{sim,area} - CV_{real,area}|}{CV_{real,area}} * 0.1$$

Here sim is for simulations, real is for either agates' experimental measurements or hydrochloric acid/sodium silicate experiment results measurements, amp is amplitude, and int for inter-pulse intervals. For example, $CV_{sim,amp}$ is coefficient of variance for amplitude values for simulations.

Similarity is simply defined as: $S=1-D$. We consider that similarity of more than 0.8 is significant.

4. Results

Two comparisons with our mathematical model were carried out, one matched these calculations with measurements of grey scale intensity of agate samples and the second with our band forming experiments.

4.1. Agates

An example of a model-calculations video showing a vivid presentation of the evolution of such band formation is given (please press [see](#) for the video).

A complete scenario of the process is vividly presented. At the beginning there is no reaction product, so the entire area is black. Then light lines appear, showing the reaction products appearing at some places. While new white lines appear, the former lines become wider and

paler, which is the result of diffusion. Grey and white lines on the black background indicate the band's creation.

Once such structures were obtained, we studied the effect of the model parameters on them, their amplitudes, widths, areas, and inter-peak intervals and used these results to obtain good similarity with experimental results.

4.2. Comparison of agates samples with simulation results

We have measured seven agates. Presented here are two examples of the actual pictures of the agates with graphs of the comparisons with our model calculations made on total lines and segmental lines measurements (Figures. 4 and 5), followed by complete showcase of CV comparison result values (Table 1) and the model parameters which have led to them (Table 2).

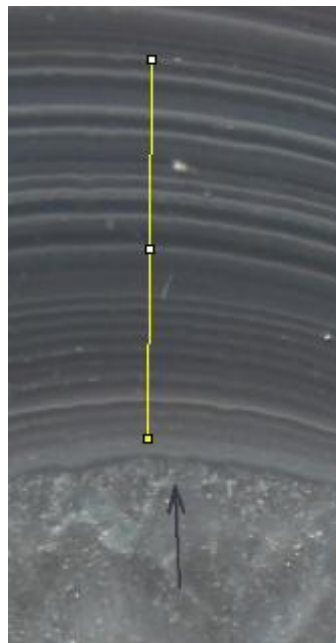


Figure 4a: Agate No. 20 – image. Bands are shown as curved whitish lines on dark background.

Vertical yellow line – line of grey scale intensity measurement shown in Figure 4b

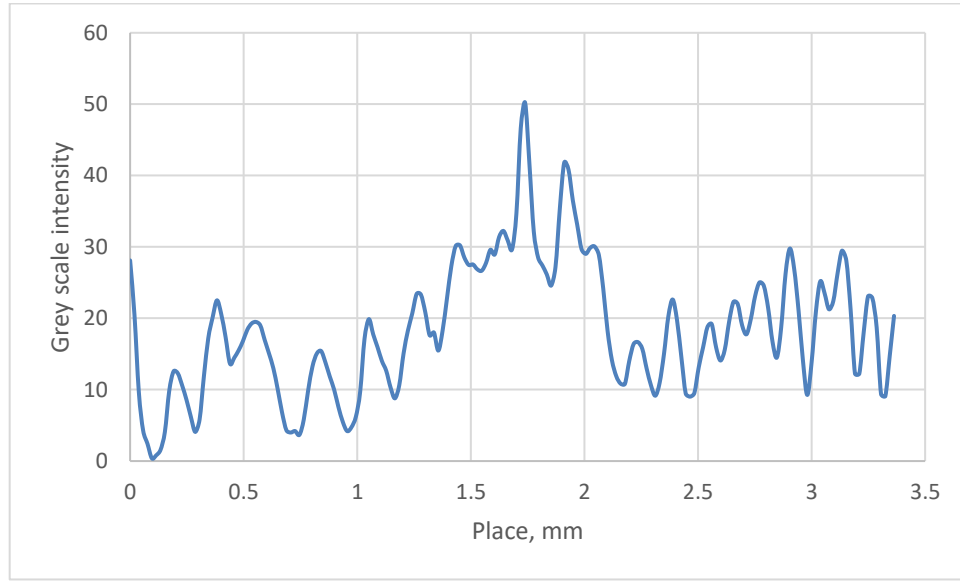


Figure 4b: Agate No. 20: grey scale intensity measurement along the yellow line in Figure 4a

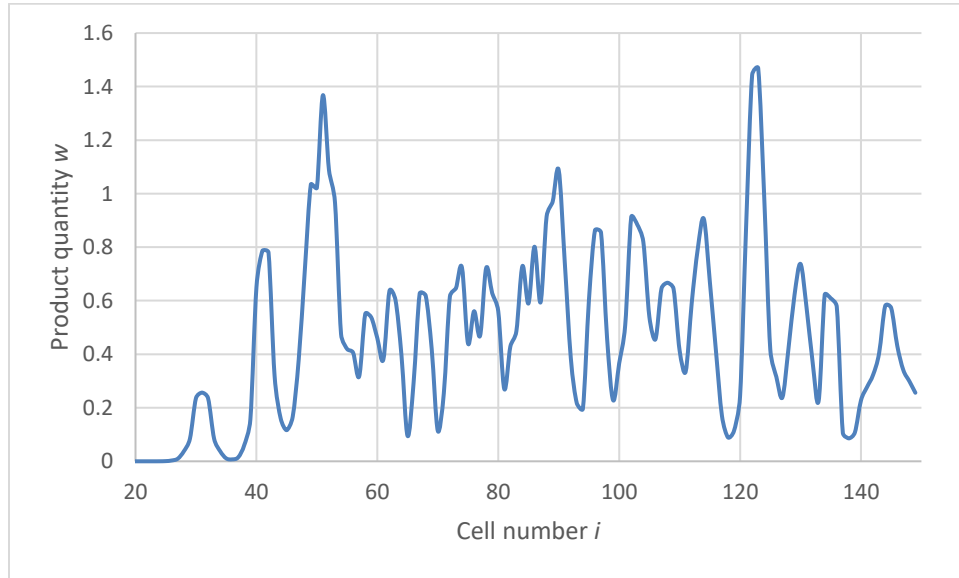


Figure 4c: Simulation of Agate No. 20 with parameters: $n=150$, $t=500$, $du=0.7$, $dv=0.01$, $dw=0.001$, $A=5$, $k=2e-7$, $t=500$, $nu=20$, $sl=40$, Moving averaged by 3.

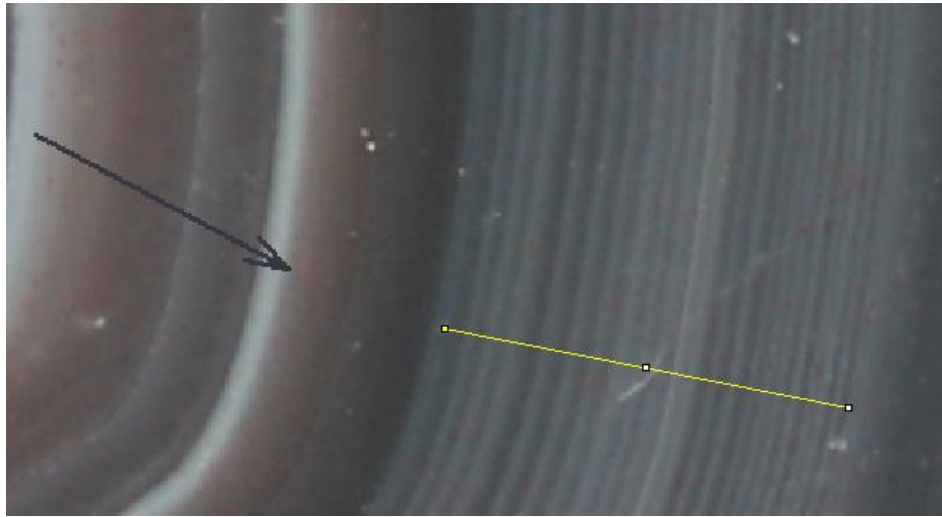


Figure 5a: Agate No. 22 – image

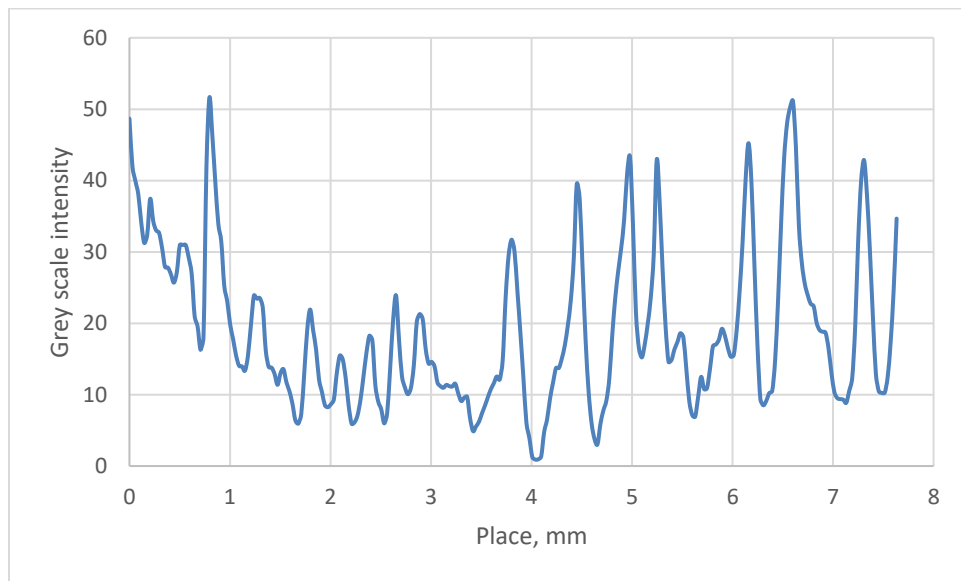


Figure 5b: Agate 22: grey scale intensity measurement - entire line

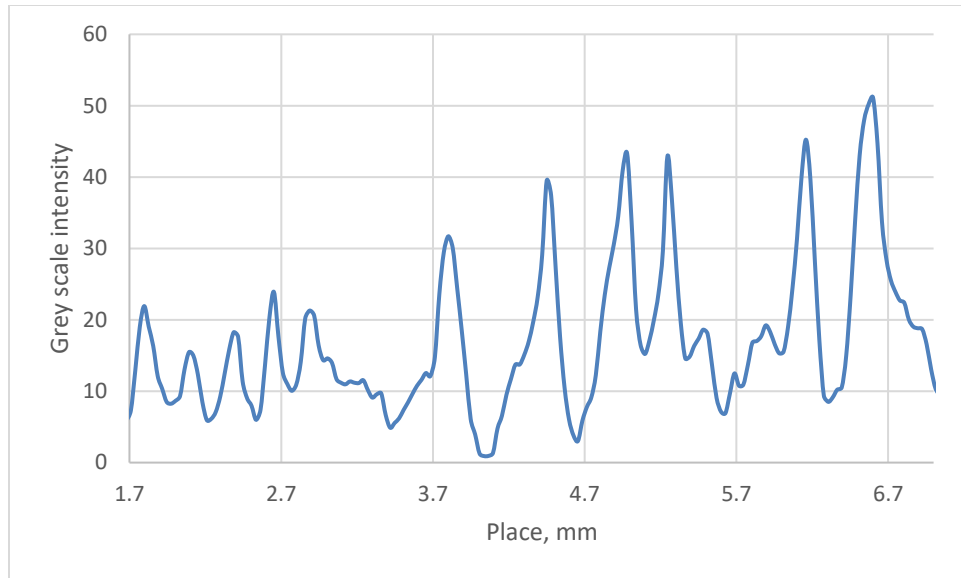


Figure 5c: Agate 22: grey scale intensity measurement - partial (between 1.7 and 6.9 mm of the line of measurement)

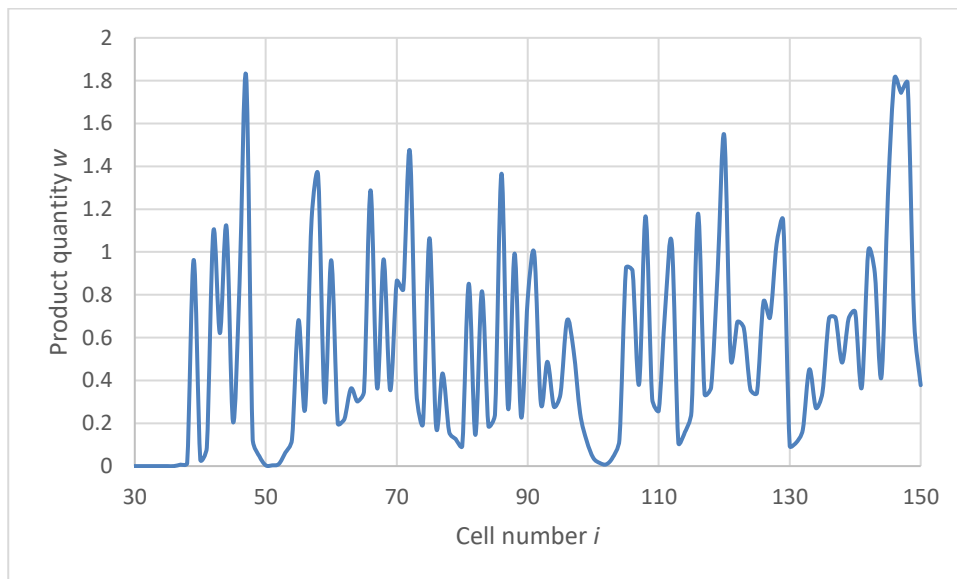


Figure 5d: Simulation Sim22 with parameters: $n=150$, $t=500$, $du=0.65$, $dv=0.01$, $dw=0.001$, $A=5$, $k=2e-7$, $ts=500$, $nu=20$, $sl=40$, no average.

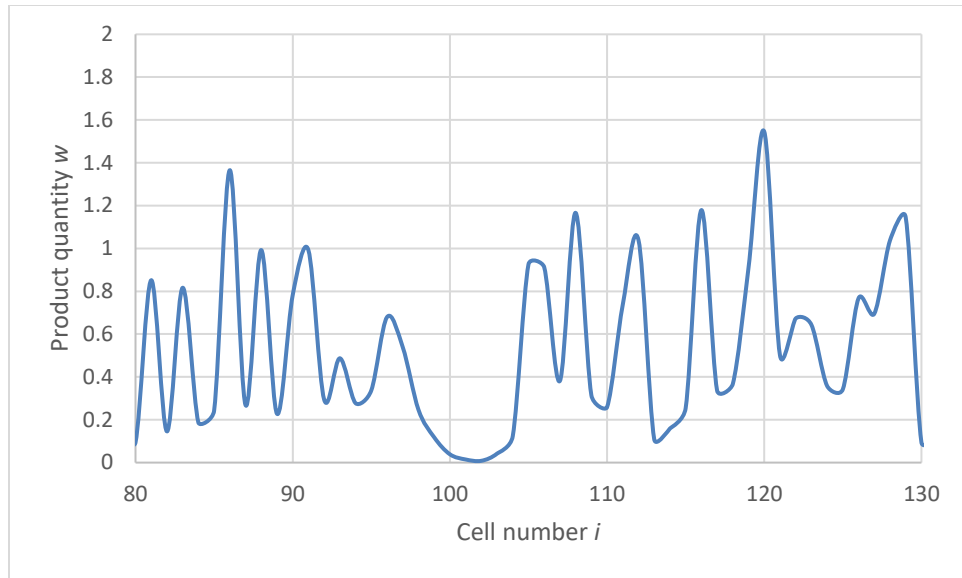


Figure 5e: Part of the simulation profile shown in Figure 5d.

Table 1: Different CV (amplitude, intervals, peak widths and areas) values and similarity for different agates and simulations.

Agate No. Sim No.	Amplitude	Intervals	Widths	Area	Similarity
Agate 3b	0.233653	0.362714	0.581311	0.826858	0.844
Sim 3b	0.355487	0.328405	0.572822	0.676913	
Agate 5 entire	0.337863	0.302626	0.454962	0.715443	0.875
Sim 5	0.384885	0.322276	0.352791	0.567186	
Agate 5 part	0.332195	0.322689	0.449248	0.677867	
Agate 6a entire	0.290147	0.292363	0.410342	0.572255	0.887
Sim 6a	0.260788	0.298765	0.335709	0.31695	
Agate 6a part	0.220461	0.287056	0.300579	0.363468	
Agate 8	0.252803	0.415096	0.416258	0.574897	0.8495
Sim 8	0.285805	0.453989	0.3546	0.352024	
Agate 20	0.36652	0.377633	0.456173	0.520713	0.893
Sim 20	0.363161	0.361884	0.317854	0.643569	
Agate 22 entire	0.352487	0.491476	0.212984	0.668175	0.918
Sim 22 entire	0.35029	0.491832	0.277671	0.535203	
Agate 22 part	0.390777	0.550289	0.253453	0.670243	0.905
Sim 22 part	0.321471	0.542881	0.271405	0.412874	
Agate 21 part	0.268687	0.826154	0.319501	0.65134	0.83

Sim 21 part	0.314038	0.593279	0.308404	0.49063	
-------------	----------	----------	----------	---------	--

Table 2: Simulation parameters for profiles mentioned in Table 1. For all of them, $n=150$, $t=500$, $A=5$, $k=2e-7$, $ts=500$, $n_u=20$, and $sl=40$.

Sim name	du	dv	dw	Average
Sim 3b	0.3	0.01	0.002	No
Sim 5	0.75	0.01	0.001	By 3
Sim 6a	0.65	0.01	0.001	By 5
Sim 8	0.65	0.07	0.0025	No
Sim 20	0.7	0.01	0.001	By 3
Sim 21	0.65	0.07	0.0025	By 3
Sim 22	0.65	0.01	0.001	No

4.4. Laboratory experiments forming bands

Here we compare the hydrochloric acid/ sodium silicate qualitative experiments (Figure 2) with our model calculations according to the similarity of CV values. An example of such similarity is given in Figure 6. CV values along with the similarity are given in Table 3.

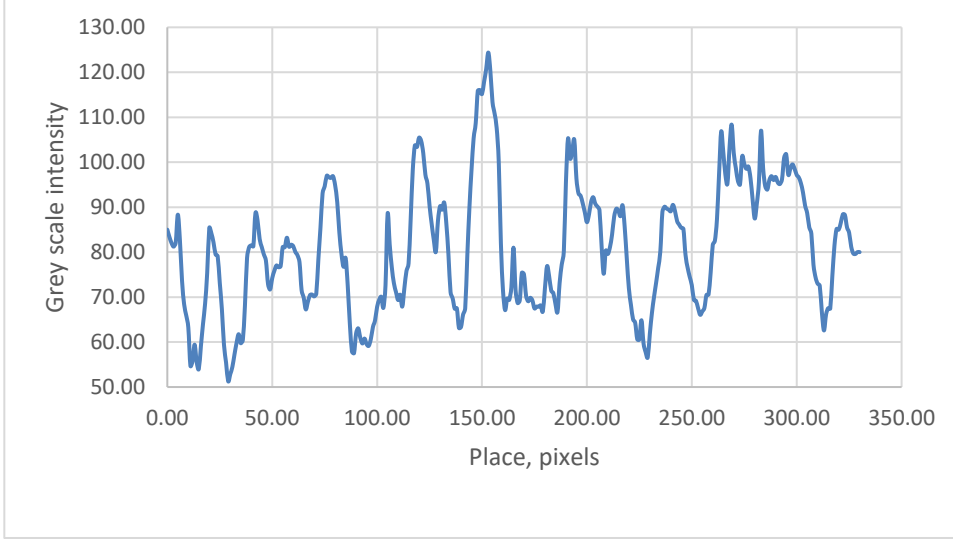


Figure 6a: Plot of – grey scale intensity of glass cell hydrochloric acid/sodium silicate experiment shown in Figure 2

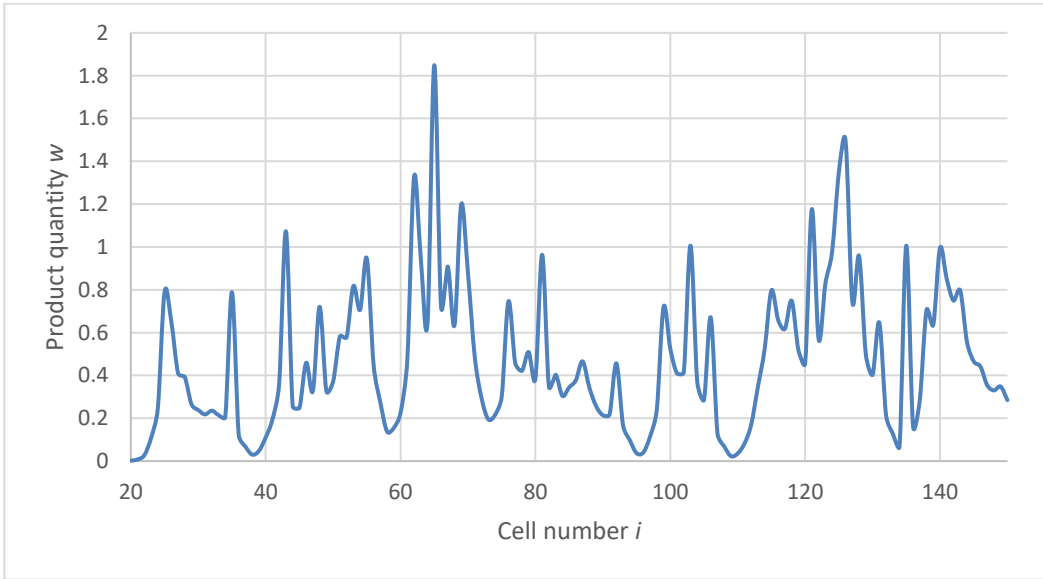


Figure 6b: Simulation with parameters: $n=150$, $t=500$, $du=0.3$, $dv=0.01$, $dw=0.002$, $A=5$, $k=2e-7$, $ts=500$, $n_u=20$, $sl=40$, no average.

Table 3: CV values for experiment and the set of simulation shown in Figure 6.

	Amplitude	Interval	Width	Area	Similarity
2015b	0.258207	0.312667	0.504285	0.783081	0.86
Simulation	0.355487	0.328405	0.572822	0.676913	

5. Discussion

There is a variety of parameters included in the model. Our results demonstrate that in order to obtain banded structure, one must choose these parameters judiciously:

5.1. Parameters influences

Banded structure is obtained for definite ranges of certain model parameters. Not all of them are equally important in their effect on the banded structure and its shape.

Results show that the effects of the model parameters on the pulse shapes are:

The advection A parameter is very crucial in creating the bands. It turns out that if the advection is either too fast or too slow, then only a few peaks or no peaks at all appear.

Pulse amplitudes: (1) diminish as the diffusion coefficient of the reaction product, dw , grows; (2) diminish as the diffusion coefficient of hydrogen ions, du , grows; (3) grow as the chemical reaction rate grows.

Pulse widths grow: (1) as the diffusion coefficient of the reaction product, dw , grows, and (2) as the chemical reaction rate grows.

Inter-pulse intervals increase: (1) as the diffusion coefficient of the reaction product, dw , grows, (2) as averaging is applied (small peaks then don't appear).

Pulse areas: (1) grow as the diffusion coefficient of the reaction product, dw , grows; (2) diminish as the diffusion coefficient of hydrogen ions, du , grows (and here the relation between the amplitude and the area is clearly seen); (3) grow as the chemical reaction rate, k , grows.

5.2. Model parameters values

Numerical values of the model parameters used in the simulations are given, and also values which show good results are chosen:

The parameter n_u , which is the size of the sample part initially occupied by hydrogen ions, must be small relative to the entire sample size n , because the bands are obtained in the other part. The value used in the simulations is $n_u=20$.

Diffusion coefficient of H^+ ions, du , for which banded structure is obtained is 0.2 –

0.75. Good results were obtained for this parameter being 0.3, 0.65, 0.7 and 0.75 (see Table 2).

Diffusion coefficient of SiO_3^{2-} ions, dv , must be much lower than du . Banded structure is obtained for its values in the range 0.005 – 0.08.

Diffusion coefficient of the reaction products, dw , for which the structure is banded, is in the range 0.001 – 0.003. For low values, the peaks are sharp and dense, while for high values they are smoother, wider and have larger distance in between.

Advection rate A , for which the structure is banded, is for $A=5$ (see Table 2). In the range 3 – 5.6 peaks were obtained but without periodicity. For smaller or larger A values, the peaks are obtained on the left or on the right of the sample only.

Proportionality coefficient k - the reaction probability, for which banded structure is obtained, is in of the order 10^{-7} . The larger the number of particles of both types per cell, the lower this parameter should be. In most of our simulations it was taken to be $2 \cdot 10^{-7}$.

5.3. Remarks

Regarding the central macro quartz crystals, we assume that they were caused by a secondary process due to dissolution of the central bands and slow recrystallization as witnessed by “bits” of bands within these crystals.

6. Conclusions

The model introduced in the manuscript can lead to banded structure and therefore can describe agates formation.

As each agate has its own unique banded structure, presumably the model parameters also vary somewhat from agate to agate. There is obviously no direct way to find the *actual* parameters of the agate formation process, but one can obtain a good relative estimation of them based on our model. Moreover, our model provides an understanding of which are the important parameters, and their individual influences and importance in shaping the bands in final structures.

References

[1] Howard CB and Rabinovitch A, A new model of agate geode formation based on a combination of morphological features and silica sol-gel experiments, European J of Mineralogy 29, 1-10, (2017).

[2] Dai C and Zhao M, Nonlinear analysis in a nutrient-algae-zooplankton system with sinking of algae, *Abstr. Appl. Anal.* 278457, 1-11, (2014).

[3] Miguez DG, Satnoianu RA and Munuzuri AP, Experimental steady pattern formation in reaction-diffusion-advection systems, *Phys. Rev. E* 73, 1-4, (2006).

Funding.

No funding was received for this project

The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.