Topological model of soap froth evolution with deterministic
T2-processes.

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Abstract

We introduce a modified topological model for the evolution of two-dimensional soap froth. The topological rearrangement associated with a T2 process is deterministic; the final topology depends on the areas of the neighboring cells. The new model gives agreement with experiments in the transient regime, where the previous models failed qualitatively, and also improves agreement in the scaling state.

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Dynamics of soap froths has attracted considerable attention among physicists [1]. Evolution of a two dimensional froth is governed by the von Neumann law [2]:

\[
\frac{da_n}{dt} = k(n - 6),
\]

where \(a_n\) is the area of any \(n\)-sided bubble. The growth rate of a bubble depends only on its topological class (TC - the number of its sides), and is completely independent of any other detail, such as the TC of its neighbors. As the froth evolves, bubbles with \(n < 6\) sides shrink and disappear: when that happens, sudden topological rearrangements (called T2 processes) take place. In the course of these processes the froth regains co-ordination number 3, and some bubbles that were neighbors of the one that disappeared may lose or gain a side. A different topological rearrangement, called T1 process, occurs by side switching, without elimination of any bubble. The total number of cells in the system decreases with time; hence the average area of the cells \(\bar{a}\) increases and the froth coarsens.

A second important finding concerning froth evolution was discovered experimentally [3–6]: after a transient period the system reaches a universal scaling state. Scaling, combined with the von Neumann law imposes that \(\bar{a} \sim t\) and that the topological distribution function is constant in the scaling regime, \(x_n(t) = N_n(t)/N(t) \rightarrow x_n^*\). The scaling state is universal in that it is independent of the froth’s initial state, the gas used, etc. These results were verified [4], other properties of the scaling state were measured [7,8] and some aspects of the transient period that precedes the scaling regime were also studied [5].

Both analytic and numerical methods have been used to address froth evolution theoretically. The analytic (mean-field) studies [8–12] yield, in general, surprisingly good agreement with experimentally measured distribution functions in the scaling state. Recently the same methodology was used to predict some more complicated aspects of froth dynamics, such as the distribution of survivors [13] in the scaling state, and the evolution of the topological distribution function from some special initial states [14,15]. For these more delicate and complex properties agreement with experiment is much weaker and only qualitative.

Surprisingly, we found that rather sophisticated topological simulation methods
are as bad or even worse in predicting the same characteristics. The aim of the present paper is to elucidate the physical reason for these discrepancies, and to present a simple modification of the simulations that improves agreement with experiment most significantly.

In one of the earliest simulations Weaire and Kermode\cite{18} described the froth in terms of the coordinates of the vertices and the gas pressures in the bubbles. By solving at each time the equations of mechanical equilibrium for all vertices, they determined the spatial configuration of the froth. The necessary computation is, however, so involved that one can not treat a large number of bubbles (they had only 500 bubbles initially - subsequently Herdtle and Aref simulated 1024 bubbles on a Cray\cite{19}). Kawasaki and co-workers\cite{20} solved a system of differential equations for the coordinates of the vertices. They were able to handle up to 24 000 cells; their results seem to be in good agreement with experiments. The von Neumann law holds, however, only approximately for this method. Potts model simulations\cite{21} are also severely restricted in the number of bubbles that can be treated.

The importance of different aspects of the microscopic dynamics and their separate effects on the macroscopic evolution of the froth are most easily studied by analysing a hierarchy of more and more simplified topological models, identifying which aspect is essential in order to obtain agreement with increasingly delicate experimental observations.

We turn now to describe and consider carefully the simplest topological model for soap froth dynamics, developed and used extensively by many investigators\cite{13,14,16,17}, which we call "model A".

**Model A:** Rather than following locations of the vertices and cell boundaries, one keeps track of the cells’ areas $a_i, i = 1, 2, \ldots N$, and their topological connectivity\cite{13,17}. Topology is contained in an adjacency matrix $T_{ij}$, which is set to be 1 if cells $i$ and $j$ are neighbors, and 0 otherwise\cite{22}. Temporal evolution is represented by integrating the von Neumann equations (1) until an area reaches the value $a_i = 0$, corresponding to disappearance of cell $i$. At this point a local rearrangement of the adjacency matrix takes place, choosing with equal probability one out of all the possible side assignments of this T2 process. Thus, even though
the precise geometry of the cells is neglected by this approach, topological correlations and the von Neumann law for temporal evolution are taken into account explicitly.

In general our simulations start with an ordered hexagonal lattice, with slightly randomized areas (i.e. set $a_i = 1 + \zeta_i$ where $\zeta_i << 1$ are taken from some distribution). A significant number of T1 transformations is performed; starting from the initial state obtained this way, and letting the froth evolve according to model $A$, we have demonstrated the following:

(a) All initial assignments of areas evolve to the same scaling state.

(b) The topological class distribution was found to be close to the experimental one, but slightly narrower; whereas the experimental value of the second moment of this distribution was $\mu_2^{\text{exp}} = 1.4 \pm 0.1$, simulations gave $\mu_2^A = 1.2$.

(c) The predicted topological distribution of the survivor cells differed from the measured one.

Regarding result (b), to our surprise mean field theory $[8]$ fits the experiments better, yielding $\mu_2^{MF} \approx 1.4$. To understand the effect of topological correlations (neglected by mean field), note that according to Aboav’s law $[23]$ a cell with a small $n$ is more likely to be the neighbor of one with a large $n$. Since ”topological dynamics”, i.e. change of TC, is caused mainly by the disappearance of $n < 6$-bubbles, clearly cells with more sides are more topologically mobile than those with small $n$. As this mobility prevalently reduces $n$, mean field, that neglects this (correlation-induced) dependence of mobility on $n$, will overestimate the number of large-sided bubbles in the (topological) steady state, thus overestimating $\mu_2$. Hence the fact that $\mu_2^A < \mu_2^{MF}$ is no surprise, but we did expect the simulation result to be the one that agrees better with experiment! Clearly some physically important aspect of the evolution (mentioned briefly in $[20,24]$ is not included in model $A$.

Important hints regarding this missing aspect came from simulations of froth evolution that start from nearly ordered initial conditions $[5,25]$ with only a few, isolated defects perturbing an ideal network of hexagonal cells. A defect is produced in the simulations by
performing a single T1 switch, replacing four adjacent hexagons by two pentagons and two heptagons. Each defect serves as a nucleation center for the growth of a cluster of non-hexagonal bubbles. Initially all the clusters evolve independently; when they become large and meet each other, they start to interact. At that time the ordered regions vanish and the froth evolves to the completely disordered, universal scaling state.

The temporal evolution of the second moment $\mu_2(t)$, as measured for these initial conditions [3], shows that the (initially very narrow) distribution broadens and $\mu_2$ increases; finally the scaling state value of 1.4 is obtained. The approach to this value is, however, non-monotonic! $\mu_2(t)$ was demonstrated [3] to exhibit a remarkable peak value of $\mu_2 \approx 2.6$. Microscopic [18] simulations [23] of evolution from a similar initial state, working with only about 500 cells, reproduced such a peak, but with the lower value of $\mu_2 \approx 1.9$.

We performed extensive simulations of evolution from similar initial conditions. Using model A, we never succeeded to produce a peak; $\mu_2$ grew monotonously (up to fluctuations that were smoothed out by averaging the data over several runs - see Fig. 1). A related deficiency of model A became evident when results of a recent study of the single cluster problem [14] were re-analyzed. This study showed by a mean field calculation and by simulations (using model A), that the topological distribution of the bubbles that belong to the growing cluster approaches a fixed form when the cluster becomes large. Weaire [15] noticed that the width of this distribution [14], $\mu_2 = 0.72$, is too small to be consistent with the experimentally obtained large peak of $\mu_2$. Indeed, as anticipated by Weaire, our subsequent simulations of a froth with isolated defects yielded only a monotonously growing $\mu_2$. This striking failure of model A prompted us to look closely also at the results (b) - (c) listed above, to identify the element that is missing from this model, and to eliminate the discrepancies by incorporating it in our topological simulations.

Model A uses the exact von Neumann equations on a topologically correct network of cells; hence this phase of the evolution is treated exactly. An uncontrolled approximation (made when bubbles disappear) is that the topological rearrangement that takes place occurs at random, selecting one of all possible outcomes with equal probability.
The assumption of random topological rearrangements is not too bad for the scaling regime, where the froth is macroscopically isotropic and homogeneous, but breaks down in the transient period of the evolution from the initial state with isolated defects. In this period the froth contains fairly isolated clusters, embedded in an inert region of small hexagons. The interior of these clusters contains large bubbles with many sides, while their boundaries contain a relatively high concentration of small \( n < 6 \) cells [5]. Typically, one of the neighbors of such a cell with \( n < 6 \) is a very large bubble, while the other \( n - 1 \) are small cells. Photographs of the froth shows that the edge shared with the large cell is nearly always much longer than the edges shared with the small cells. As a result of this, the cell with the large area rarely loses a side during the topological rearrangement that follows the disappearance of the \( n < 6 \) cell. This correlation between the areas of the neighbors and the topological rearrangement that takes place in a T2 process was completely neglected by model A. These correlations can have a considerable effect when the areas of the neighbors of a disappearing cell are significantly different [26]. Since area is correlated with the number of sides [4,8] (Lewis’ law) the effect described above will reduce the rate at which cells with high \( n \) loose sides, which, in turn, will increase their number and broaden the topological distribution. To incorporate these correlation we now examine closely the manner in which a T2 process occurs. It has been argued recently [24] that when a disappearing bubble becomes much smaller than its neighbors, its shape is retained while shrinking. Therefore the identity of the shortest side is preserved till the moment when its length becomes comparable to the width of a vertex. At this point the potential barrier for a T1 switch of the shortest side decreases significantly and the froth immediately lowers its energy by a T1 process. Thus we postulate that a T2 process for pentagons starts with the disappearance of the shortest edge by a T1 process, turning a pentagon first into a rectangle, which again executes a T1 switch of its shortest edge and turns into a triangle, which simply shrinks to a point. A sequence of these processes is illustrated in Fig. 2. A similar way of executing T2-processes has been used by Weaire and Kermode [18]. This procedure eliminates all stochasticity from the froth’s evolution: once the initial state is set, evolution is completely deterministic.
In order to include the modified T2 process described above in a numerical algorithm, we need information regarding the length of the edges $l_{i,j}$ separating two neighboring cells $i$ and $j$. To extract this information from our topological model, we looked for a way to relate the lengths, $l_{i,j}$ to those properties of the bubbles that were followed anyway in our simulation, namely the cells’ connectivity and areas. To estimate $l_{i,j}$ consider a typical bubble $i$ with $n_i$ sides. Its perimeter $P_i$ is related to its area $a_i$ as $P_i^2 \sim a_i$; assuming then, as first approximation, that $l_{i,j} \sim P_i/n_i$, we have $a_i \sim (n_i l_{i,j})^2$ which, in turn, implies $l_{i,j} \sim \sqrt{a_i}/n_i$.

On the other hand, the side $l_{i,j}$ belongs to the cell $j$ as well, so that $l_{i,j} \sim \sqrt{a_j}/n_j$. Therefore, $l_{i,j} = x_{i,j} \sqrt{a_i} \sqrt{a_j}/n_i n_j$, where $x_{i,j}$ depends on the forms of the cells. Our approximation is now to assume that the $x_{i,j}$ do not vary too much from cell to cell and from side to side, i.e. $x_{i,j} \approx x_0$, where $x_0$ is the same for all sides in the froth. Since we need only estimates of the relative sizes of the sides of a cell, we hope that the error of our rough estimate is not critical. The factor $x_0$ can be dropped, and we can rewrite the result in the following final form:

$$l_{i,j} = \frac{\sqrt{a_i} \sqrt{a_j}}{n_i n_j}.$$  \hspace{1cm}  \text{(2)}

This prescription suffices to construct our modified, deterministic topological model:

**Model B** differs from model A only in the way the T2-process is performed. When a shrinking bubble reaches a critical size we calculate the lengths of its sides, using (2), and perform a T1 switch of the minimal side, until the shrinking cell is a triangle, which is reduced to a point.

$\mu_2(t)$, obtained from simulations that start with an ordered array of hexagons of slightly randomized areas, perturbed by a small concentration of randomly scattered defects, is presented in Fig. 1. The main qualitative distinction between the results of the two models is the existence of the pronounced peak. In addition, the value of $\mu_2$ in the scaling regime is now also in agreement with the experimentally obtained $\mu_2 = 1.4 \pm 0.1$. Our success in eliminating these discrepancies between experiment and the previously used topological model indicates that we have indeed identified correctly the source of the disagreement.
On the other hand, it should be noted that the magnitude of the peak, $\mu = 1.76$, differs from the experimental value $\mu_2 = 2.6$, but is rather close to 1.9, the result of Weaire and Lei [25]. Apparently these two approaches have a common reason for the discrepancy, and the difference between our simulations and the experiment is not due to the approximation implicit in the purely topological nature of our approach.

At early stages when the froth consists of well-separated well developed clusters, there are very large differences between the areas of the cells in the clusters’ interior versus perimeter and exterior. The control parameter $\sqrt{a/n}$ is much larger for the large bubbles, and the modified rearrangement rules have a considerable effect. In the scaling state of the froth, when there are no such huge differences between the areas of the neighbors, the control ratio is nearly constant for all $n$ that occur with significant density [27]. Therefore in the scaling state the various topological rearrangements occur more or less randomly with equal probabilities, and model A describes the scaling regime rather well. Nevertheless, the control ratio still increases slightly [27] with $n$, making bubbles with large $n$ less likely to loose a side when model B is used, which explains why $\mu_B^2 \approx 1.4 > 1.2 \approx \mu_A^2$.

We used model B on two other problems where model A has failed. First, we simulated the single cluster problem. We found that as in our previous study (that used model A), the topological distribution function of the growing cluster approaches a fixed form. As one could expect, model B gives a broader distribution than model A; $\mu_A^2 \approx 0.7 < 1.1 \approx \mu_B^2$.

Lastly, we rerun simulations of a large number of cells, and measured again the topological distribution of the survivor population [13]. Preliminary results indicate that the distribution obtained using model B is in excellent agreement with experiment, whereas that of model A was significantly off [27].

Note that mean field neglects all correlations - topological, as well as those introduced here (that depend on the areas). As discussed earlier, topological correlations tend to increase the rate at which cells with large $n$ shed their sides (sharpening the topological distribution), whereas the area-dependent correlations reduce this rate (broadening it). Thus the two effects act with opposite signs, which explains why mean field gave, in the scaling
state, a distribution whose width was closer to experiment than that obtained by model A.

In summary, we demonstrated that the manner in which the topological rearrangement that follows a T2 process is performed has a strong effect on the dynamics. The previously used natural choice of selecting the rearrangement at random, assigning equal probability to every possible outcome, gives sometimes qualitatively incorrect results. In real froth dynamics the outcome of the T2-process is strongly correlated with the areas of the neighbors of the disappearing bubble. The effect of these correlations is especially pronounced in the transient period of the evolution from a highly ordered initial state. In this case the experiments show a remarkable peak of $\mu_2(t)$, the width of the topological distribution function, which cannot be reproduced without taking into account the area-dependence of the T2-processes. We succeeded to incorporate these correlations in our topological model without making it more involved computationally. The results of the new model agree much better with a variety of experimental results than the previous model.

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FIG. 1. The second moment of the topological distribution of the froth, $\mu_2$ vs. the mean area of the cells, for models A (full squares) and B (circles). In all simulations the initial configuration contains 1000 defects, placed randomly in a regular array of 40000 hexagons. Each curve presents data averaged over 6 runs. The curve obtained using model B exhibits a peak and gives an asymptotic value in agreement with the experimental one measured in the scaling state (1.4).
FIG. 2. Disappearance of a pentagon occurs in three stages: Solid line: just before the T2-process; Dashed line: after a T1 switch of the shortest side the pentagon turns into a rectangle; Dotted line: after a T1 switch of its shortest side the square becomes a triangle, which then shrinks to a point.