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Tile automaton in the well-mixed medium

Tomoyuki Yamamoto [a,*], Kunihiko Kaneko [b]

[a] School of Knowledge Science, Japan Advanced Institute of Science and Technlogy, 1-1 Asahidai, Tatsunokuchi, Ishikawa 923-1292, Japan
[b] Department of Pure and Applied Sciences, University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8902, Japan

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Abstract

By introducing a mean-field version of the tile automaton model introduced in earlier works, growth of molecules through chemical reaction networks is studied with explicit consideration for molecule shape as a “tile”. Tiles are picked up randomly to collide, and with a certain rule they react to form new tiles. A non-trivial growth pattern, called joint growth is found, with which tiles grow by combining tiles successively. This joint growth leads to a power-law distribution of tile sizes, by forming a positive feedback process for reproduction of tiles through cooperative relationship among large tiles. This effective growth is achieved by spontaneous differentiation of time scales: quick process for an autocatalytic network and a slower process with joint growth. We also discuss the relevance of the present results to the origin of life as a loose set of reproducting chemicals.

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Keywords: Non-trivial growth process; Differentiation of time scales; Cooperative relationship; Origin of life; Threshold phenomenon

1. Introduction

While chemical activity of biological molecules are well studied, it is still unclear how the chemical evolution has progressed: especially, we are interested in the origin and evolution of the metabolic system.

The metabolic system is sustained by enzymes, which establish the specificity of the chemical reaction network against side reactions. However, a high specificity from the first stage of life is rather unlikely. Hence, we assume that early life (or a pre-biotic chemical reaction network system) is based on non-specific chemical reactions and its flexibility allows for the search of a reaction with higher specificity, efficiency, stability, or complexity.

In the present paper, we try to realize such evolution by modifying the tile automaton models [14–16]. In the model, the reaction pathways depend on the shape of molecules and configuration (i.e., the angle of collision). Then, diverse pathways are potentially included by making use of the combinatorial variety of shapes. We think that this diversity played an important role in early chemical evolution.

Here we take a model with a well stirred “soup” by adopting the random collision rule and disregard spatial variation, in contrast with the original tile model, where “mechanical” behaviors emerge through the spatial arrangement of molecules (i.e., tiles) [16]. The spatial aspect is included only as the shape of tiles and the collision angles.

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[*] Corresponding author. Tel.: +81-761-511748; fax: +81-761-511149.
E-mail address: t-yama@jaist.ac.jp (T. Yamamoto).

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Note that the possible number of configurations increase rapidly as tiles become larger and their shape become more complicated. Then, we expect that some pathways are spontaneously selected through the reproduction of molecules, depending on the chemical network. As we will show, we find the formation of cooperative relationship among large tiles to maintain their growth against decomposition (see Section 3.4.2), which may correspond to the emergence of enzymatic function.

This feature may correspond an exploitation of combinatorial complexity, since we expect that the number of possible configurations and of the reaction pathways increases as large tiles are formed. The algorithmic chemistry by Fontana [5,6] discusses a similar problem. In Fontana's models, a formula of λ-calculus resembles a chemical molecule and the application between two "molecules" stands for the chemical reaction. Then the combinatorial variety of calculus is used and the result of reaction can be diverse. The most remarkable difference between Fontana's models and our models lies in the assumption of the time scale of the reaction. In Fontana's model, the reaction is allowed to take infinite time (i.e., until the calculation ends) and large modifications of molecule shape is allowed. In other words, this model assumes relaxation for each reaction. In contrast, in our model, only local changes of shape are applied and a short time scale is assumed for each reaction. Relaxation is not assumed and single reaction in our model corresponds to the intermediate stage of Fontana's models. Then by our model, it is possible to see the dynamical aspect of the reaction.

As a result, an interesting feature is found in our model with explicit consideration of the shape; while the polymerization in a well-mixed medium is thought to be difficult since alignment is rarely satisfied, the growth of molecule is obtained in our model. As described later (see Section 3.4), such growth in size can be realized as a side effect.

Note that there are autocatalytic pathways among tiny tiles. Such small tiles work as depolymerizing agents and any large tile can be decomposed. It follows that the growth of tiles against decomposition is not easy. The most important driving force for the growth, as we will find, comes from the formation of a "cooperation" between large tiles. Unlike Kaufmann's autocatalytic network [12], this cooperation is not based on pre-defined catalytic pathways, but depends on specific shape and configuration (i.e., angle of collision). Also, this cooperation emerges from diverse patterns of reactions and has a non-trivial positive feedback process, unlike the pattern-matching catalysis of Bagley et al. [1,2].

The organization of this paper is as follows. Section 2 describes the model. The behavior of the model is given in Section 3. In Section 4, we discuss the mechanism for the growth and cooperative relationship. Finally, conclusion is stated in Section 5.

2. Model

The tile, which represents a molecule, is represented as a set of connected unit squares (i.e., cells). No internal state in a molecule is considered. All tiles are kept in a "soup" and random collision is adopted.

Chemical reactions are represented as a change of tiles' shape and size, induced by collisions. Tiles are selected randomly to collide and the configuration for the collision (i.e., angle of collision) is also chosen at random. As described below, the outcome of a reaction is given by the application of deterministic transition rules, similar to cellular automata.

The protocol of the model is shown in Fig. 1. After tiles are chosen and a complex of random configuration is formed, the overlapping length is checked. Complex that are too dense are not allowed to react. This reaction rule is based on the previous tile automaton models [14–16].

We assume that a period of time is required for reaction and dissolution of a complex. Complexes wait in the tank in an intermediate state. Note that the complexes may collide again (i.e., be chosen again) during this wait, and a three-body reaction is possible. It follows that a densely packed complex can react through multiple collisions. After the reaction or dissolution of a complex, the tiles are put back to the soup.

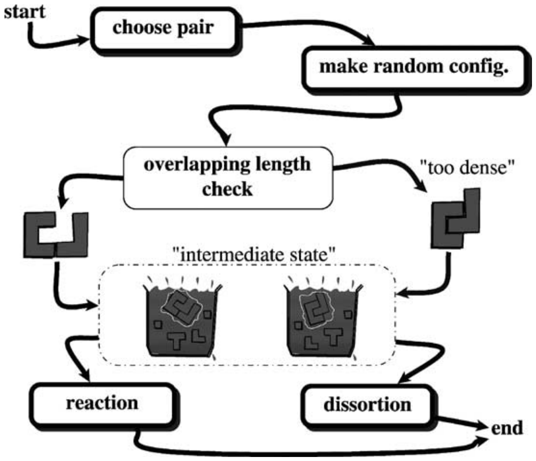

Fig. 1. The protocol of the model. See text for detail.

Boundary conditions are chosen as follows. There are upper limits for both population and density, to keep approximate chemostat condition. Also, tiles no larger than 5 are preserved, once they appear. We suppose such tiles are supplied as input flux. Since this model is not based on population dynamics but on individual population, amplification is required to support the evolution of pathways. The effect of this feature is discussed later (see Section 3.4.1).

We assume there are only a few small tiles in the beginning. The typical initial condition consists of tiny tiles only (size 1 or 2). For more details of the model and parameters, see Appendix A.

2.1. Reaction rule

The reaction is restricted by the reacting zone (i.e., the neighborhood of colliding sites), as shown in Fig. 2. The use of local reaction rules allows for the extension of single body reactions to multibody reactions, by simply joining the reacting zones.

Similar to the tile automaton model, the rule of reaction inverts the states within the reacting zone (see examples in Figs. 3 and 4). Here, each cell has a state of either 0 (empty space) or 1 (occupied by a cell). Note that the total area is not conserved by the reaction.

The tiles are rearranged after the reaction. Depending on the configuration, the tiles may join, break, or new tiles may be created.

2.2. Rate rule

The occurrence of the reaction could be suppressed. After a complex is formed, the overlapping length is evaluated by the rate rule and reaction is prohibited when the length is big (i.e., densely packed). The overlapping length is represented by the “cell ratio” (the ratio of occupied cells in the reacting zone) and upper limit is adopted for allowing the reaction.

This rule suppresses the decrease of total mass of tiles, because the production rate is given by the ratio of occupied cells in the reacting zone. The upper limit of the cell ratio (r_H) is usually 0.55, where decrease of total area is allowed.

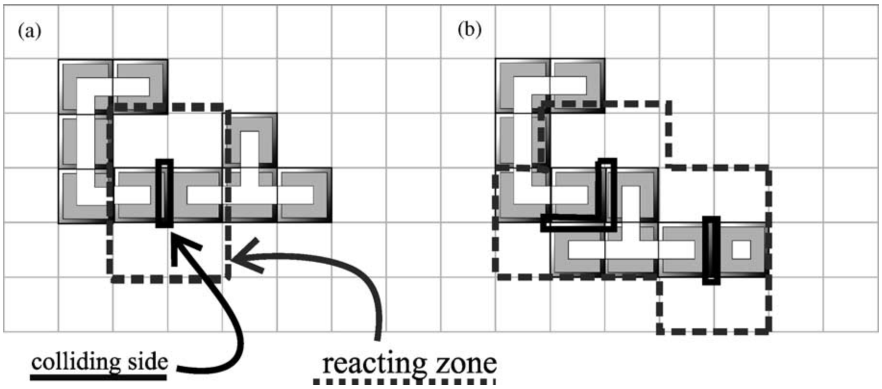

Fig. 2. (a) The colliding side and the reacting zone are shown. The reacting zone is the nearest neighbor of the colliding side. (b) When there are more than one colliding side, the corresponding reacting zones are simply joined.

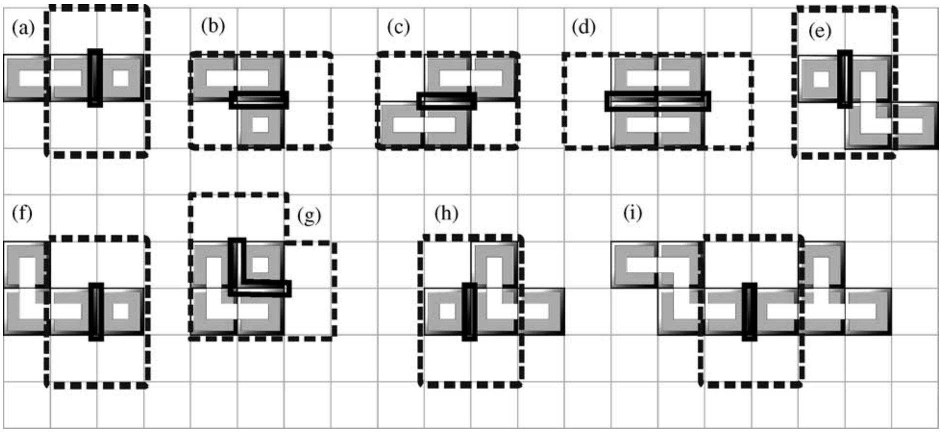

Fig. 3. Before the reaction. The areas covered by the reacting zones vary, depending on the configuration.

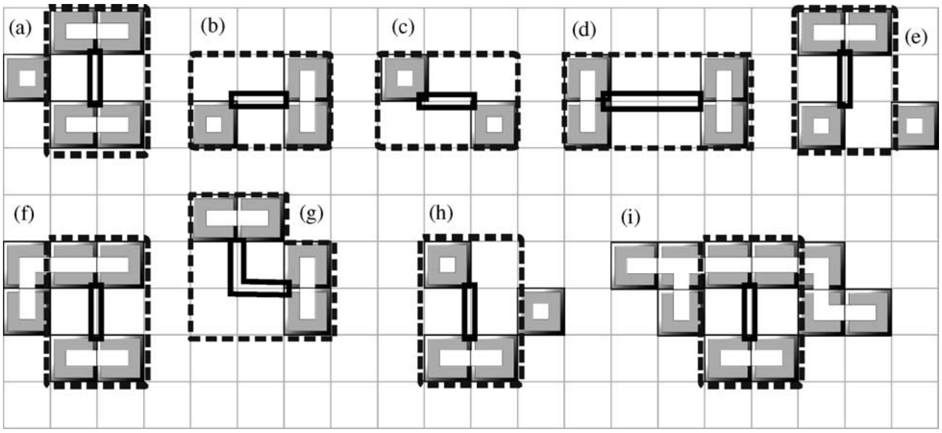

Fig. 4. After the reaction. Differences on the configurations result in a large difference. (a) A rectangle is reproduced. (b, d) The total area is conserved and tiles are also conserved, though rotated. (c) The total area decreases. (e, g, h) The total area is conserved, but L-shape is broken. (f) An L-shape is extended. Note that from all possible configurations of an L-shape and a square, only one case preserves a curved shape. The importance of L-shape area is shown in case (i), where two tiles join.

Examples are shown in Fig. 5. Note that the ratio depends on configurations, in the cases (a)–(e), the difference of configurations give different respective cell ratios. Besides, in (d) and (e), the reaction is suppressed in the case (e) and whether a reaction occurs or not is controlled by a small tile on the left hand side.

3. Results

3.1. Overview

A typical snapshot of the simulation of our model is shown in Fig. 6. While specific shapes of tiles that are created depend on the initial conditions including random seeds the diversity of size of tiles is almost same. The average size of the largest tile is about 120. The growth of tiles is generally observed (see Fig. 8), and sustained in the presence of random elimination of tiles.

The population sizes of “tiny” tiles (size 1 or 2, see below for the definition) are large, which replicate by autocatalytic process as will be shown. Tiles of size 3–5 cannot reproduce by themselves, and are supplied. We show later that, according to the present rule, there is no autocatalytic pathway except the tiny tiles of size 1–2 (see Section 3.2).

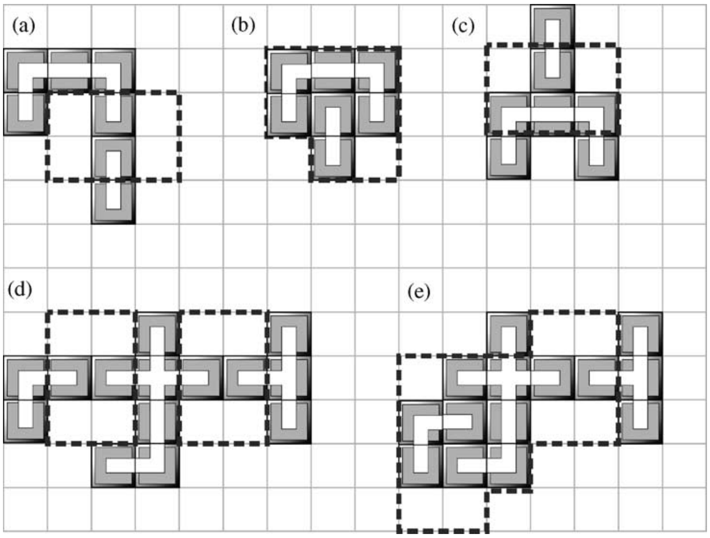

Fig. 5. The cell ratio depends on the configuration. The cell ratios are, respectively (a) 1/3, (b) 7/8, (c) 2/3, (d) 1/3 and (e) 10/17. When r_H is 0.5, the reaction is allowed for (a) and (d). Since the tiles are identical for (a)–(e), respectively, the reaction pathway largely depends on the configuration. Also, on (d) and (e), the position of an L-shaped tile determines if the reaction occurs or not.

When a large tile reacts by colliding with a tiny tile, it is more likely to be decomposed (see Fig. 11) than grow. If there is no input flux, any tile is decomposed into tiny ones and only tiles of size 1–2 remain. In other words, the system relaxes to an equilibrium state consisting only of tiny tiles. Hence, the growth of tiles is not a trivial process. Later, we see that there are two different mechanisms for growth: one is the “joint growth”, growth by joining large tiles (i.e., larger than about 20) where a cooperative relationship among them is observed. The other is the aggregation process by adding tiny tiles in a step-by-step manner, as an independent process for each growing tile. Of course, collision with a tiny tile is most frequent and aggregation is widely seen for all kinds of tiles. However, such collisions may lead to decomposition. Hence the growth by aggregation is rather slow, as shown later (see Section 3.4.2). In contrast, the configurations of collisions resulting in joint growth is limited, and patterns of joinable shapes are also limited. While the speed of joint growth is significantly faster than that of aggregation, once achieved, the probability of occurrence of a configuration or distribution of tiles that allows for joint growth is small. Indeed, the growth of tiles is accelerated by achieving the distribution of tiles, so that they survive from collisions with tiny tiles. Joint growth works only for large tiles.

Now we examine the conditions for joint growth. Conditions are satisfied and maintained only if the distribution of large tiles reaches some level, and joint growth has a threshold-type dependence on the input flux of small tiles (see Section 3.4.1). In Section 3.4.2, we will show that this threshold-type behavior is originated in “cooperative” relationships among large tiles, leading to a positive feedback process that produces larger tiles.

Although the growth itself looks similar to what is observed by Bagley et al. [1,2] in an autocatalytic network, there is an important difference. Bugrey et al. explicitly implemented the catalysis in advance, so that the growth was possible. In our model, since the shapes change by reactions, and the product of each reaction does not necessarily continue further: the larger the tiles grow, the less prone against decomposition they become, and a cooperative relationship (i.e., joint growth) among large tiles emerges. In fact, this difference in the growth mechanism leads to a drastic change in the distribution of tile sizes. In our case the

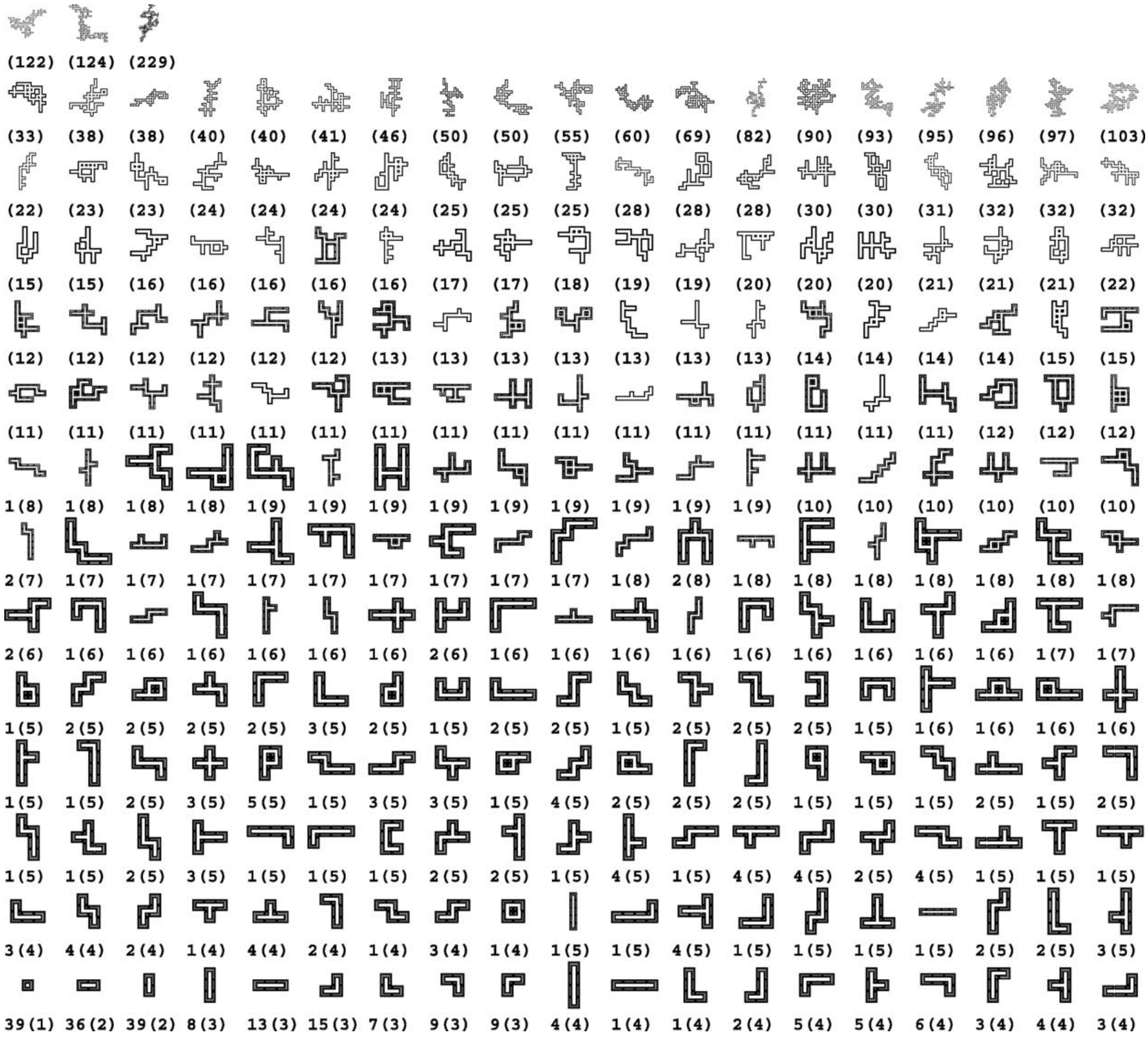

Fig. 6. A snapshot of simulation. The tiles are sorted the size, from bottom left to top right. The number in brackets is the size and whenever it appears the number outside the brackets is the population size.

distribution of size has a long tail with a power law, while in the study by Bagley et al., the distribution decays exponentially. This demonstrates the efficiency of joint growth.

The effective growth of tiles proceeds, with the reaction pathways shown schematically in Fig. 7. Two cases for growth, aggregation, and joint growth are shown by the arrows, where the bifurcation of branches of a pathway is due to the reaction at a different configuration of collision. As we show later, the tiles are classified into four zones with regards to the growth pattern, depending on the size of tiles.

- Zone A (tiny tiles; size 1 and 2): the tiles form an autocatalytic network of reproduction. Within the network of all possible two-body reactions, these tiles form a closed set and no other tile is created by two-body reaction. On the other hand, all tiles with

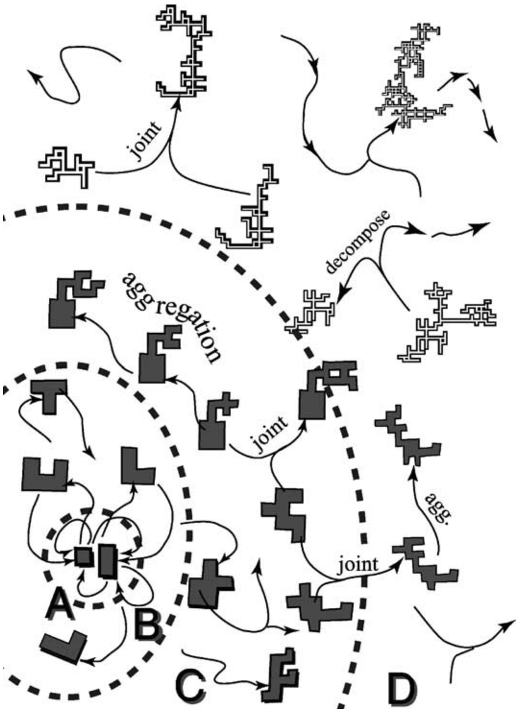

Fig. 7. A schematic picture of the reaction pathways. Zones are classified by tiles' sizes. A: 1–2, B: 3–5, C: 6–19, D: ≥20 (shown in shadowed letters). Schematic images of joint growth and aggregation are also shown (denoted by "joint" and "aggregation", respectively). Note the difference in reaction products between joint growth and aggregation.

size 1 or 2 reproduces by themselves through autocatalytic process. If there is no input flux, only this network remains since larger tiles are decomposed while the tiles of zone A are preserved by autocatalytic reactions. Accordingly, the network of zone A is called the minimal network (see Section 3.2 for details).

- Zone B (small tiles; size 3–5): the tiles in zone B are supplied as input flux, as shown in Section 2. Small tiles do not disappear once created.

  Indeed, the input flux is necessary to keep the growth of tiles, since curved tiles, which are essential for growth, are included in this zone. We should note that there is no autocatalytic pathway outside zone A. Small tiles are supplied but they do not replicate. They are consumed to produce larger tiles.

- Zone C (medium tiles; size 6–19): the tiles in this zone are not supplied from the outside; instead they are formed from the reaction of small tiles of zone A and B. In this zone, tiles are not large enough to continue joint growth. The tiles have some joinable parts but they cannot continuously keep on growing.

  During a collision with a tiny tile, the tiles are easily decomposed. If two tiles in this zone successfully join to form a tile in the next zone, the larger tile can continue joint growth.

- Zone D (large tiles; 20 or larger): most tiles have several parts that allow for joint growth (see Fig. 12), and they grow efficiently with joint growth (see Section 3.4). Zone D tiles are large enough to maintain their size against collisions with tiny tiles. As shown in Section 3.4.1, a positive feedback process appears: the larger a tile grows, the more stable it becomes against for the decomposition. Since a large tile may have many joinable parts with a complicated shape, the reaction with tiny tiles is suppressed by the rate rule (see Section 2.2). Although a tile may be broken into pieces (see Fig. 11), its fragments can grow again by joining with a larger tile. While the aggregation process is still working in this zone, its contribution to the growth is minor, when compared with joint growth.

We should note that joint growth includes a non-trivial growth process. Fig. 8 shows the distribution tiles' size. To obtain the histogram, we accumulated data from 70 runs. The population size distribution has a tail with a power law. The region of power-law distribution extends to a larger size with time (compare with the histograms at time 10 and 50). The increase of the power-law tail clearly shows a non-trivial growth process, supported by a positive feedback process (for more detail, see Section 3.4.2).

3.2. *The minimal network*

The minimal network is a closed subset of pathways that reproduce themselves through autocatalytic reactions. In the present model, the minimal network consists of all tiles of size 1 or 2, within which all possible reaction pathways are closed and form an autocatalytic pathway (see Fig. 9). Without

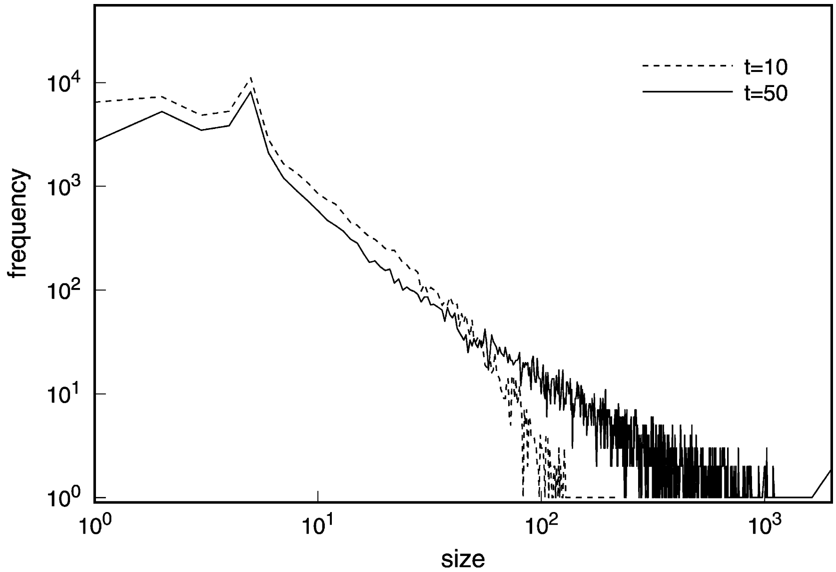

Fig. 8. Histograms of mass of tiles. Log–log plot. Two snapshots are imposed ($t = 10$ and 50). For each plot 70 runs are accumulated.

input flux (i.e., the supply of small tiles), only tiles in this network remain. Also, if only tiny tiles exist at the beginning, the diversity of tiles does not increase and only tiny tiles can reproduce. This state corresponds to an equilibrium state; no polymerization resulting in the growth of tiles is seen and only tiles that belong to the minimal network exist.

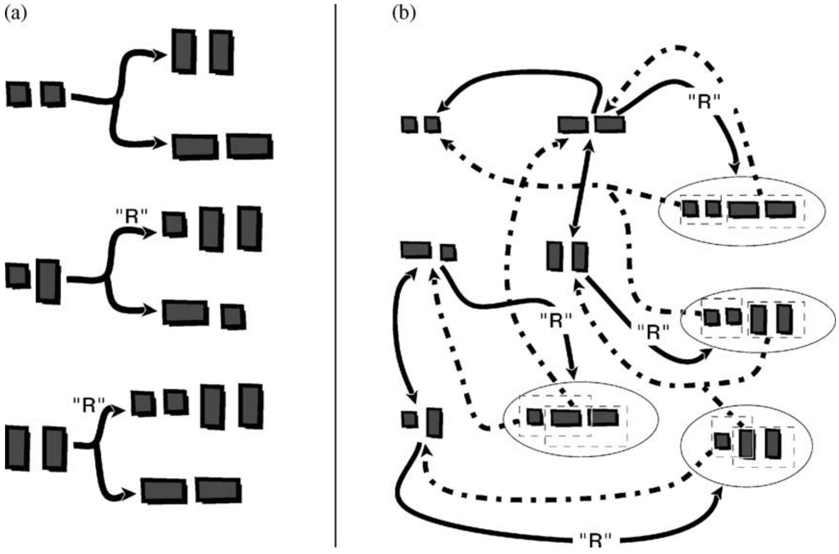

Fig. 9. The minimal network. (a) All two-body reaction pathways between tiny tiles. When the reaction paths bifurcate, they are due to collisions with different configurations. See Figs. 3 and 4 for details. (b) The minimal network. Solid lines stand for transitions due to a reaction. Dashed lines connect identical pairs. The label "R" indicates a reproducing path. Note that the minimal network is closed within tiny tiles.

The diversity of tiles shown in Fig. 6 is supported by the input flux and partially multibody reaction (see below). Note that a small tile is not supplied until it appears here at least once. The diversity is triggered by the multibody reaction. For making the diverse tile shapes by joining, at least one L-shaped tile is necessary, which is not included in the minimal network (compare case (i) of Figs. 3 and 4).

A tile is often decomposed by a reaction with tiny tiles of size 1 or 2 (see Section 3.3). Since smaller tiles are more fragile, they need to be supported by an external supply source. Then, it is important to understand how the population of larger tiles is sustained without external supply, and in spite of the decomposition by the tiny tiles. This mechanism is examined in Section 3.3.

To enhance the pathways beyond the minimal network, at least one small tile is required. In particular, an L-shaped area is required for joining two tiles. Fig. 10 shows how an L-shaped tile is made only with tiny tiles through a multibody collision. However, the large tile is fragilised by collisions with tiny tiles. In Figs. 3 and 4, out of all possible configurations for collisions ((e)–(h)), only one case (f) preserves the curved shape. The curved tiles of small size may be decomposed before they join and increase their respective size. Then, to obtain diverse pathways, the small tiles have to be supplied in order to start further growth process (see Section 3.4.1).

3.3. Joint growth vs. decomposition

As generic features of reactions, we suggest two tendencies. One is decomposition, whereby a tile is broken by reacting with tiny tiles. The other is growth, which contributes to diversity and comes against decomposition. In this section, we study both tendencies in detail and discuss how they oppose each other. Although growth is supported by the input flux, it is robust to a certain extent, as is described below.

The conflict between growth and decomposition may correspond to two stable equilibria of Dyson's model [3] of the origin of life. In his model, there are two equilibrium states: one is an active state where peptides are "alive" in an autocatalytic manner and the other is an inactive state which corresponds to a "dead" state. In our model, those two equilibria correspond to states with growth and decomposition, respectively. Also, in Dyson's model, there is an unstable equilibrium state between them. Indeed a jump from the "dead" state to the "alive" state is possible. While its driving force is the size of polymer in Dyson's model, in our model, the driving force will be shown to be a "cooperative" relationship between large tiles: the possibility for the jump is defined as the probability of collision between large tiles. Although this probability is defined by the density of the input flux, we should note that the cooperative relationship

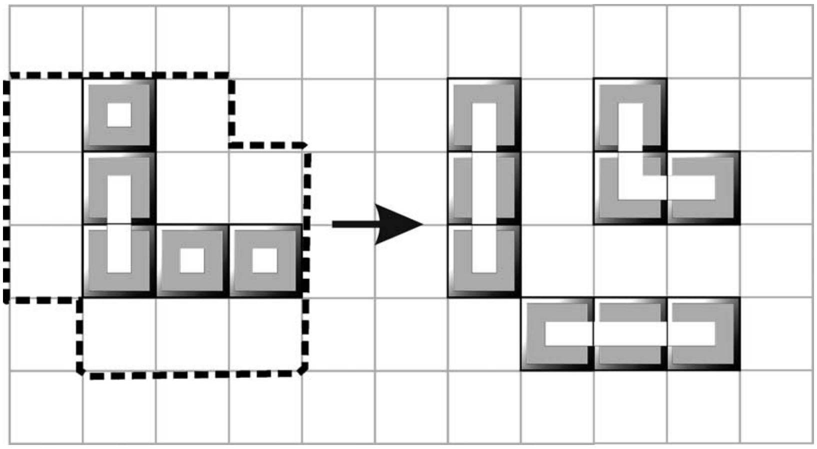

Fig. 10. An example of formation of L-shaped tile. This shape cannot be formed by a two-body reaction between tiny tiles.

between large tiles is not explicitly defined by the rule of reaction and hence is an emergent behavior.

Next, let us study the mechanisms for growth. In fact, there are two mechanisms; joint growth and aggregation. The former is a quick growth process of tiles realized by combining large tiles. The latter is a rather trivial and a slower process, like diffusion limited aggregation (DLA) [8]. Joint growth progresses faster than decomposition and works well even if the input flux is low. This feature is important, since the decomposition has a driving force to bring back the system to the "dead" equilibrium. A strong counter force is thus required to keep the system "alive".

While the joining of tiles is ultimately allowed by the reaction rule, a continuous joining process is not a trivial phenomenon. Since tiles are continuously decomposed, collisions between large tiles should take place frequently. For instance, if there is only one large tile, it cannot maintain its size. While large tiles may be formed by aggregation, they must also meet together in order to sustain their size. Since the configuration of collision is randomly chosen and appropriate configuration for joining is limited, joint growth must be quite unstable in the beginning. Then, a threshold-like phenomenon is expected (see Section 3.4.1); as the number of large tiles increases by joint growth, a positive feedback process sustains itself (see Section 3.4).

Conversely, decomposition is a much more stable process than joint growth. Decomposition is likely to occur when some tile reacts with a tiny tile. While the tiles may join to form a single tile, their mass increases only little. Since the reaction is restricted to the neighborhood of colliding sites and the mass increases at most by the size of reacting zones. A step-by-step growth is difficult (see Section 3.4.1 for simulation) when the input flux is low. Also, the tiny tiles form the minimal network and they usually occupy a large proportion of the total population. Hence the collision with a tiny tile occurs with higher probability. The decomposition process must thus be very efficient.

In the worst case, a large tile can be cut into two parts. Fig. 11 shows that even a large tile can be easily broken when reacting with a tiny tile. A W-shaped region, as shown in Fig. 11(f), is a typical vulnerability for a large tile. With this type of reaction, the size of the tile decreases drastically. In fact, a tile can be decomposed into tiny tiles after a few steps.

3.4. Joint growth

We now study joint growth in more detail. Generally speaking, joint growth is faster when the reaction involves larger tiles. As in zone D (see Section 3.1 and Fig. 7), a rapid growth is possible by joining large tiles, when a reaction occurs between two complex-shaped tiles. In Fig. 12, several examples of joint are shown. Note that L-shapes are required on the same side as the collision. Furthermore, both tiles must be larger than the reacting zone (2×3 cells in one-side collision) and be curved to include an empty area within the reacting zone. If such joinable shapes are part of tiles, a larger tile is formed (see Fig. 16). Of course, the occurrence of joins depends on the configuration. It is not easily satisfied, and "joinable shapes" are often broken by a reaction with other configurations. In spite of this difficulty, the rapid growth obtained by joining reactions starts to appear at the zone D, which continuously supplies joinable large tiles.

This joint growth is based on a positive feedback process. The coalescence of large (i.e., joinable) tiles increases the population ratio of joinable large tiles and the probability of joint growth is increased. Also, a larger tile requires longer time to be decomposed into smaller ones. As a rough estimation, the feedback process producing larger tiles works when there are several tiles of size larger than 20. This gives the boundary between zones C and D (see Section 3.4.1). Once there is a sufficient number of tiles in zone D, joint growth becomes stable. Indeed, growth is possible even when the input flux is cut off. Even if large tiles are cut into two parts, the fragments can join with other tiles to make a stable growth again.

Figs. 13 and 14 show snapshots when the input flux is cut off. At time 15, when a rich diversity of tiles exists, we cut the input flux. Then, at time 25, tiles of intermediate sizes (i.e., zone C) have already disappeared but large tiles remain, and even grow. We should note that no stable tile keeps on existing for a long period, but large tiles continue to exist by changing their size and shape. The quick change of shapes

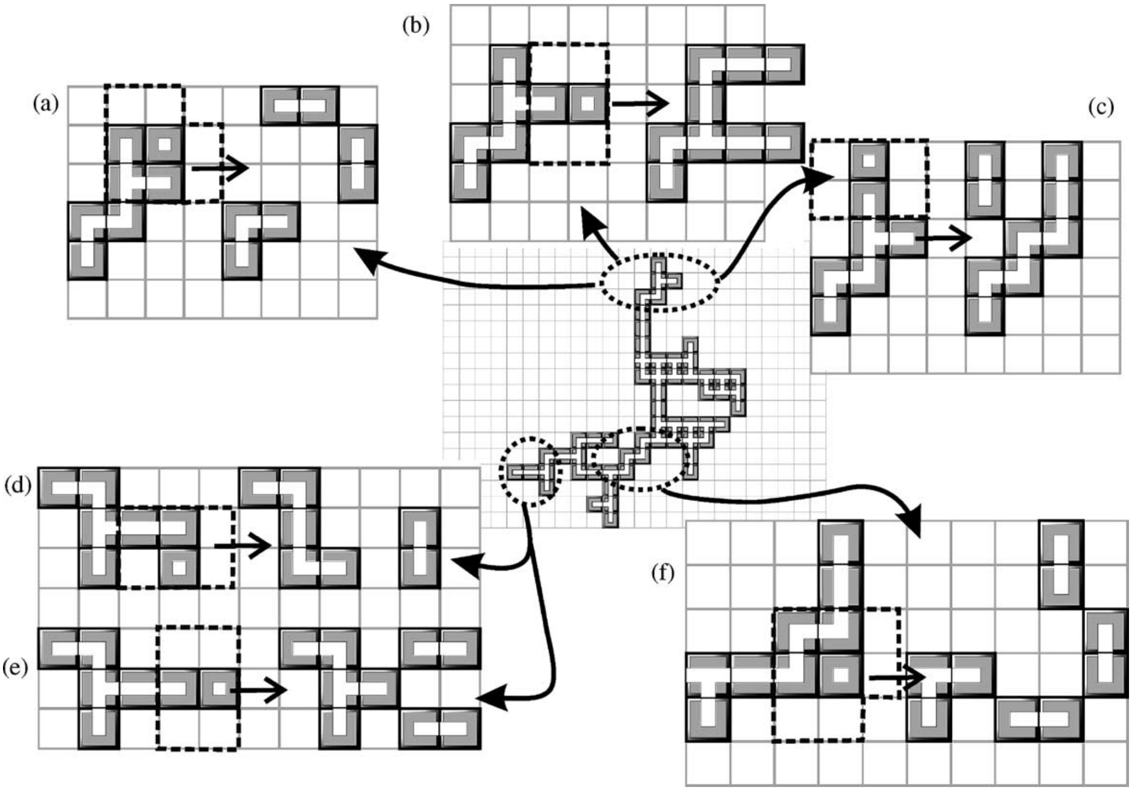

Fig. 11. A large tile can be decomposed by the reaction with smaller tiles. (a)–(c) shows a collision with the upper arm. A bulge can work as a connector, but it is not stable against a reaction with "wrong configuration". (a) A caved area is broken and three cells (L-shaped area) are disintegrated. (b, c) This configuration works as a connector, but a square is not joinable and is also broken. In case (c), the arm is transformed into a W-shape, which has weak parts (see also case (f)). (d, e) A long bulge is not joinable, but they are transformed into a short one, which has connectability. The mass is however decreased. (f) A W-shape is the weakest point and the tile is dissolved into two parts.

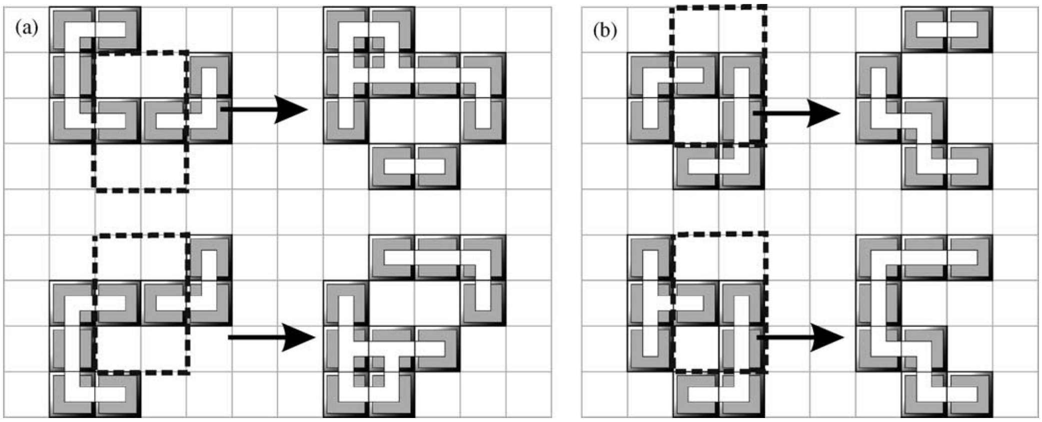

Fig. 12. Examples of joinable shapes and their dependence on the configuration. (a) The two tiles join together at the top, but not at the bottom. (b) The larger number of curved areas a tile has, the likelier it grows. Roughly speaking, the combination of a notch and an L (or U) shape gives a joinable part.

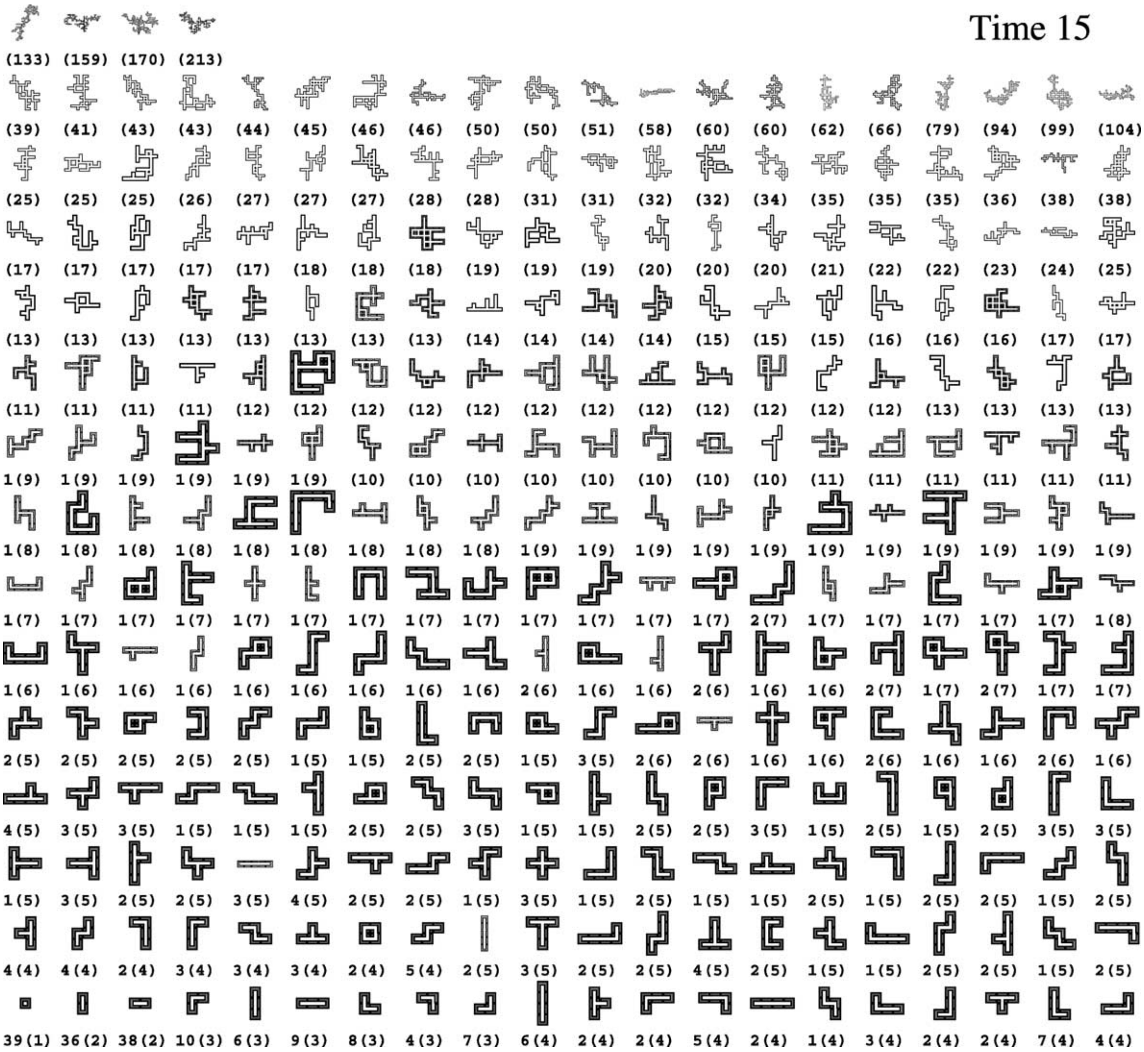

Fig. 13. A snapshot at time 15. The input flux is cut off at this moment. Shown in a similar manner as in Fig. 6.

is shown in the figures. At time 50, see Fig. 14, tiles are clearly divided into a small one (at zone A, B) and a large one (zone D). Roughly speaking, the tile size of the larger group is greater than 20, which gives an estimate for the lower size limit of joint growth.

The large tiles remain for more than 100 time units; much longer period than when the input flux is applied (15 time units). Although the shape of remaining large tiles depends on the initial condition, this behavior is commonly seen. Then, we can conclude that a set of joinable large tiles is a non-trivial self-sustaining state (i.e., maintain joint growth).

To sum up, joint growth has the following two distinctive features. First, the unit of growth is a large tile. Tiles larger than some threshold are required to keep this joint growth, stably against decomposition. Second, joint growth is provided by reactions with other large tiles or smaller fragments broken from them. Thus, the growth starts only after the population of tiles reach as a condition given by zone D. This condition is given by the distribution of tiles. Unlike DLA,

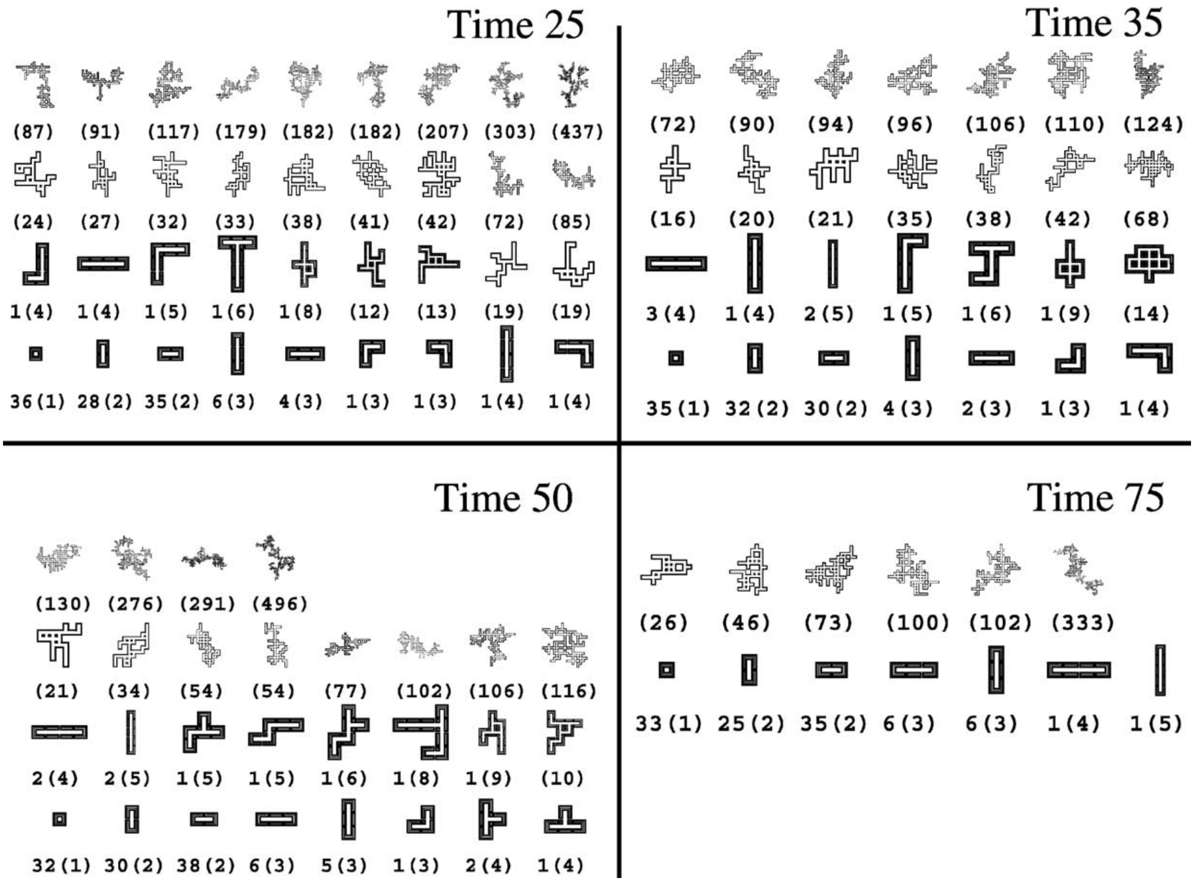

Fig. 14. Snapshot at times 25, 35, 50 and 75. After the cut off, large tiles remain with their shape and size changed.

joint growth is not possible when there is only one large tile. In Figs. 15 and 16, examples of the aggregation (i.e., DLA like process) and joint growth are, respectively, shown.

The feedback process requires a sufficient number of large tiles. It is expected that the state is reached only if the initial input flux is larger than a certain threshold. Without positive feedback process the probability to form tiles would gradually increase with the input flux, while a threshold-type dependence on the input flux is expected under the presence of a positive feedback process. The existence of the threshold-like behavior, to be shown in the next subsection, also implies the existence of a lower limit for joint growth, which gives the border between zone C and D.

3.4.1. Threshold-like dependence of joint growth on the input flux

We now examine joint growth more closely. To study the dependence of joint growth on the input flux, the percentages of such events over 100 runs that the largest tile exceeds each given limit (10, 20, 30, 50, 70 and 90) against the probability of input flux (P_s) (see Fig. 17). Here the input flux P_s is defined as follows: if a tile no larger than 5 disappears from the reaction, it is supplied with the probability P_s.

From the figure, a threshold-like behavior is clearly discernible. As P_s increases, the maximum size increase rapidly around $P_s > 0.40$. Note that for none of the runs, the maximal tile size reaches 90 when $P_s = 0.35$, while for all runs it reaches 90 when $P_s = 0.45$. This threshold-like behavior is observed for tile sizes

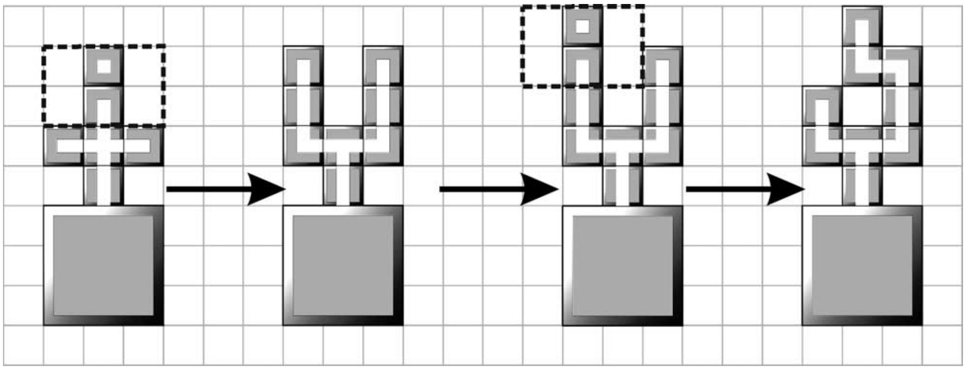

Fig. 15. An example of the aggregation process. Two consequent reactions are shown. The increase in mass is small, although the shapes change significantly.

larger than 20, while tiles of size 10–20 are commonly found around the threshold, $P_s = 0.35$–0.45. Tiles of this size are thought to supply the rapid joint growth of tiles, thus producing larger tiles.

In Fig. 18, histograms of the mass of tiles are plotted for several values of P_s, obtained from samples over 100 runs. A horizontal dotted line is the average population size 1, the minimal value expected for continuous existence. Since we expect more than one large tiles to be required to start joint growth, the lower limit for joint growth is estimated by looking for the point where the histogram for the threshold value of P_s crosses the dotted horizontal line.

As shown above, the threshold for the growth is estimated around $P_s = 0.40$–0.35. We compare the histograms for both sides of the threshold. The two histograms cross the dotted line at about size 20. For $P_s \geq 0.40$, more than one tile of size 20 exists, while none do for $P_s \leq 0.35$. Accordingly, we estimate that joint growth requires tiles of size larger than about 20. The border between zones C and D is defined by this size.

The threshold-like behavior demonstrates a positive feedback process. First, joint growth requires large tiles. As shown in Fig. 16, some special “joinable” shapes (e.g., L-shaped area) and configurations are required for coalescence. However, if a tile has an

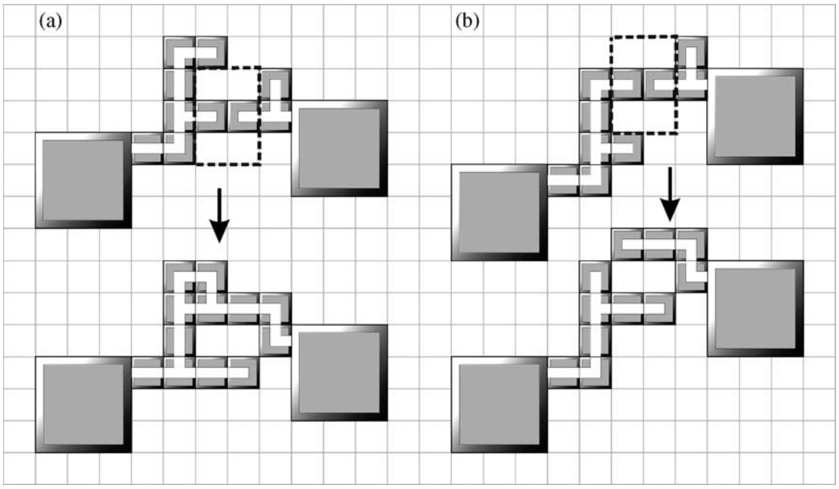

Fig. 16. (a) An example of joint growth. (b) Depending on the configuration of the collision, the same tiles as case (a) are unable to join.

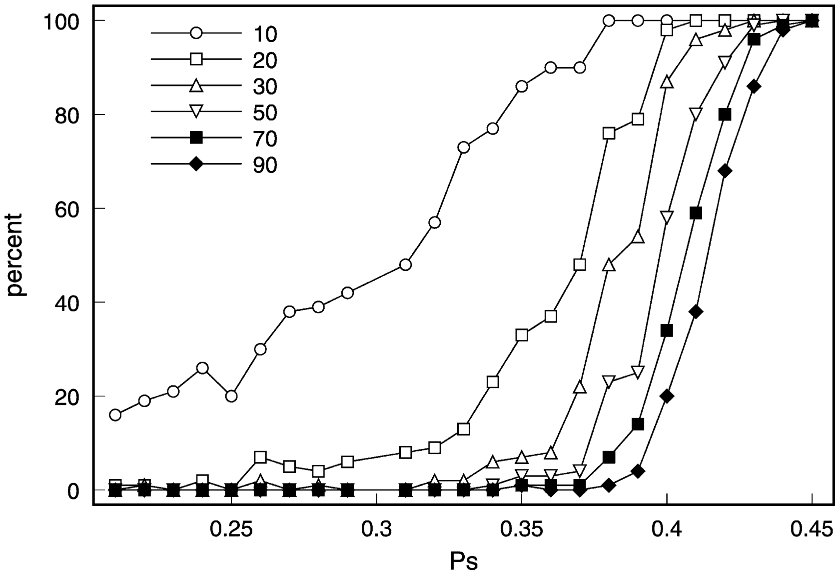

Fig. 17. The percentage of cases which have tiles larger than the listed size. Note that the plots converge as the limit size increases. One hundred samples are taken for each probability P_s.

L-shape area, it may be broken by a reaction depending on the configuration for the collision. Then, in order to continuously form a larger tile, it is important to have as many joinable shapes as possible; hence a larger tile is more advantageous for joint growth. Indeed, tiles of threshold size 20 often have several joinable areas.

Second, as a tile grows up, its stability against decomposition increases, since it has a large surface area and a complex shape. Then, by the rate rule, it is less likely to react with a tiny tile. While these large tiles have weak parts (see Fig. 11), the probability for decomposition decreases generally.

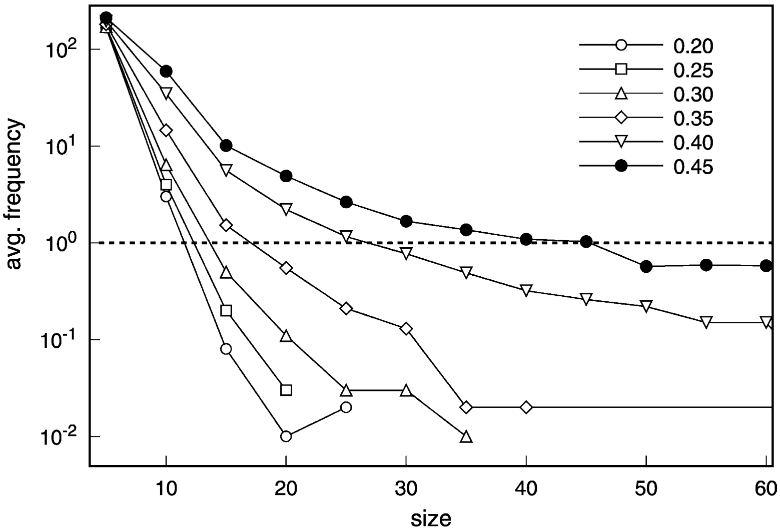

Fig. 18. Histograms of the mass of tiles with the change of P_s with semi-log scale. Averaged over 100 runs. The dotted horizontal line gives the size 1 for the average population.

Third, with the increase in population of the large tiles, the probability of collision between large tiles increases (see Section 3.4.2 for detail), contributing to joint growth. To sum up the above three features, it is expected that once a sufficient number of large tiles appear, growth is accelerated: tiles easily join together and become stable against decomposition. The growth is maintained by this positive feedback process, which supports the threshold-like behavior.

3.4.2. *Joint growth vs. aggregation*

To isolate the effect of joint growth, we modified the model by preventing joint growth. We have imposed the following two restrictions on the reaction: one prohibit the reaction between large tiles, and the other prohibits the reuse of fragments from large tiles. With these restrictions, the only possible way for the growth is the aggregation process, by successively putting together small tiles. To be more specific, the restrictions are as follows:

1. Prohibiting the reactions between large tiles: if there are more than one tiles larger than the limit l_L (typically 20), the reaction is prohibited. Here, to suppress the joining process, two tiles larger than l_L (i.e., in zone D) cannot react. However, a reaction between a tile in zone C and one in zone D is still allowed.
2. Killing fragments: among the products of the reaction involving a tile larger than the limit l_K (typically 20), all tiles smaller than l_K are eliminated. This restriction prevents cooperative relationship between a large tile and fragments from the collapse of a large tile. A fragment does not show joint growth by itself, but it may join together with a small tile or another fragment to come back to zone D. With this restriction the distinction between joint growth and the aggregation is made clear, since the reuse of fragments works as a “gray zone” between the two zones.

When the probability of the input flux is low, the latter restriction is effective: as the fragments could be used as a source for joint growth if the restriction is not included. Then, with this restriction, the threshold value for the growth is shifted to a higher probability P_s. On the other hand, the former restriction prevents large tiles from joining. Quick growth is hence suppressed.

As mentioned above, by adding these restrictions, we have plotted in Fig. 19 the probability that a maximal tile reaches a given size. Now, the plots

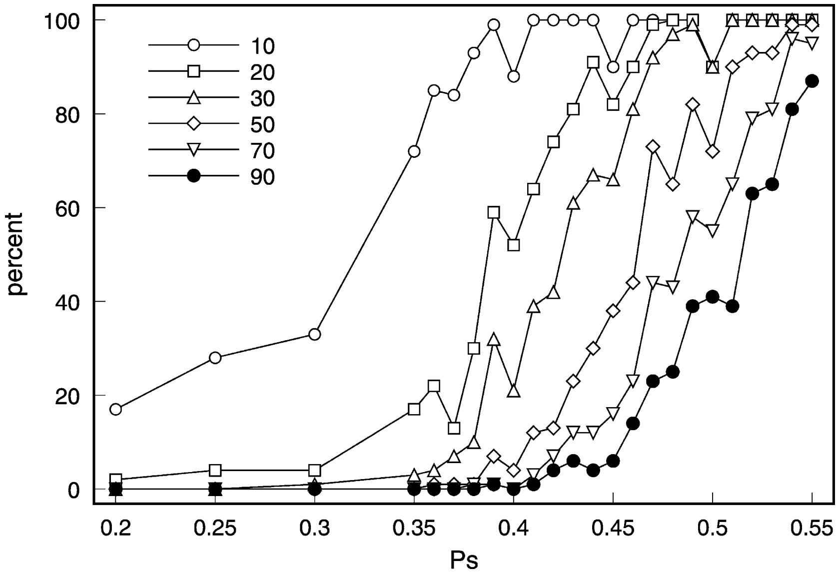

Fig. 19. Same plot as Fig. 17 with two restrictions added to eliminate joint growth. Note that more input flux is required to obtain large tiles.

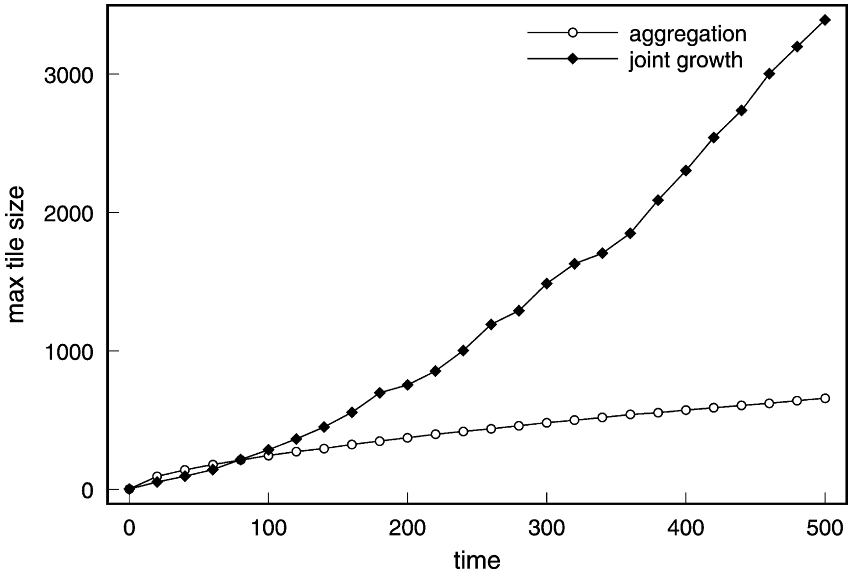

Fig. 20. The time series of the sizes of the largest tile. Averaged over 100 samples for each case.

exhibit a large fluctuation, since the aggregation process depends only on the probabilistic input flux. Threshold-like behavior is not observed. Here, we should note that the aggregation is supported by small tiles, not by tiny tiles, since the latter process always exists, due to the autocatalytic minimal network, even when P_s is zero.

Comparing Figs. 17 and 19, the aggregation process is suppressed, when P_s is low ($P_s = 0.45$) and only joint growth works. To see the difference between the

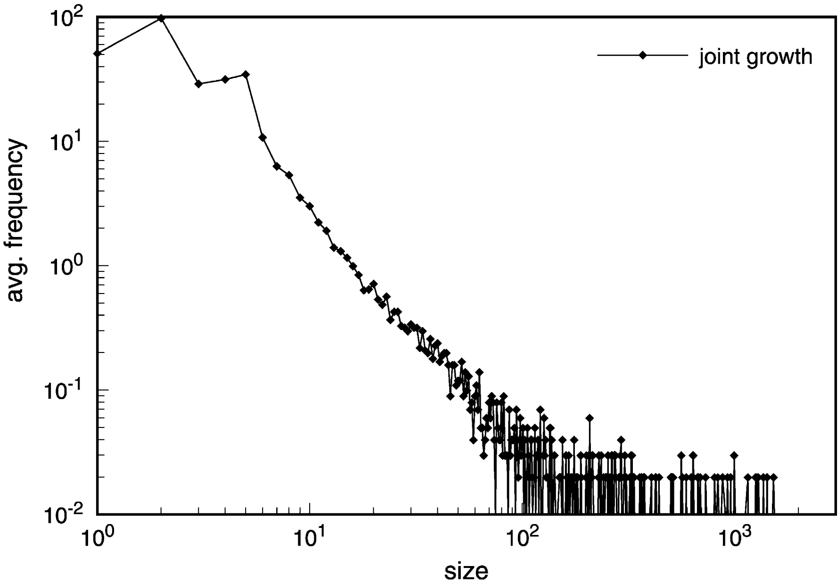

Fig. 21. Histograms of mass of tiles when $P_s = 0.45$ (joint growth case), averaged over 100 samples at time 500. Log–log plot. The plot is similar to Fig. 8.

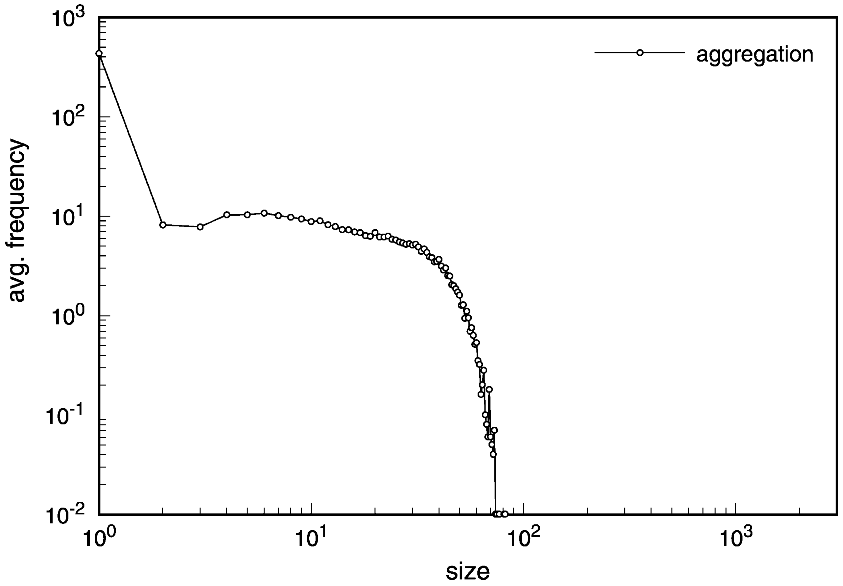

Fig. 22. Histograms of mass of tiles when the two restrictions are adopted (aggregation case), averaged over 100 samples at time 500. Log–log plot. The plot saturates, implying a slow growth.

two growth mechanisms, the following two cases are compared:

- Joint growth: P_S is set at 0.45 without additional restrictions.
- Aggregation: the above two restrictions are imposed to suppress joint growth, while P_S is set to 1.0 to amplify the aggregation.

In Fig. 20, the time series of size of the largest tile are shown for both cases, by averaging over 100 samples. The difference is clear. With aggregation only, the maximal size is suppressed. The aggregation process is slow in spite of high P_S.

The histograms of mass of tiles are shown in Fig. 21 (joint growth case) and Fig. 22 (the aggregation case), again obtained over 100 samples. Note that, for the latter "aggregation case", small tiles are supplied at a high rate (with large P_S) so that the total number of tiles is much higher. However, the mass distribution in this case is not extended to large sizes, and decays rapidly. On the other hand, for the former "joint growth" case, the distribution shows a tail with a power-law-like behavior as in Fig. 8. This power-law tail suggests the existence of a non-trivial feedback process within joint growth.

The positive feedback process leading to the power-law mass distribution can be summarized as follows; the larger a tile grows, the more frequently and stably joint growth occurs. This feedback process is strong enough to overcome decomposition.

We should note that this positive feedback process is not found in earlier models of pre-biotic evolution such as in Bagley et al. [1,2]. In fact, in their model, the mass distribution is exponential, without a power-law tail, and can be explained by a random aggregation process.

4. Discussion

In the present paper, we have studied a model of reacting molecules (tiles), to see the emergence of reproduction out of a 'soup' of molecules. We have found that growth of tiles is achieved through a positive feedback process by reaction among tiles. Notice that, in the present model, and in the absence of input flux, the system can only go to a equilibrium state, where only tiny tiles exist. The equilibrium state is brought by the minimal network, which is a closed network among tiny tiles. The tiny tiles form an autocatalytic network and increase the population which provides a supply for larger tiles. On the other hand, any large tile is easily broken apart by a collision with tiny tiles (see Fig. 11). Hence, tiles tend to be decomposed into tiny ones. To attain a non-trivial structure within the reaction network, some mechanism is essential to maintain the size of polymers (tiles).

The growth processes, the aggregation and joint growth are regarded as the driving forces to bring the system out of the equilibrium. While the former process is rather trivial, the latter one introduces a positive feedback process among the reactions, and cooperative growth among tiles is made possible, leading to a power-law distribution for tile sizes.

4.1. *Joint growth*

First, let us recall how joint growth is possible. Joint growth emerges through a cooperative behavior among tiles and is sustained by a positive feedback reaction process. We should emphasize that this cooperativity is most important in the present model, since it brings about fast and robust growth.

The cooperativity is based on joint growth of large tiles. In Fig. 20, tiles grow faster than linearly over time. Indeed, if we assume that the largest tiles join at each time step, the maximum size would increase exponentially over time. Of course, the supply of large tiles is limited, and this assumption is invalid. Hence this exponential growth does not occur, but the system still maintains a high growth speed as in our case.

Due to the positive feedback process, the reaction of large tiles does not crucially depend on the input flux. Although joint growth is supported by the input flux, large tiles keep on growing over a long time span, even when the input is cut out (see Figs. 13 and 14). Here large tiles recycle the fragments made by decomposing reactions and use them as a resource for further growth. This recycling process is also possible even when the input flux is low (see Figs. 13 and 14). Accordingly, joint growth works under a lower input flux condition than the aggregation. With this joint growth, spontaneous polymerization to form a large molecule is accelerated.

Next, let us discuss the condition to allow for joint growth following our numerical result. First, there is a selection pressure for a complicated shape. Since a tile with a simple shape is more vulnerable to a collision with tiny tiles, the tile shape becomes complicated as it grows. The formation of such complicated shapes brings about parts suitable for joint reactions.

Second, the reaction pathways have diversity, since the reaction depends on the angle of collision. The variety of possible configurations of collisions increases as tiles become larger. A larger tile can have richer pathways.

Only limited number of tile parts can join with other tiles. In order to keep continuous joint growth, the existence of several such parts is necessary, since many types of collision do not contribute to joint reaction. A large tile can have several spare joinable parts as “buffers”, to sustain joint growth against decomposition reactions. Hence a positive feedback process takes place: the larger a tile grows, the more likely it is to sustain joint growth. Among a huge variety of possible reactions, joint growth is selected under the pressure of decomposition reactions.

While the shapes allowing for joint reaction are the most important factor for the growth, the selection of specific shapes is not necessary here. Since the tile shape keeps on changing through reactions, there exists a large variety of reaction pathways. Also we should note that there is no genuine self-replication, except within the minimal network. Hence, it is difficult to attribute a given function to the shape of given individual tile, and similarly to distinguish a tile that can grow by joint process from one that cannot.

In spite of this difficulty, the population of tiles formed by the joint growth shows that the power-law-like size distribution of tiles is a remarkable difference with the exponential distribution obtained by aggregation only (see Section 3.4.2). The growth of tiles is accomplished, even though a function for each individual tile (unit) is not assigned. The growth is a collective behavior of the tiles.

The emergence of complex tiles that helps each other’s growth may suggest the spontaneous emergence of enzymatic activity. The soup of tiles in our model keeps the activity for further reproduction. Note that the reproduction here is not the accurate replication adopted by DNA and/or RNA. Our results suggest that the cooperative loss reproduction is easier to be evolved as a generic phenomenon of reacting polymers, as has also been proposed by Dyson [3] for the origin of life.

4.2. Evolution without template and emergence of temporal differentiation

Several models of autocatalytic reaction networks have already been proposed to study the origin of life [1,2,12]. These studies focus on the faithful replication of molecules (or the ensemble of molecules). In these studies, any large molecule is synthesized at once, not step-by-step. The possible reaction pathways are pre-defined by a given rule for a catalytic network. For example, the possible reaction network is defined by pattern matching of a string representing a polymer in the Bagley's model.[1] While the inversion rule in our model defines a possible reaction pathway, our rule is given only for a local reaction process. During a reaction, the modification of shape is local to the part that has collided (i.e., within the reacting zone). This prohibits trivial replication of a large tile (i.e., a tile larger than the reacting zone). There is no template that is preserved by the reaction.

Instead of using the external template for the replication, joint growth emerges from our model, through a cooperative process followed by the positive feedback process mentioned above. To make this process possible, both joint growth and a minimal network to provide small molecules are necessary. To make the coexistence of the minimal network and joint growth, the separation of time scales is important, i.e., the fast process of the minimal network and the slow process of joint growth.

In our model, the separation of time scales is achieved as follows. In the minimal network, replication of tiny tiles is completed in a single reaction, and thus the process is fast. In contrast, joint growth of a large tile is very slow, since joint reaction is possible only within a limited configuration for the collision, and its probability of occurrence is quite low. Furthermore, the growth is suppressed by the collision with tiny tiles, which can lead a large tile to decompose into tiny tiles. Indeed, decomposition is faster than growth.

Here, the size of a large tile provides a long time scale before the "relaxation" to the complete decomposition. Since joint growth is slow, a tile must be large enough to maintain its size by keeping joint growth running. The size of a large tile plays a role to separate the time scale of the two processes: the fast decomposition and the slow joint growth. On the other hand, threshold-like behavior on the input flux and the positive feedback process are supported by the separation of the time scales of the two processes.

Generally speaking, we expect that the differentiation of time scales is essential to maintain a living organism. A metabolic system has a variety of reaction pathways with different time scales organized hierarchically; energy is supplied into slower cycles from faster cycles, as seen from glycolytic to protein synthesis cycles. The resources of the slow reaction processes are supplied from fast reaction networks with the energy source.

This coexistence of different time scales is not seriously taken into account in previous models of reaction networks for the origin of life. In the hypercycle [4], the reaction rate is fixed for a cycle. There, a parasitic process can break the whole cycle, if its reaction rate is faster than its host. Then slow reaction cannot be added to the existing network. Also, other models of reaction networks such as the algorithmic chemistry [5,6] or tape-machine network [9] assume a single reaction time scale for reproduction of each molecule. Although the reaction network is topologically complex, there appears no temporally differentiation in reaction pathways.

In reality, however, the time scale for the synthesis of a large molecule would require a much longer time scale. Living organisms, in some sense, exploit the coexistence of different time scales. One possibility to include a different time scale, of course, is to

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[1] The polymerization corresponds to the growth of tile in our model.

include the compartmentization of a cell, and that cell division occurs in a much slower time scale [7,10,11]. This approach will be relevant to the study of cell differentiation and development, but here we are interested in the origin of a cellular system itself. In our study, we did not impose an external condition for a cell. Still, a longer time scale for growth is separated spontaneously.

We should also mention that explicit treatment of shape for the study of RNA world seems to be promising. In a spatially resolved model of RNA world by Yamamoto and Hogeweg [13], the shape (i.e., secondary structure) of RNA molecules is included and the "cooperative" relationship of short molecules is obtained, as an "assembly" process to reproduce long polymers. By adopting an explicit function of folded molecules, a positive feedback process may be generated.

4.3. Comparison with the spatial model

As mentioned earlier, the present "well-mixed" model is derived from the original spatial model [16]. The most remarkable difference between the two models lies in their treatment of motion. While we adopted Newtonian motion for the spatial model, the present well-mixed model assumes random collisions. This difference between the two models comes from the difference in the estimated mean free path between the collisions; it is about the unit length for the spatial model, and is about the total system size for the well-mixed model. In this sense, these two models are at the extreme limits for the mean free path.

In the spatial model, the Newtonian motion is adopted. A cluster, called factory, in which tiles keep on producing new tiles, is formed as a result of "entanglement" between two different aspects: the shape and the motion. The hooking function of a large tile is essential for realizing a factory. Since large tiles must be built within a cluster, there is a feedback process between the increase of the tile size and the growth of a cluster. Also, as the number of tiles within a cluster increases, some mechanical functions emerge, such as the formation of a rigid wall or the division of a cluster. Note that the size of a cluster determines the range of its interactions. Large tiles within a cluster increase possible configurations of collisions and the diversity of possible reaction pathways. This growth of diversity is accelerated combinatorially. Through this feedback process, the complexity of the reaction pathway increases.

The increase of possible reaction pathways is also seen in the present well-mixed model, as tile sizes increase. However, the size growth works in a different manner. As mentioned (see Section 3.4.2), the size influences the lifetime of a tile. Although most reaction processes occur among tiny tiles with a fast time scale, joint growth of a large tile has a much longer time scale.

To sum up, the growth of tiles supports the positive feedback process for the reproduction of tiles for both models. In the spatial model, this is possible by the interplay between the spatial structure and the motion, while in the present model it is achieved through the separation of time scales. Both aspects will be important to design a life-like machine.

5. Conclusion

Our result implies that chemical activity can be changed during the evolution. While major tendency of our model is to drive the system back to the equilibrium state consisting only of the minimal network, once several large tiles are formed, a positive feedback process sustains joint growth which bring the system to a non-trivial state. Large tiles join together to form a larger tile and reuse their fragments. Thus a cooperative growth of tiles is possible and the pathways that work effectively change in time.

These large tiles have complex shapes, because several parts for joining reaction are formed and a simple shape is easily decomposed by the collision with tiny tiles. The emergence of complex tiles that help growing each other may suggest the spontaneous emergence of enzymatic activity. The soup of the tiles in our model keep the activity for further reproduction. Note that the reproduction here is not an accurate replication adopted by DNA and/or RNA. Our result may suggest that the cooperative loose reproduction is easier to be evolved as a generic phenomenon of reacting polymers, as has also been proposed by Dyson [3] for the origin of life.

While we have not found a behavior corresponding enzymatic reaction, it would be interesting to adopt an external definition of enzymatic reactions. The present "well-mixed with shape" modeling allows a realistic behavior of an enzyme.

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Appendix A. Parameters and conditions

The total population is bounded by the population limit (typically 400) and the maximum density is also bounded by the density limit (typically 0.1). The population is rescaled when the total population exceeds twice the population limit. T_w (typically 0.2) gives the period of a complex, after then it either collides with a tile, or it is disintegrated. The time step is given by assuming $\mathrm{d}t = 1/N_\mathrm{tile}$, where N_tile is the total number of tiles. This assumption keeps the collision rate per tile constant.

Each time step, n_r (typically 10) pairs of tiles or complexes are selected for collision. This parameter determines the population density of complexes, which is relative to the probability of many-body reaction. Small tiles (see Section 3.1) are assumed to be supplied, and at least one of each tile with size ≤ 5 is preserved, as long as once they appear: the minimum population size is kept to 1.

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