Mathematically Modeling Parameters for a Stable RNA World

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Background on Abiogenesis

The origin of life is one of the greatest scientific mysteries of our time. Scientists have long sought a way to recreate life in the laboratory and after the Miller and Urey experiment showed that amino acids could spontaneously organize from inorganic molecules under the right conditions, (Miller, 1953) the prospect seemed closer than ever before. Many researchers attempted to push the boundaries, but issues arose in trying to go further than synthesizing simple organic molecules.

The environmental conditions necessary for the process of abiogenesis to occur have been theorized. Formation of organic molecules, the necessary components for abiogenesis, require an abundance of chemicals, extreme pressure, and a significant source of energy. These requirements serve as the guidance in determining what environment would be most likely for abiogenesis to occur in. There are competing ideas for the environmental system that is best suited to provide these conditions. Most notable are the ideas of the Darwinian pond system and the hydrothermal vent system. The Darwinian pond system posits that organic molecules were created in warm pond systems when they were exposed to energy from a source such as a lightning strike. The hydrothermal vent system however has become the prevailing idea for an environment that could lead to abiogenesis. The hydrothermal vent system posits that a constant flow of chemicals and heat energy being pushed out from a deep-sea vent from the center of the Earth coupled with the high pressure of being deep underwater creates the optimal conditions for abiogenies. The hydrothermal vent system is the system we will use when creating our model.

With the publishing of his paper, “Selforganization of Matter and the Evolution of Biological Macromolecules,” Manfred Eigen had created a new problem in the study of the origin of life, “the error threshold” which formed the basis of what is now known as the “Eigen Paradox”. This posited that RNA molecules would need error correcting enzymes to reach a length of over 100 base pairs, only for an RNA molecule to code for error correcting enzymes the RNA would need to be far larger than 100 base pairs (Eigen 1971). Thus, new ways of modeling the origin of life were necessary and many mathematical models have been put forth since.

Some recent mathematical models have used dynamical systems models such as one by Goldenfield et al., which focused on the horizontal gene transfer as being a possible solution to the Eigen paradox. We seek to represent horizontal gene transfer using a different model than what was used in this paper.

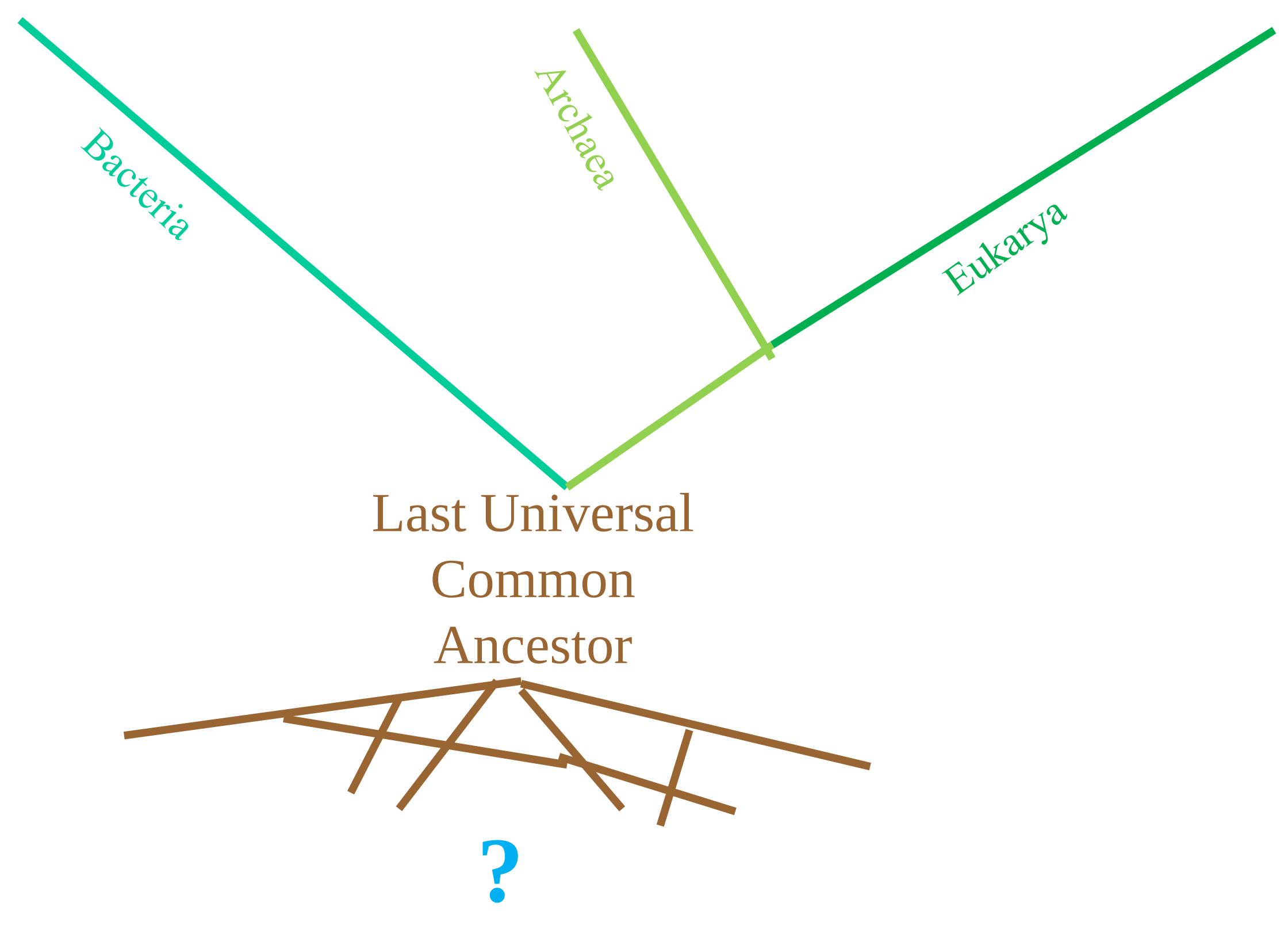

Figure 1: The conceptual evolutionary tree of life. Evolution posits that life descended from a common ancestor. How that common ancestor developed is the focus of origin of life studies.

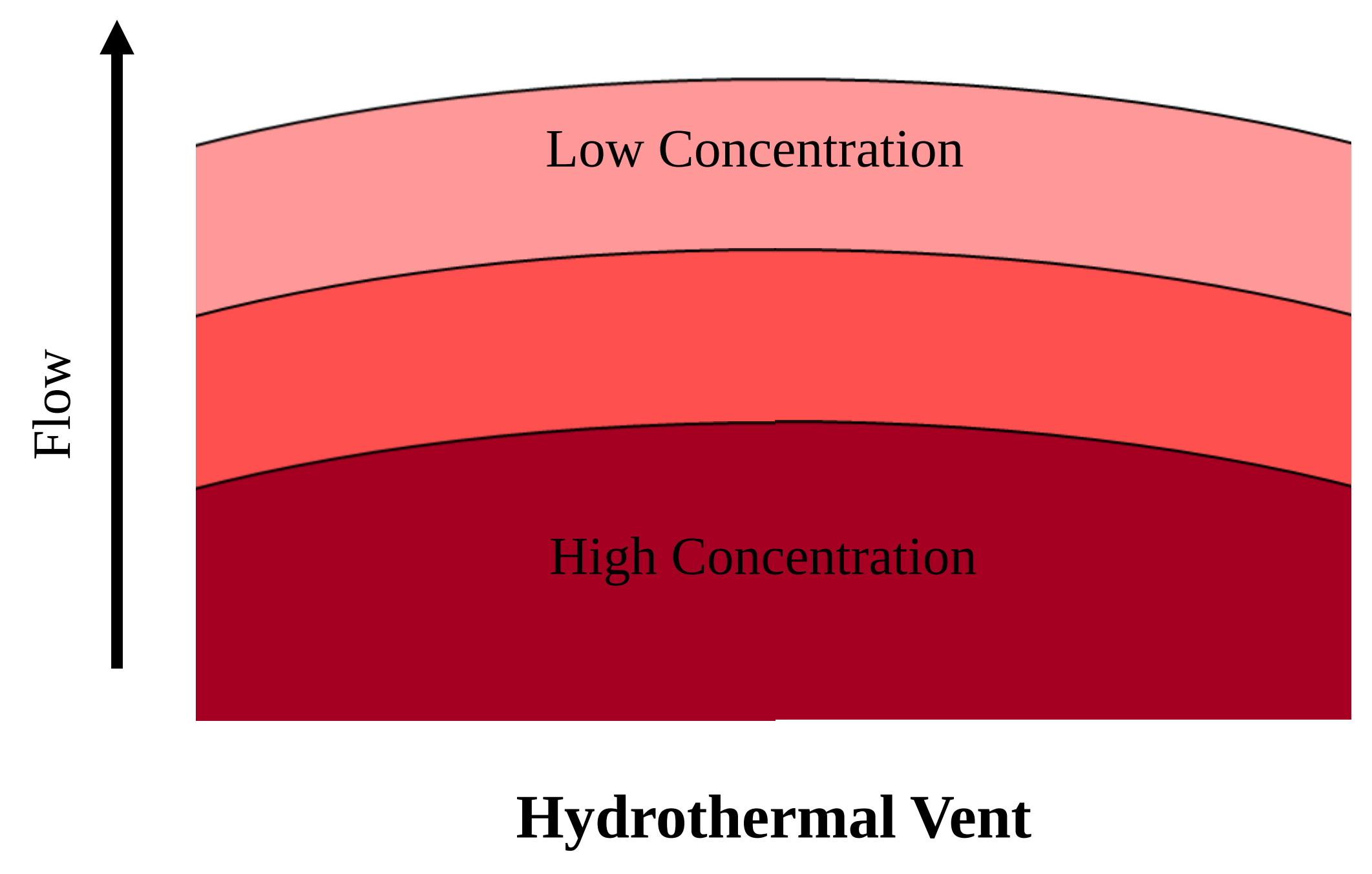

Figure 2: A visual model of a hydrothermal vent system, showing the flow of energy and organic molecules from the vent and concentration of these molecules as they diffuse out into the sea.

The Reaction Diffusion Model

Reaction diffusion systems are a widely applied model for representing interactions of subjects in a system. When modeled these systems create patterns, called Turing Patterns after Alan Turing introduced the concept in his 1952 paper, “The chemical basis of morphogenesis.” These patterns can be used to draw conclusions by observing the distribution and concentrations of the subjects of study.

We will use a reaction diffusion system to model theoretical early Earth conditions of RNA molecules in a hydrothermal vent environment. Small RNA molecules will form closest to the vent and flow away from the vent creating a concentration gradient. The RNA will diffuse and develop over time within this system. We will then try to find the parameters necessary for a stable system.

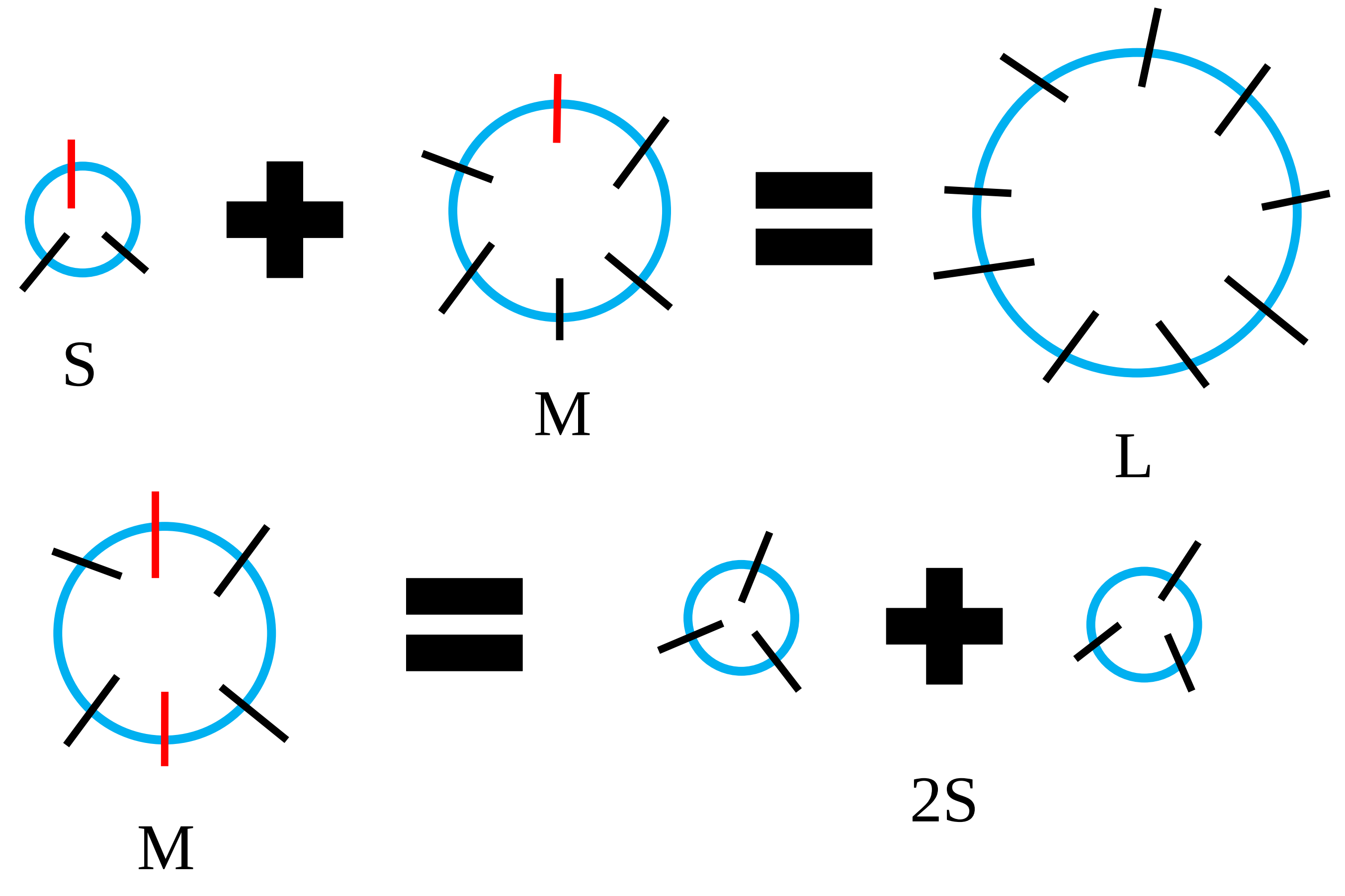

Figure 3: Visual representation of how the RNA, represented as plasmids, combine and disintegrate in the confines of the model. The combination of RNA serves as a way to represent horizontal gene transfer. Top Row: One small plasmid and one medium plasmid combine to form one large plasmid. Bottom Row: One medium plasmid disintegrates into two small plasmids.

Methods

We will use the Julia Programming Language to create reaction diffusion models with the following factors:

- Dependent Variables: RNA amounts by size (S, M, and L)
- Independent variables: Rates of recombination: γ_{SS} and γ_{SM}. Rates of disintegration: γ_M and γ_L.
- Parameters: Diffusion coefficients: D_S, D_M, and D_L ($D_S>D_M>D_L$).

$$\frac{dS}{dt} = DS\nabla^2 S - \gamma_{SS}S^2 + \gamma_M 2M - \gamma_{SM}SM + \gamma_L L$$

$$\frac{dM}{dt} = DM\nabla^2 M + \gamma_{SS}S^2 - \gamma_M M - \gamma_{SM}SM + \gamma_L L$$

$$\frac{dL}{dt} = DL\nabla^2 L + \gamma_{SM}SM - \gamma_L L$$

What does this mean?

- The rates of disintegration and recombination are independently manipulated in the models.
- Two small RNA combine at a certain rate to create one medium RNA and one medium RNA disintegrates at a certain rate to create two small RNA. One small RNA and one medium RNA combine at a certain rate to create one large RNA. One large RNA disintegrates at a certain rate to create one small RNA and one medium RNA.

We created reaction diffusion models with varying rates of recombination and disintegration to find the most stable systems, i.e., systems that can maintain mostly constant concentrations of each RNA size.

In the reaction diffusion model:

- The rate of disintegration increases as the length increases.
- The rate of recombination of RNA is not affected by length.
- Rates of disintegration increase, and rates of recombination decrease as the RNA move further away on the concentration gradient due to less access to both organic molecules and other RNA to interact with.
- The rate of diffusion on the gradient decreases as length increases.

Aims and Considerations

Our results will allow us to apply the necessary parameters to theories of early earth conditions to offer guidance on whether a possible theory is mathematically possible. If a certain system contains molecules that do not combine or diffuse at rates necessary to sustain the system, then that system would not be a possible and theorists could move on to creating a different system that fulfills the necessary parameters for stability. Our model will not be inclusive of every possible factor that could affect the necessary rates for stability, but the significance of these possible factors could be calculated to determine if they are necessary for inclusion or not. This is one possible model of a phenomena that cannot currently be observed, and the model could be revised in the future.

Future expansions of the model could include adding more RNA sizes to the model to better mimic the reality of how many different sizes of RNA molecules there are. More factors could also be added to the model, such as specific amounts of organic molecules available to the RNA molecules, to more accurately fine tune the parameters necessary for stability.

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