CONSTRAINING THE PREBIOTIC CELL SIZE LIMITS IN EXTREMELY HOSTILE UV ENVIRONMENTS: IMPLICATIONS FOR THE EARLY EARTH.

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THE AIM

- To study the abilities of spherical vesicles to harbor an appreciable population of a determined types of replicator according to the vesicle size in extremely hostile UV environments.

Replicator-> a chemical species able to produce copies of itself in the interaction with an appropriate substrate

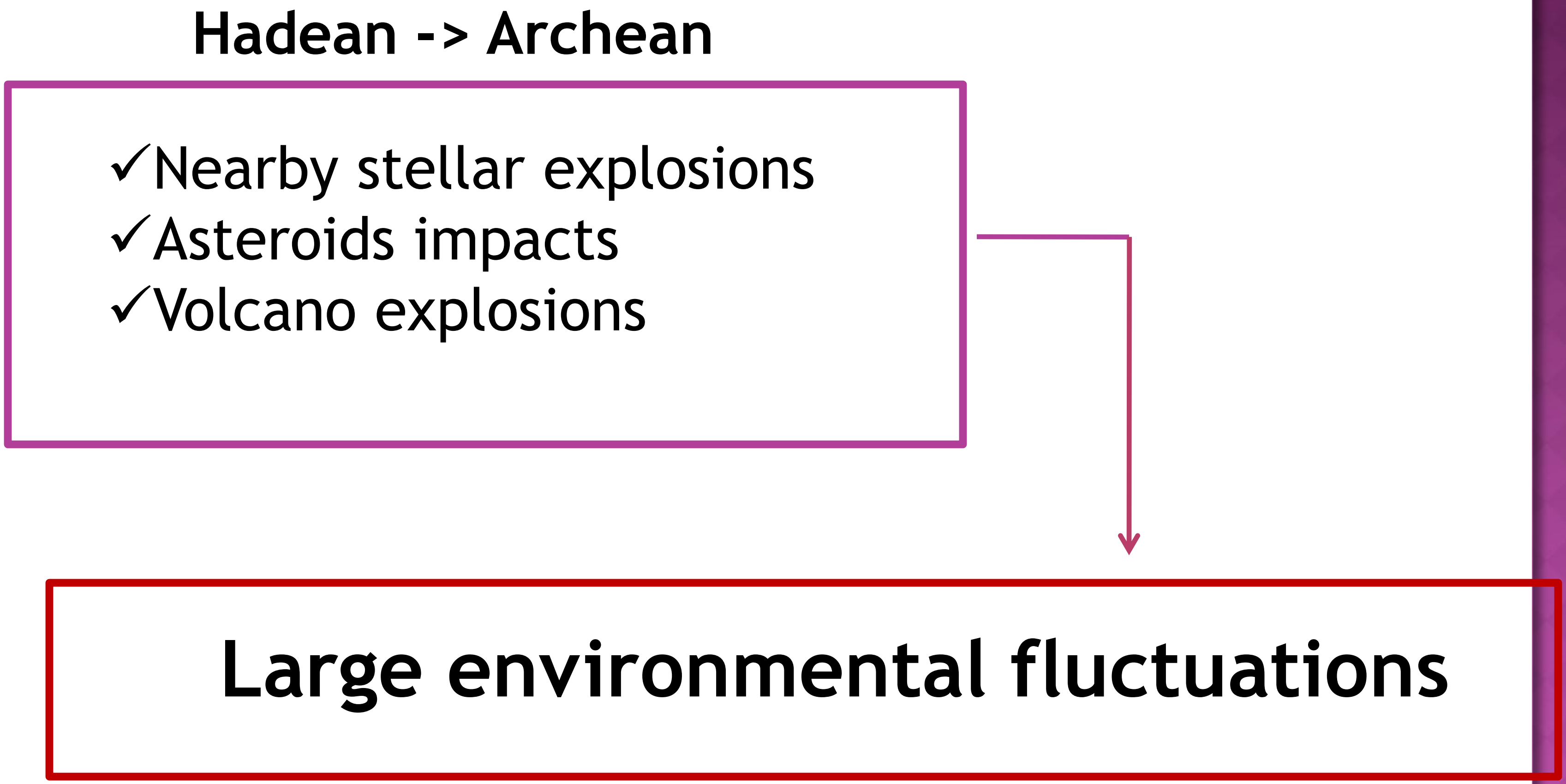
THE ORIGIN OF LIFE AND THE EARLY EARTH:
A HOSTILE ENVIRONMENT

Hadean -> Archean

- ✓The influence of a young Sun
- ✓An almost anoxic atmosphere
- ✓The lack of an ozone layer

Large UV levels at the surface of the planet

THE ORIGIN OF LIFE AND THE EARLY EARTH:
A HOSTILE ENVIRONMENT



Hadean -> Archean

✓Nearby stellar explosions
✓Asteroids impacts
✓Volcano explosions

Large environmental fluctuations

THE ROLE OF VESICLES

- Provides an appropriate micro-environment for the chemical process that take place in the cell. Vesicles play a major role stabilizing physical conditions (for instance, reducing the UV levels) and impeding the input of strange compounds able to interfere in the cellular processes. These features are keys to preserve functioning processes like the molecular replication, an intrinsic mechanism of all known living beings.

THE MODEL

- As a model of the prebiotic cell we considered a spherical vesicle delimited by a selective membrane. The vesicle is immersed in a medium where the content of nutrients remains constant. Two different chemical species are considered in our analysis. On one hand, a substrate that flows by diffusion inside the cell from the exterior; on the other hand, a replicator that feeds on the substrate and that is readily destroyed in the external medium surrounding the vesicle.

THE EQUATIONS

$$\frac{\partial u}{\partial t} = D_1\left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r}\right) - a\,uv = 0$$

$$\frac{\partial v}{\partial t} = D_2\left(\frac{\partial^2 v}{\partial r^2} + \frac{2}{r}\frac{\partial v}{\partial r}\right) + a\,uv - d_n\,v^n = 0 \qquad n = 1,2$$

D_1 D_2 are the diffusion constants for each species

$d_n = \{d_1, d_2\}$ are the *reproduction* and *mortality* (first and second order) rate constants respectively.

TYPES OF REPLICATORS

- **Model M1**: a linear decay (n=1) is assumed of the form representing the intrinsic degradation rate of the replicator. A linear decay is presumable the right choice for such replicator systems where the spontaneous, thermal or photolytic decomposition play the major role.

- **Model M2:** a nonlinear decay of the form when is associated with the underlying chemistry of the system. In this particular case, we presume the formation of a new inactive chemical species in the reaction of two replicator molecules.

NONDIMENSIONAL VARIABLES

$$u = C_0 \frac{\tilde{u}_r}{\tilde{r}}; \qquad v = C_0{}^{3-n} \frac{a}{d_n} \frac{\tilde{v}_r}{\tilde{r}}; \qquad r = \left(\frac{D_2}{a\, C_0}\right)^{\frac{1}{2}} \tilde{r}$$

THE NONDIMENSIONAL EQUATIONS

$$\left(\frac{D_1}{D_2}\right)\left(\frac{d_n}{a\,{C_0}^{2-n}}\right)\frac{\partial^2\tilde{u}_r}{\partial\tilde{r}^2}-\frac{\tilde{u}_r\tilde{v}_r}{\tilde{r}}=0$$

$$\frac{\partial^2\tilde{v}}{\partial\tilde{r}^2}+\frac{\tilde{u}_r\tilde{v}_r}{\tilde{r}}-\left(\frac{d_n}{a\,C_0}\right)^{2-n}{\tilde{v}_r}^{n}=0 \qquad n=1,2$$

BOUNDARY CONDITIONS

$$\tilde{u}_r(\tilde{R})=\tilde{u}_0;\quad \tilde{v}_r(\tilde{R})=0$$

$$\tilde{u}_r(0)=0;\qquad \tilde{v}_r(0)=0$$

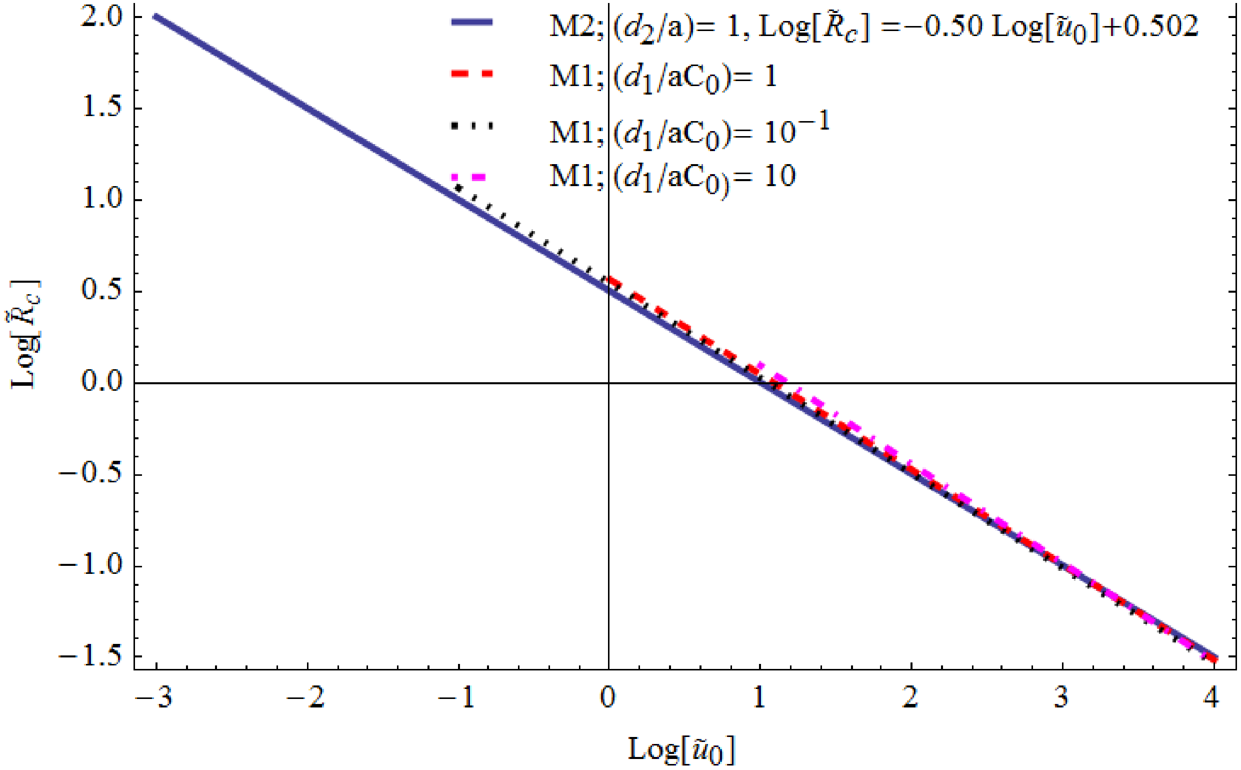
CRITICAL RADIUS AND HABITABILITY

- For the three models we find the existence of a critical radius under which the replicator population is not longer viable.

- Furthermore, the three studied models display approximately the same tendency when the critical radius correlates with the substrate concentration in the medium.

- The value is independent of the ratio deaths/ births excepting the **M1 model.**

CRITICAL RADIUS AND HABITABILITY OF THE VESICLE



For models M1 and M2, the critical radius scales approximately as the inverse of the square root of substrate concentration at the cell boundary.

A DIMENSIONAL EXPRESSION FOR THE CRITICAL RADIUS

$$R_C = 3.181\left(\frac{D_2}{a\,u_0}\right)^{\frac{1}{2}}$$

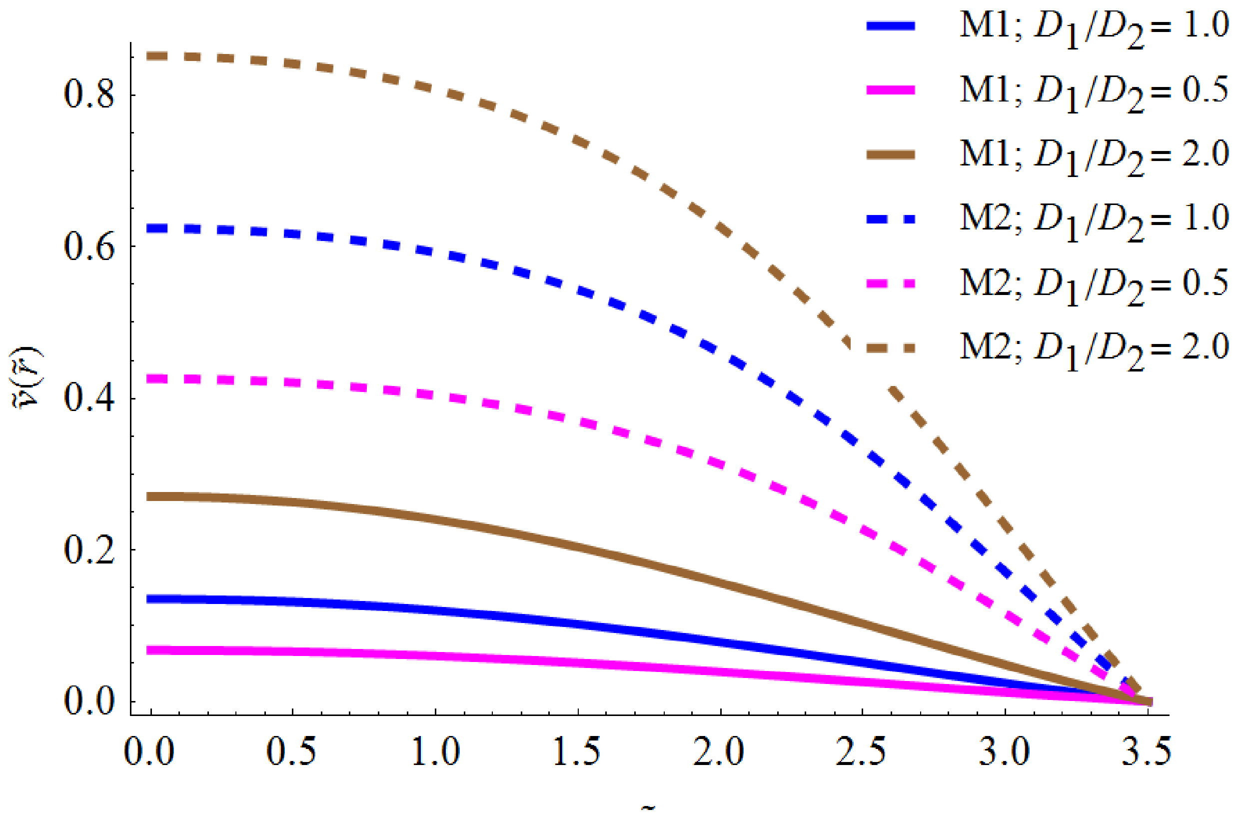
The three main factors that determined the habitability of a vesicle

- The diffusion constant of the replicator
- The reproduction coefficient
- The availability of substrate in the medium.

OTHER FACTORS AFFECTING THE POPULATION OF REPLICATORS

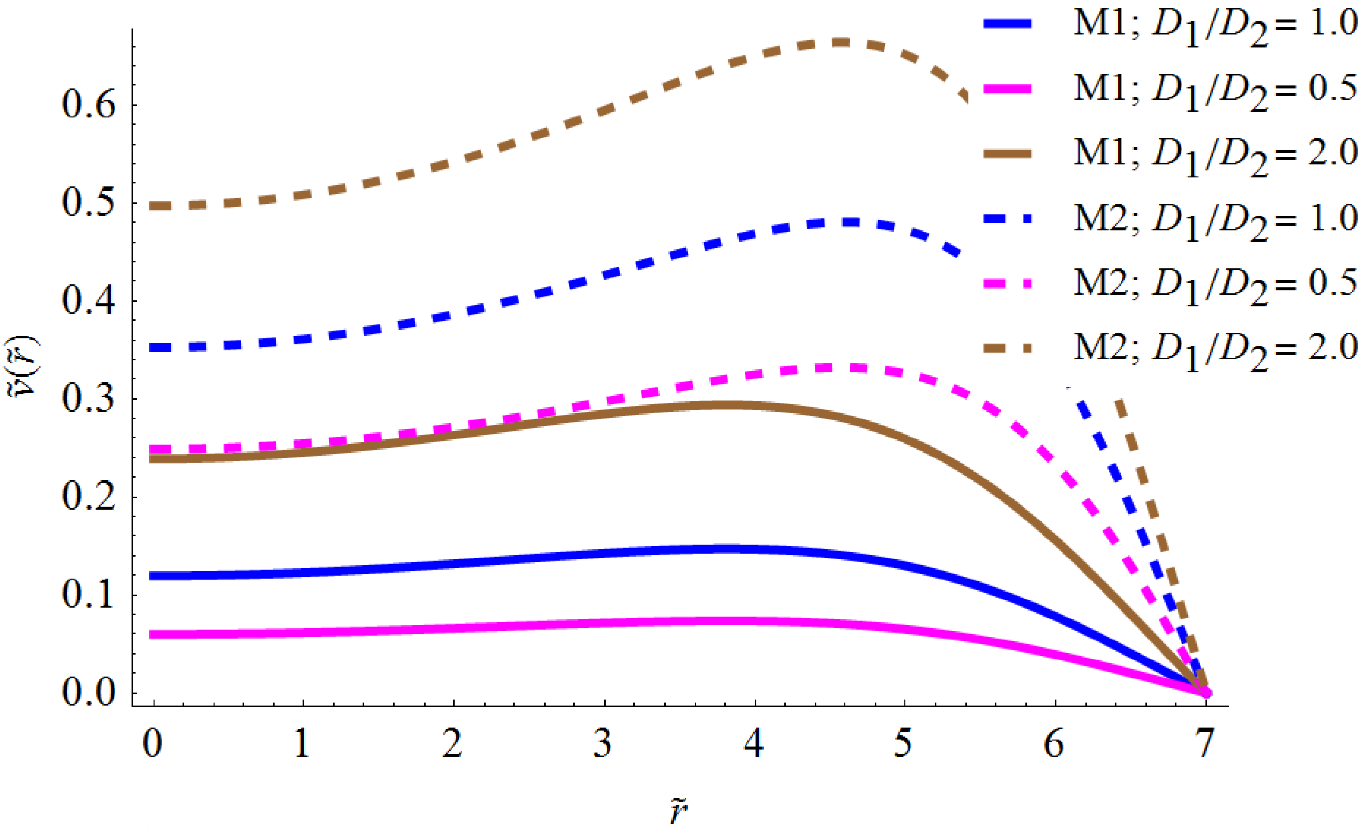
- According to the concept of kinetic stability introduced by Pross (Pross 2005a; Pross 2011; Pross and Khodorkovsky 2004) , the size of replicator population at steady state could be considered as a direct measure of the robustness of the system. Let us discuss briefly how the different parameters influence in the population according to the different models, even when some of them do not have a direct impact on the value of critical radius.

DIFFERENCES IN THE ABILITY TO DIFFUSE BETWEEN SUBSTRATE AND REPLICATOR (SMALL VESICLE)



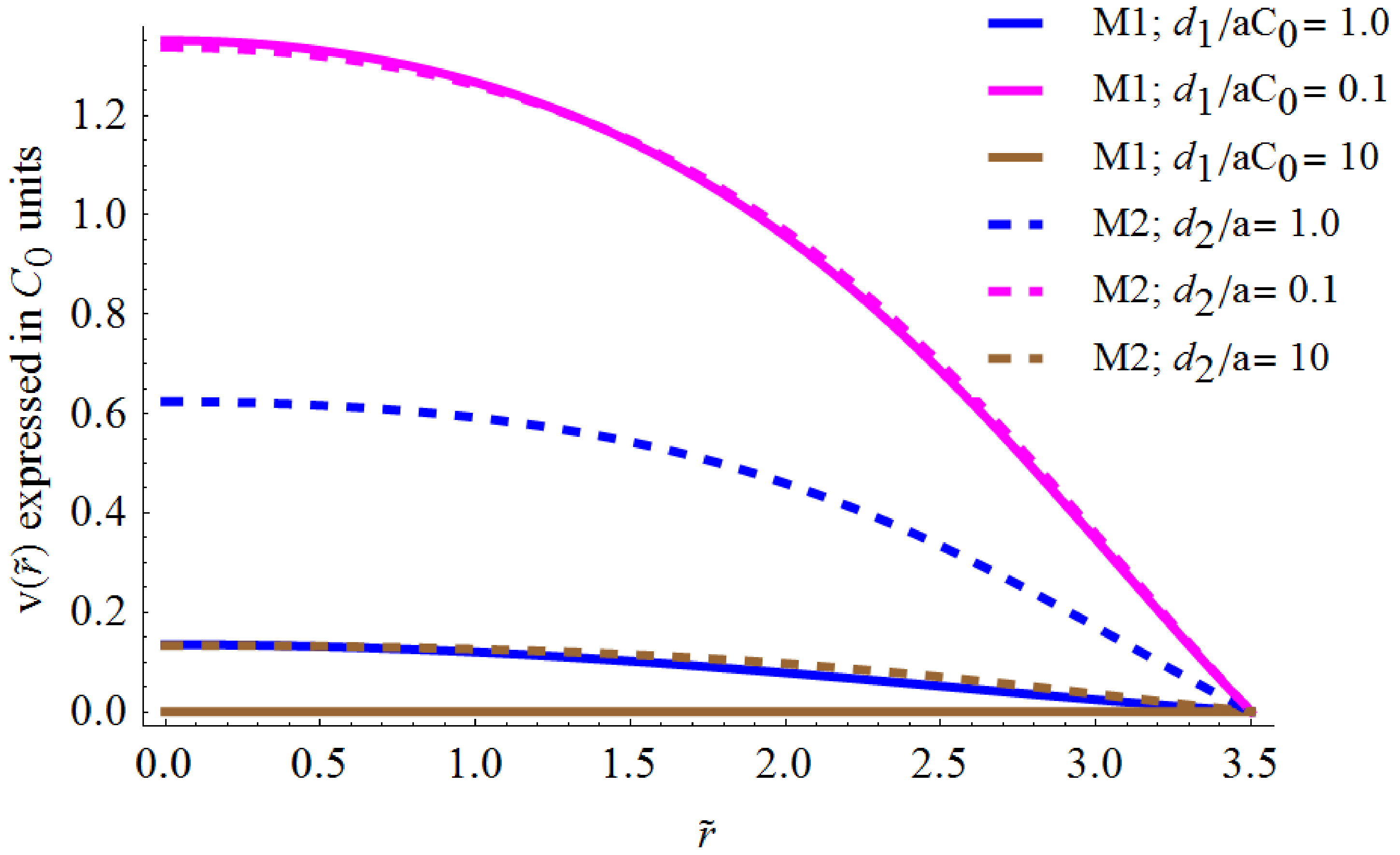
The influence of the ratio D1/D2 in the nondimensional concentration profile for the replicator.

DIFFERENCES IN THE ABILITY TO DIFFUSE BETWEEN SUBSTRATE AND REPLICATOR (LARGER VESICLE)



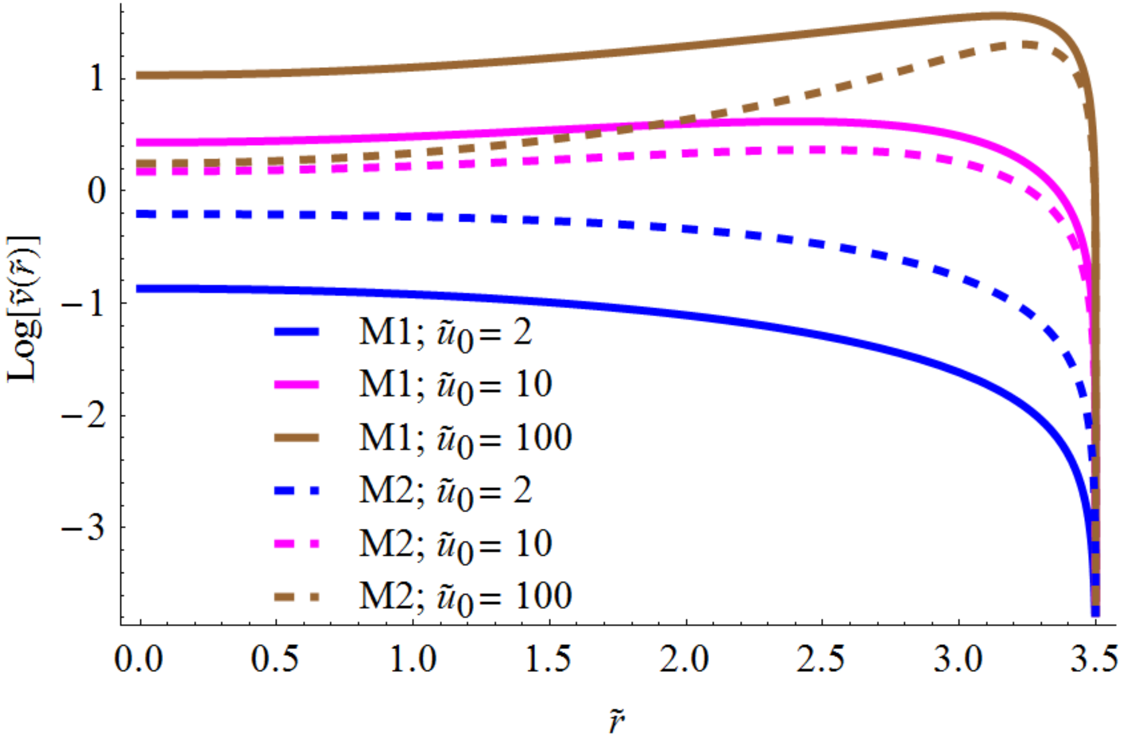
The influence of the ratio D1/D2 in the nondimensional concentration profile for the replicator.

CHANGES IN THE BIRTHS/DEATHS RATIO



The influence of the deaths/births ratio in the dimensional concentration profile for the replicator.

THE IMPACT OF SUBSTRATE CONCENTRATION (SMALL VESICLE)



The influence of substrate concentration in the concentration profile for the replicator species.

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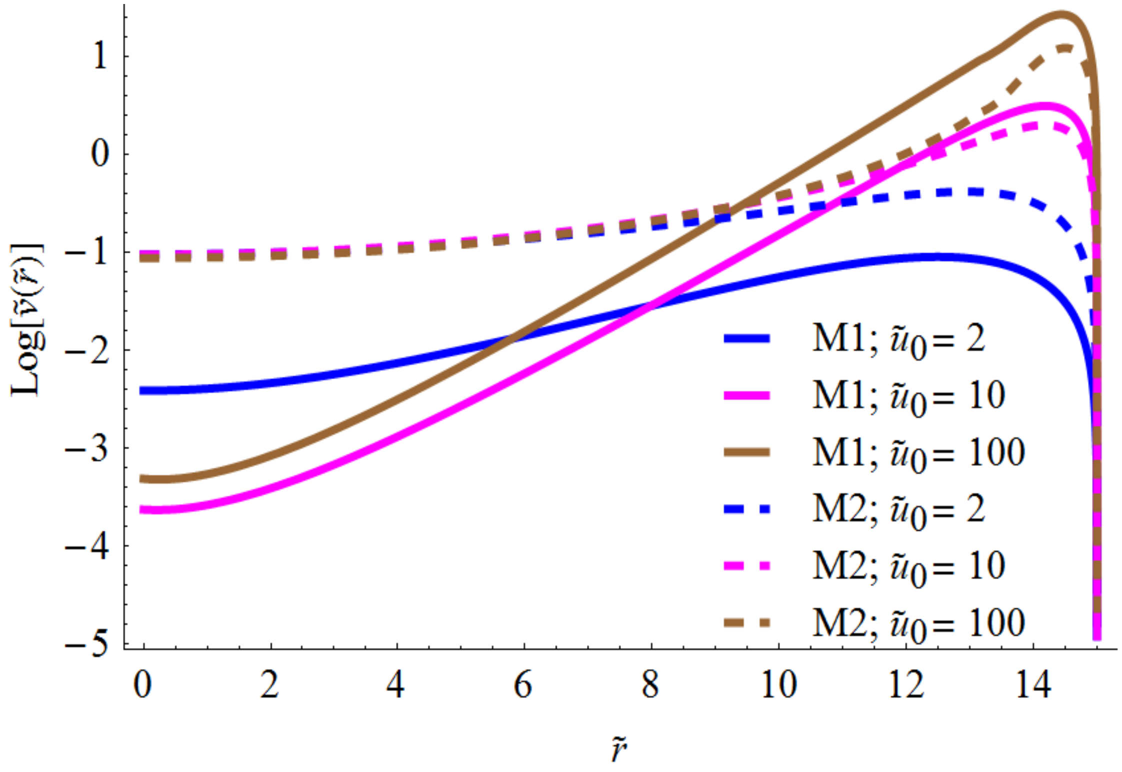

The influence of substrate concentration in the concentration profile for the replicator species.

CONCLUSIONS

- The abilities of chemical replicator to inhabit a vesicle in extreme environments may be restricted at some minimal length scale even when the processes of compartmentalization are usually considered as an effective mechanism of entropy reduction and self-organization in a biological system.

- The minimal size is controlled in our case by the availability of substrate, the diffusion constant of the replicator species and the effectiveness of the replication process codified in the reproduction rate constant.

- Despite the differences with other approaches, once again the availability of substrate emerge as a central problem to understand the origin of life on Earth

- Inhabit extremely large vesicles is also improbable due partially to a substantial dilution of the replicator species in the inner volume