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How can we validate and improve this model for self-organised limestone-marl alternations?

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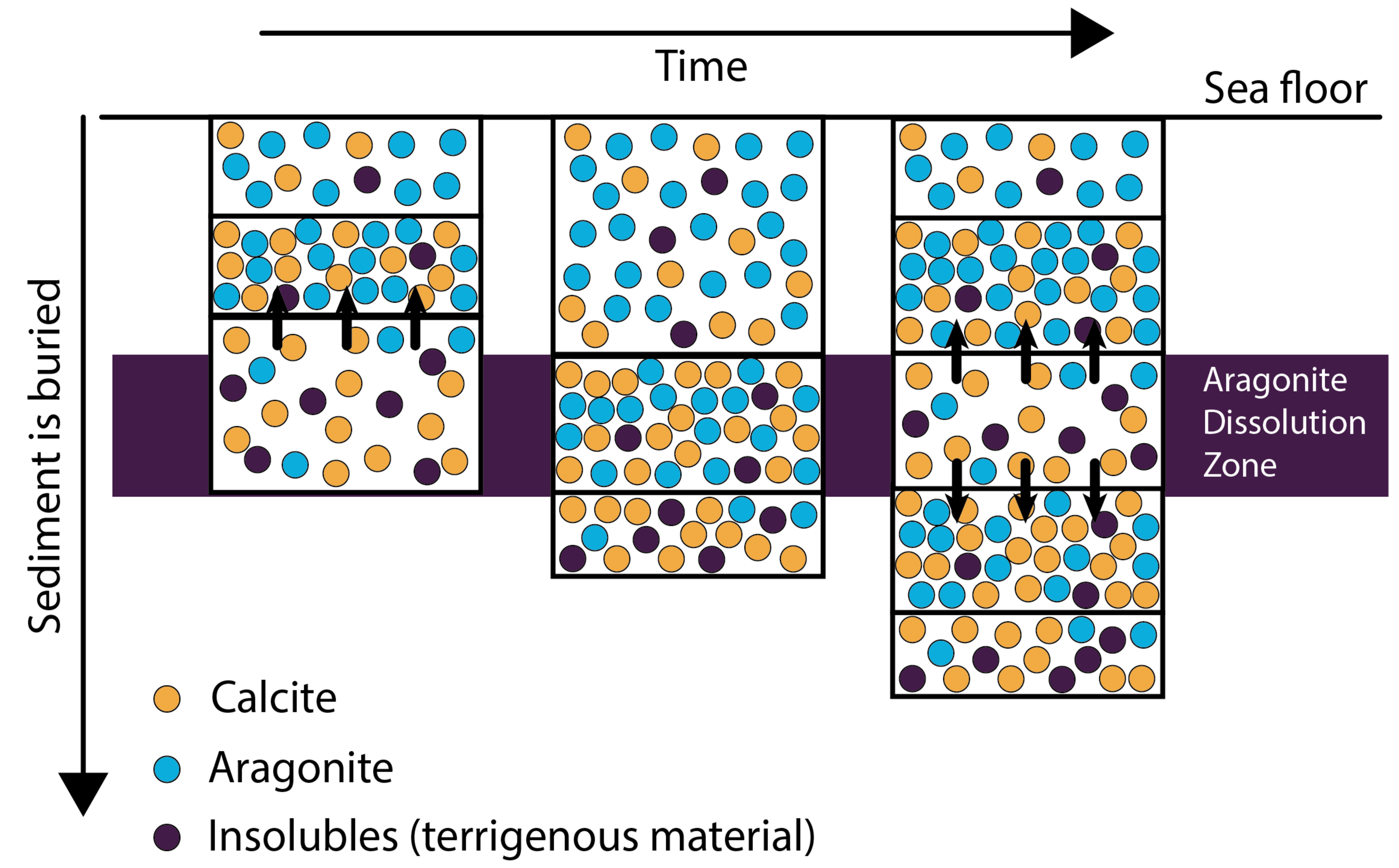
Abstract

Geological evidence for self-organisation in limestone-marl alternations[1,2] inspired Ivan L'Heureux[3] to derive a reactive-transport model for the formation of these banded patterns. This model not only describes reaction and advection of two minerals – aragonite and calcite – but also takes into account the aragonite dissolution zone (ADZ). The ADZ is microbially induced: at these depths - modelled to extend from 50 to 150 cm -below the water-sediment interface bacteria dissolving aragonite-bearing sediment are most active. In this zone calcium Ca^{2+} and carbonate CO_3^{2-} ions are released and precipitate somewhere else in the sediment and cement it. The advection of these ions is governed by the flow of the pore water, which depends on the porosity. The model is special because the porosity is a dynamic quantity: it changes in time due to compaction, dissolution and cementation. L'Heureux derived right-hand sides for the time derivatives of five quantities: the aragonite and calcite compositions, the concentrations of two ions in the pore water and the porosity. We have attempted to reproduce the results of his model, particularly the oscillations, but until now we only succeeded in reproducing a single solution, without oscillations.

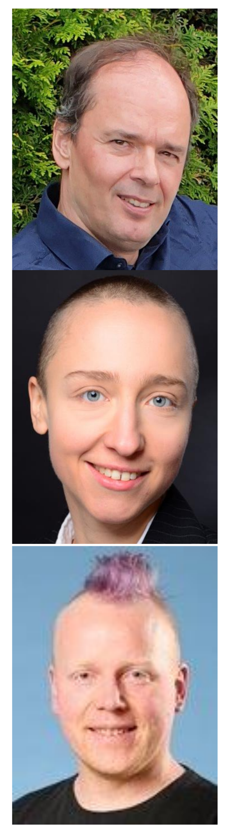
1) "Limestone-marl alternations as environmental archives and the role of early diagenesis: a critical review", by Hildegard Westphal (2006).
2) "Self-organized rhythmic patterns in geochemical systems", by Ivan L'Heureux (2013)
3) "Diagenetic Self-Organization and Stochastic Resonance in a Model of Limestone-Marl Sequences", by Ivan L'Heureux (2018).



We are seeking help with respect to:

1) The physical correctness of these equations.
2) The most stable and adequate numerical scheme for integrating them.
3) Does something similar to a "ground truth" exist, i.e. a scenario, which the model should reproduce?
4) Should we see oscillations in time for one or more of the five fields, e.g. for high initial and surface porosities?

Please approach one of these authors if you have any suggestions!



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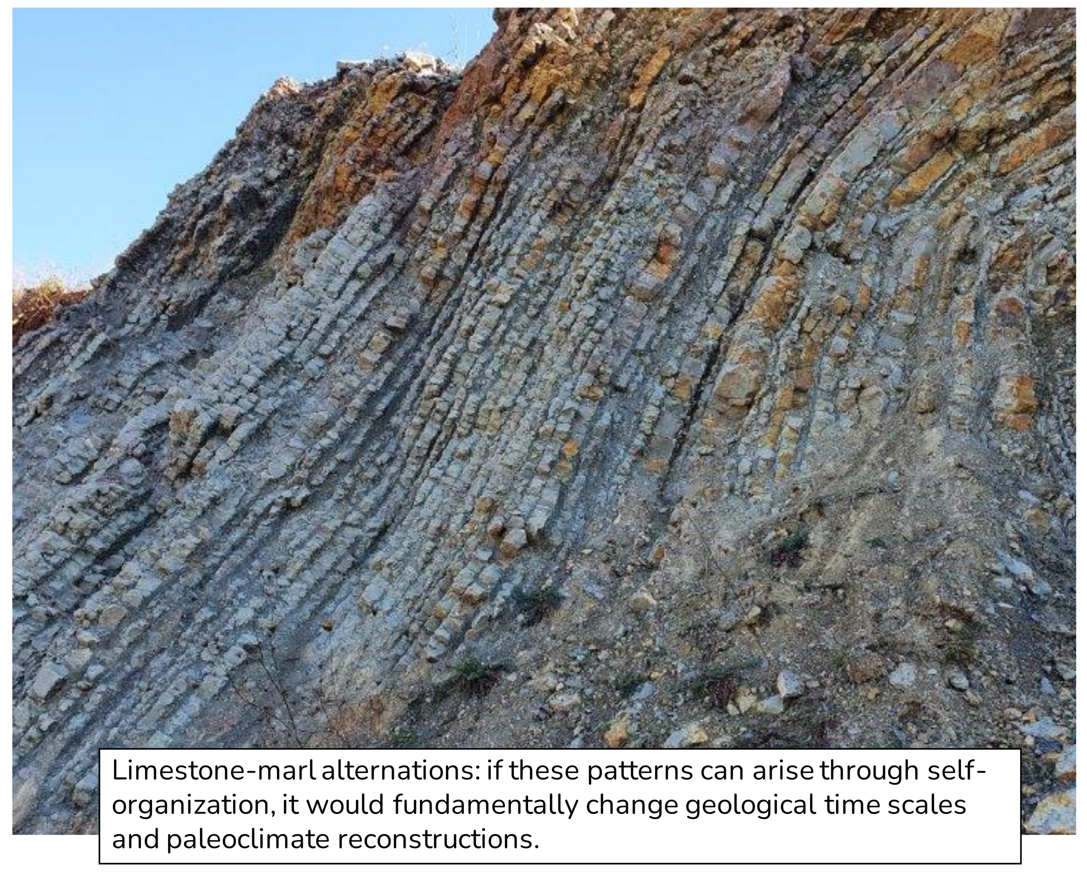


Limestone-marl alternations: if these patterns can arise through self-organization, it would fundamentally change geological time scales and paleoclimate reconstructions.

1 Description

The model describes the evolution of the concentrations of five variables:

1. Solids: two minerals which dissolve and (re)precipitate from/to the **same** solutes. They are expressed as proportions of the solid phase, and must accordingly be non-negative, and their sum must be smaller or equal to one.
   (a) C_C - Proportion of calcite in the solid phase
   (b) C_A - Proportion of aragonite in the solid phase
2. Solutes $\hat{c}_k$, where $k \in \{Ca, CO_3\}$
   (a) $\hat{c}_{Ca}$ - calcium concentration in pore water
   (b) $\hat{c}_{CO_3}$ - carbonate concentration in pore water
3. Porosity ϕ

Equation numbers refer to the equations in the original publication.

2 Equations

$$\frac{\partial}{\partial t}C_A = -U\frac{\partial}{\partial x}C_A - \mathrm{Da}\left[(1-C_A)C_A(\Omega_{DA}-\nu_1\Omega_{PA}) + \lambda C_A C_C(\Omega_{PC}-\nu_2\Omega_{DC})\right] \quad (40)$$

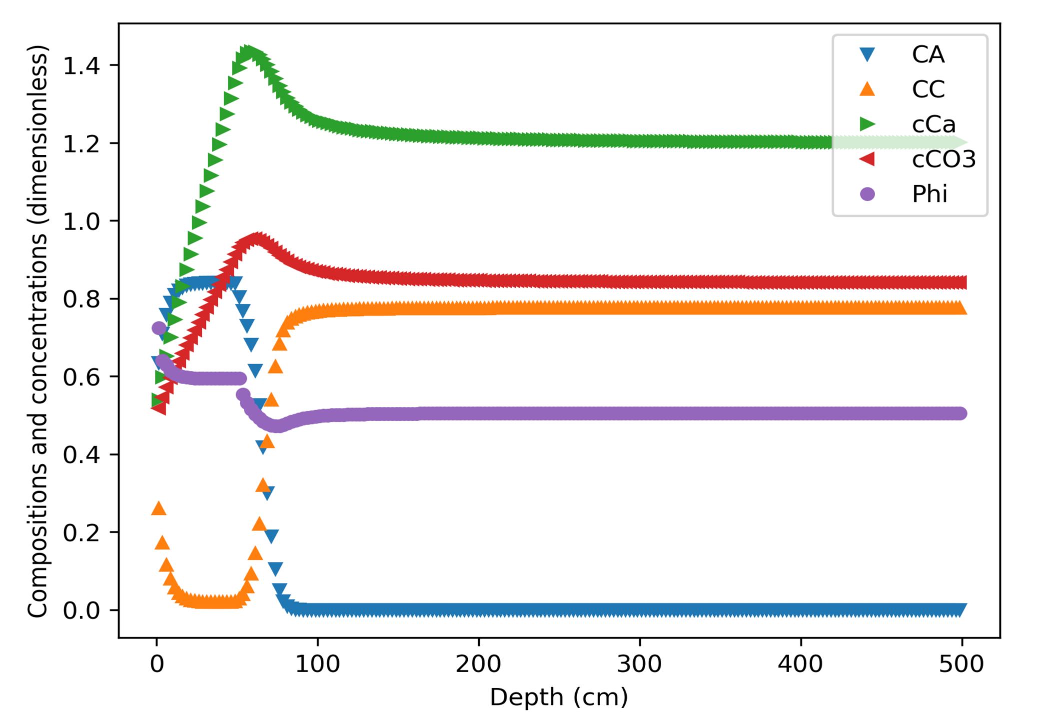
$$\frac{\partial}{\partial t}C_C = -U\frac{\partial}{\partial x}C_C + \mathrm{Da}\left[\lambda(1-C_C)C_C(\Omega_{PC}-\nu_2\Omega_{DC}) + C_A C_C(\Omega_{DA}-\nu_1\Omega_{PA})\right] \quad (41)$$

$$\frac{\partial}{\partial t}\hat{c}_k = -W\frac{\partial}{\partial x}\hat{c}_k + \frac{1}{\phi}\frac{\partial}{\partial x}\left(\phi d_k \frac{\partial \hat{c}_k}{\partial x}\right) + \mathrm{Da}\,\frac{(1-\phi)}{\phi}(\delta-\hat{c}_k)\left[C_A(\Omega_{DA}-\nu_1\Omega_{PA}) - \lambda C_C(\Omega_{PC}-\nu_2\Omega_{DC})\right] \quad (42)$$

The third equation solves for two quantities, $\hat{c}_k$ being a rescaled concentration of dissolved species, Ca and CO_3. Both these quantities appear in the definitions of Ω_i (which are therefore functions of x).

$$\frac{\partial}{\partial t}\phi = -\frac{\partial}{\partial x}(W\phi) + d_\phi\frac{\partial^2\phi}{\partial x^2} + \mathrm{Da}(1-\phi)\left[C_A(\Omega_{DA}-\nu_1\Omega_{PA}) - \lambda C_C(\Omega_{PC}-\nu_2\Omega_{DC})\right] \quad (43)$$

Distributions after 13190 years, with Phi(surface)=0.6, Phi(Initial)=0.5



Check https://github.com/MindTheGap-ERC for all our software.

Sharing is encouraged

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