

Supporting Information for “Reaction-diffusion waves in hydro-mechanically coupled porous solids as a precursor to instabilities”

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1. Linear stability analysis

The proposed system of reaction-cross-diffusion equations (equation 9 and 10 in the main text) describing the porous material behavior post yield are high-order nonlinear partial differential equations, for which no analytical solutions can be obtained. To conduct the linear stability analysis, we first consider a set of solutions described by a small perturbation (denoted with *) around the steady state $(\tilde{p}_{s0}, \tilde{p}_{f0})=(0, 0)$:

$$\tilde{p}_s(\tilde{x}, \tilde{t}) = \tilde{p}_{s0}(\tilde{x}, \tilde{t}) + \tilde{p}_s^*(\tilde{x}, \tilde{t}), \quad (1)$$

$$\tilde{p}_f(\tilde{x}, \tilde{t}) = \tilde{p}_{f0}(\tilde{x}, \tilde{t}) + \tilde{p}_f^*(\tilde{x}, \tilde{t}), \quad (2)$$

The perturbation satisfies the following linearized version of the cross-diffusion equations given by:

$$\frac{\partial \tilde{p}_s^*}{\partial \tilde{t}} = \tilde{D}_M \frac{\partial^2 \tilde{p}_s^*}{\partial \tilde{x}^2} + \tilde{d}_H \frac{\partial^2 \tilde{p}_s^*}{\partial \tilde{x}^2} + \tilde{a}_{11} \tilde{p}_s^* + \tilde{a}_{12} \tilde{p}_f^* \quad (3)$$

$$\frac{\partial \tilde{p}_f^*}{\partial \tilde{t}} = \tilde{d}_M \frac{\partial^2 \tilde{p}_s^*}{\partial \tilde{x}^2} + \tilde{D}_H \frac{\partial^2 \tilde{p}_s^*}{\partial \tilde{x}^2} + \tilde{a}_{21} \tilde{p}_s^* + \tilde{a}_{22} \tilde{p}_f^* \quad (4)$$

where $\tilde{a}_{11} = \left. \frac{\partial \tilde{R}_1}{\partial \tilde{p}_s} \right|_{\tilde{p}_s=\tilde{p}_{s0}}$, $\tilde{a}_{12} = \left. \frac{\partial \tilde{R}_1}{\partial \tilde{p}_f} \right|_{\tilde{p}_f=\tilde{p}_{f0}}$, $\tilde{a}_{21} = \left. \frac{\partial \tilde{R}_2}{\partial \tilde{p}_s} \right|_{\tilde{p}_s=\tilde{p}_{s0}}$, $\tilde{a}_{22} = \left. \frac{\partial \tilde{R}_2}{\partial \tilde{p}_f} \right|_{\tilde{p}_f=\tilde{p}_{f0}}$ are the first order derivatives of the normalized reaction terms.

By applying a space Fourier transform to the above equations, the perturbation can be expressed as:

$$\tilde{p}_s^*(\tilde{x}, \tilde{t}) = \tilde{p}_s^* \exp(ik\tilde{x} + s_k\tilde{t}) \quad (5)$$

$$\tilde{p}_f^*(\tilde{x}, \tilde{t}) = \tilde{p}_f^* \exp(ik\tilde{x} + s_k\tilde{t}) \quad (6)$$

where k denotes the wavenumber in space while s_k is the growth rate of the perturbation. By substituting Eq. (5) and Eq. (6) into Eq. (3) and Eq. (4), the applied perturbation translates into:

$$\begin{bmatrix} s_k + k^2 \tilde{D}_M - \tilde{a}_{11} & k^2 \tilde{d}_H - \tilde{a}_{12} \\ k^2 \tilde{d}_M - \tilde{a}_{21} & s_k + k^2 \tilde{D}_H - \tilde{a}_{22} \end{bmatrix} \begin{bmatrix} \tilde{p}_s^* \\ \tilde{p}_f^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (7)$$

which leads to the following condition:

$$\det \begin{bmatrix} s_k + k^2 \tilde{D}_M - \tilde{a}_{11} & k^2 \tilde{d}_H - \tilde{a}_{12} \\ k^2 \tilde{d}_M - \tilde{a}_{21} & s_k + k^2 \tilde{D}_H - \tilde{a}_{22} \end{bmatrix} = 0 \quad (8)$$

From Eq. (8), we derive a characteristic equation of s_k :

$$s_k^2 - \text{tr}_k s_k + \Delta_k = 0 \quad (9)$$

where $\text{tr}_k = (\tilde{a}_{11} + \tilde{a}_{22}) - k^2(\tilde{D}_M + \tilde{D}_H)$ and $\Delta_k = \tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{12}\tilde{a}_{21} + k^4(\tilde{D}_M\tilde{D}_H - \tilde{d}_M\tilde{d}_H) - k^2(\tilde{a}_{11}\tilde{D}_H + \tilde{a}_{22}\tilde{D}_M - \tilde{a}_{21}\tilde{d}_H - \tilde{a}_{12}\tilde{d}_M)$. Thus, the solution of Eq. (8) is expressed as

$$s_k = \frac{\text{tr}_k \pm \sqrt{\text{tr}_k^2 - 4\Delta_k}}{2} \quad (10)$$

Based on material stability theory, the system becomes unstable in the Lyapunov sense if there exists $\text{Re}(s_k) > 0$ since the perturbation would increase with time in this case. Moreover, if s_{k_c} is a real number upon the occurrence of an instability (i.e. $s_{k_c} \geq 0$ for the critical wavenumber k_c), the system undergoes a saddle-node bifurcation or the so-called Turing bifurcation, along with the previous stable nodes in the phase space changing to the unstable saddle. However, if s_{k_c} is a pure complex number upon the occurrence of instability, the system undergoes a Hopf bifurcation as the previous stable focus in the phase space changes to an unstable one. Based on the above derivation, we present in the main manuscript a detailed discussion of these typical types of instabilities as well as a newly discovered quasisoliton wave type in relation to reaction-diffusion waves in the context of poromechanics.

2. Parametric space and its possible application

To discuss the geoscientific implications of our newly proposed nonlocal reaction-diffusion equation, we map the three fundamental classes of instabilities - Turing-, Hopf-, and cross-diffusion waves - in the parametric space $\tilde{a}_{11} - \tilde{a}_{22}$ (Fig. S1). The control parameters \tilde{a}_{11} and \tilde{a}_{22} represent the first-order coefficients of the solid and fluid pressure reaction rates \tilde{R}_1 and \tilde{R}_2 . Although we need an order 3 expansion for the mechanical reaction term to obtain cross-diffusion waves, these first-order terms fully control the onset of cross-diffusion wave instabilities. We find that the appearance of the cross-diffusion wave corresponds to a narrow domain (highlighted polygon in Fig. S1) where \tilde{a}_{11} is negative and the magnitude of the coefficient for fluid pressure rate \tilde{a}_{22} is small. Interestingly, cross-diffusion waves are even possible for very small negative \tilde{a}_{11} , corresponding to very small values of solid overstress rate (low tectonic loads).

The fact that in our stability analysis cross-diffusion waves are expected for such low values in mechanical reaction rates \tilde{R}_1 coupled with low reaction rate \tilde{R}_2 (slow production of fluid pressure source from chemical reactions) implies that such cross-diffusion waves are common features. An example for such low fluid pressure source terms is the dissolution-precipitation reaction during diagenesis or metamorphic breakdown which occurs on long time scales. These reactions are therefore expected to trigger slow cross-diffusion waves which may be interpreted geologically as the first step in a long road to failure.

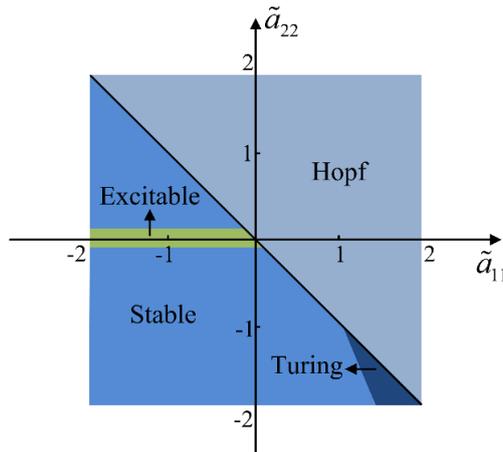


Figure S1. Parametric \tilde{a}_{11} versus \tilde{a}_{22} space of three fundamental instabilities: Turing-, Hopf-, and cross-diffusion waves

The modification of an originally homogeneous material into a structured one may, under continued geodynamic loading, lead to further amplification of the applied stress, resulting in the activation of high-stress micro-deformation processes such as crystal-plastic dislocation creep. Zaiser and Hähner (1997) describe a range of processes in this dislocation regime which can lead to an oscillatory response. These oscillatory phenomena en-

countered in metals and alkali halides have been identified as an excitable wave phenomenon (Zuev & Barannikova, 2010) based on the particle-like discrete foundation of their slip systems.

Similar to the self-cross-diffusion waves, the Turing instability occupies only a narrow domain of parameters while the Hopf instability covers the largest section of the mapped space (Fig. S1). One would therefore expect Hopf bifurcations to be most common in nature because they cover the largest parameter space. Hopf waves occur for either a positive \tilde{a}_{11} or a sufficiently large \tilde{a}_{22} in the case of a negative \tilde{a}_{11} . Hopf and Turing bifurcations have been applied to explain the rhythmic layering observed in many geological/chemical systems as found in experiments where oscillatory reactions occur in solid solutions grown from aqueous solutions (L'Heureux, 2013).

Hopf- and Turing-style instabilities in geomaterials have first been described by Dewers and Ortoleva (1990). The authors formulate a mathematical model for interaction between chemical and mechanical thermodynamic forces and fluxes that appear in randomly varying mixtures of mechanically strong and weak reacting minerals in the presence of an applied stress field. Stress concentrations in the stronger phase were described to increase the chemical potential and lead to transport down chemical potential gradients into regions initially depleted in the strong phase. This positive feedback between chemical and mechanical thermodynamic forces leads to chemo-mechanical oscillations where textural variations become amplified. In their introduction, Dewers and Ortoleva (1990) describe many observations of metamorphic patterns, resulting from a change in the structure of an initially random material into a strongly layered medium.

In our analysis, we found that Hopf waves do not reflect from boundaries but dump their energy into them. This property could become important as a potential mechanism for pre-seismic slip on a future major fault. While in this simulation the Hopf waves focus cumulative damage on the opposite boundary, in a more realistic geological scenario damage accumulation can occur on pre-existing faults or fractures, which can act as internal elastic-plastic system boundaries embedded in the large-scale plastic zone. The Hopf bifurcation is therefore here interpreted to prepare a given internal structure for failure. In this sense, we may speculate that, in terms of geological interpretation, Hopf bifurcations could be a mechanism for generating distributed fault damage zones as defined in Table 1 in (Peacock et al., 2017).

For the Hopf bifurcation, our simulations show two regimes with an irregular pattern: a transient regime prior to the wave reaching the opposite boundary with exponentially decaying frequency-amplitude relationships, and a post-boundary interaction regime with a stable orbit (Fig. 2 of the main manuscript), also with an exponential frequency-magnitude relationship (Fig. 1c of the main manuscript). Similar patterns have been reported in the geological literature (Elphick et al., 2021). For the application of the approach to geology, L'Heureux (2013) emphasizes the caveat that it is impossible to differentiate between the dynamic or stable-orbit type of solution. The time sequence of the pattern development requires careful microstructural and field geological analysis which is beyond the scope of this contribution.

The quasi-soliton (cross-diffusion) wave solution has the interesting property that the velocity of the wave is a material property and not affected by initial conditions. Once the wave is triggered by perturbations, it continues and sustains itself (at perpetuity if the coefficients do not change) as a self cross-diffusion wave. The quasi-soliton wave is argued here to be the most often encountered in nature as chemical fluid-release reactions are often very slow, thus favouring the nucleation of cross-diffusion waves. It may be seen to prepare the material for Hopf- or Turing bifurcations or directly lead to catastrophic instabilities.

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