Brine channel formation in sea ice by phase separation

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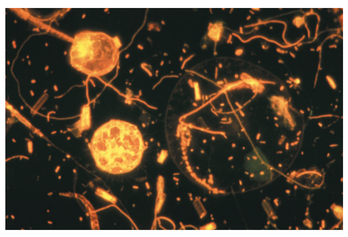
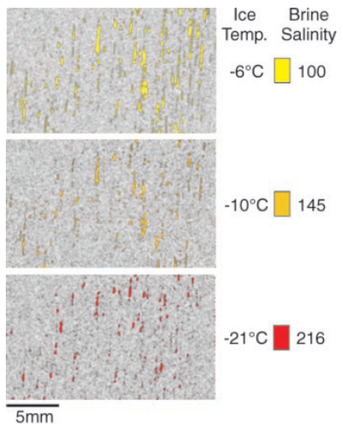
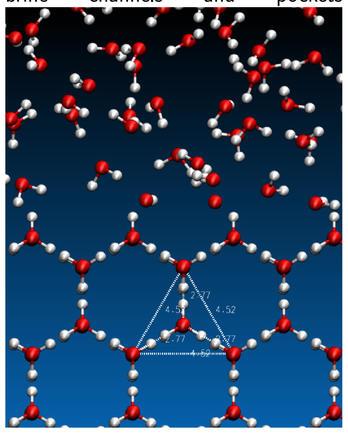
Introduction



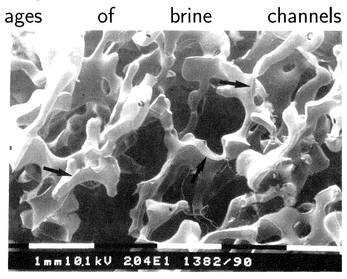
Psychrophilic bacteria in brine channels and pockets



Magnetic-resonance images of brine channels



Molecular structure of water and ice



Cast of brine channels (Weissenberger)

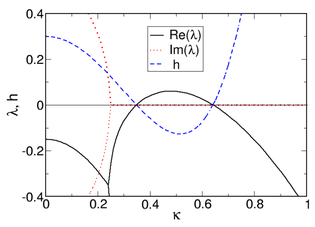
Reaction-diffusion model (Turing)

$$\frac{\partial\psi(\xi,\tau)}{\partial\tau} = \alpha_1\psi - \psi^3 + \delta\psi^5 + \rho + \frac{\partial^2\psi(\xi,\tau)}{\partial\xi^2}$$
$$\frac{\partial\rho(\xi,\tau)}{\partial\tau} = -\alpha_2\rho - \psi + D\frac{\partial^2\rho(\xi,\tau)}{\partial\xi^2}$$

α_1 = temperature-dependent rate
α_2 = desalinization rate
δ = measure for specific heat

Linear Stability Analysis

$$\begin{pmatrix}\bar\psi\\ \bar\rho\end{pmatrix} = \begin{pmatrix}\bar\psi_i\\ \bar\rho_i\end{pmatrix} exp(\lambda(\kappa)\tau + i\kappa\xi)$$



Dispersion of the linear stability versus the dimensionless wave number κ for $\alpha_1 = 0.7$, $\alpha_2 = 1$, $D = 6$ together with the function $h(\kappa)$

steady state

$$\lambda(\kappa)^2 + [\kappa^2(1+D) + \alpha_2 - \alpha_1]\lambda(\kappa) + h(\kappa^2) = 0$$

with $h(\kappa^2) = D\kappa^4 + (\alpha_2 - \alpha_1 D)\kappa^2 - \alpha_1\alpha_2 + 1$

Turing space

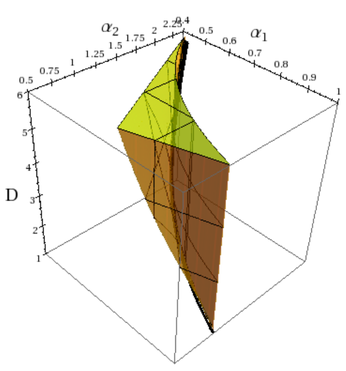
homogeneous phase stable if eigenvalues negative

$$\text{condition I}: \quad \alpha_2 > \alpha_1 \text{ and } \alpha_1\alpha_2 < 1.$$

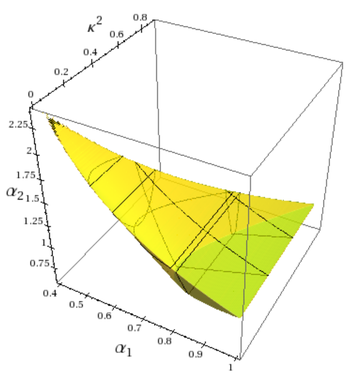
spatial inhomogeneous case, $\kappa^2 > 0$ some spatial fluctuations may be amplified and form macroscopic structures, i.e. the Turing structure, modes growing in time$\mathrm{Re}\lambda(\kappa) > 0$

$$\text{condition II}: \quad D > \frac{(1+\sqrt{1-\alpha_1\alpha_2})^2}{\alpha_1^2}.$$

$$\text{cond. III}: \quad \kappa^2 \in \frac{1}{2D}\left(\alpha_1 D - \alpha_2 \pm \sqrt{(\alpha_1 D + \alpha_2)^2 - 4D}\right)$$



The Turing space where spatial structures can occur, lower limiting line, $\alpha_2 = 1/\alpha_1$, $D = 1/\alpha_1^2$ (thick)



The possible wave numbers κ^2 where spatial structures can occur for $D = 6$ in dependence on α_1 and α_2

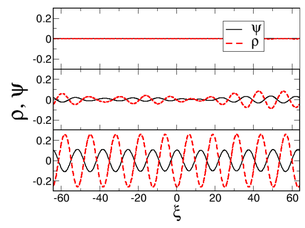
Critical modes

critical wavenumber from largest modes

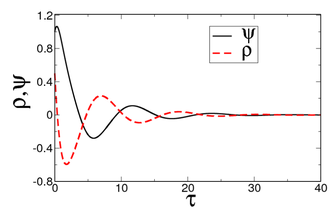
$$D_c = \frac{(1+\sqrt{1-\alpha_1\alpha_2})^2}{\alpha_1^2}$$

with the critical wavenumber determining size of structure $\frac{2\pi}{\kappa_c}$,

$$\kappa_c^2 = \frac{D_c f_\psi + g_\rho}{2D_c} = \frac{D_c\alpha_1 - \alpha_2}{2D_c}$$

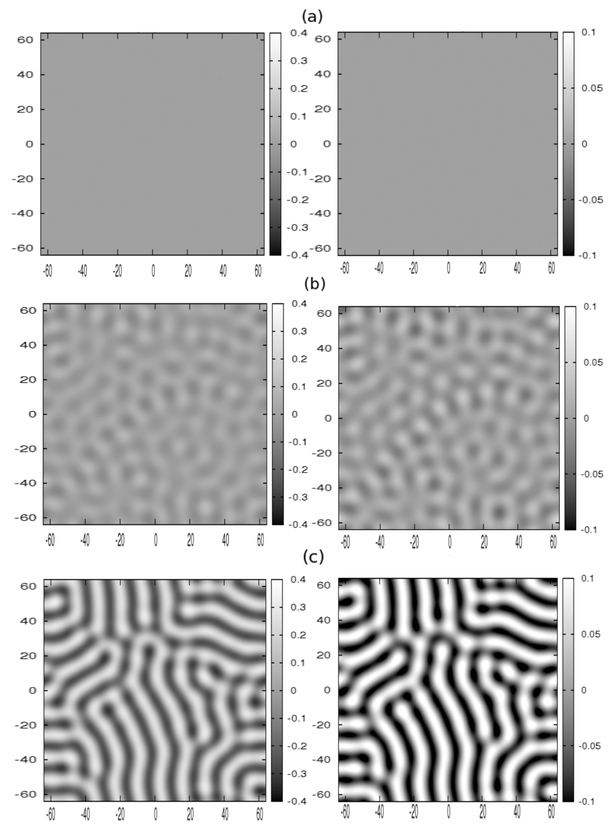


Time evolution of the order parameter ψ and salinity ρ versus spatial coordinates for $\tau = 100, 170, 400$ (from above to below)for $\alpha_1 = 0.7$, $\alpha_2 = 1$, $\delta = \frac{3}{16\alpha_1}$, $D = 6$ with the initial condition $\rho(\tau = 0) = 0.5 \pm 0.01N(0,1)$ and periodic boundary conditions



Time evolution of the order parameter ψ and the salinity ρ for $\alpha_1 = 0.7$, $\alpha_2 = 1$, $\delta = \frac{3}{16\alpha_1}$ and the initial order parameter $\psi(\tau = 0) = 1$ and the dimensionless salinity $\rho(\tau = 0) = 0.5$

Time evolution (Turing)



Structure formation for 3 time steps $\tau = 100, 170, 400$ (from top to bottom, a-c) for the order parameter Ψ (left) and the salinity ρ (right). The parameters are $\alpha_1 = 0.7$, $\alpha_2 = 1$, $\delta = \frac{3}{16\alpha_1}$, $D = 6$ with the initial condition $\rho(\tau = 0) = 0.5 \pm 0.01N(0,1)$ and periodic boundary conditions

Link to experimental data

Experimental data	critical wave number	model parameter
$D_1 = 10^{-5}\frac{cm^2}{s}$	$\frac{2\pi}{\kappa_c} = 12.6 = \frac{2\pi}{k_c}\frac{\sqrt[4]{b_1 b_2}}{\sqrt{D_1}}$	$b_1 b_2 = 2.5 \times 10^6 s^{-2}$ $a_1 = \sqrt{b_1 b_2}\alpha_1 = 1111 s^{-1}$ $a_2 = \sqrt{b_1 b_2}\alpha_2 = 1587 s^{-1}$ $D_2 = D_1 D = 6 \times 10^{-5}\frac{cm^2}{s}$
$\tau_d = 10^5 s^{-1}$	$a_1 \sim \frac{T_c - T}{T_c}\frac{1}{\tau_d}$	$a_1 \sim 1107 s^{-1}$

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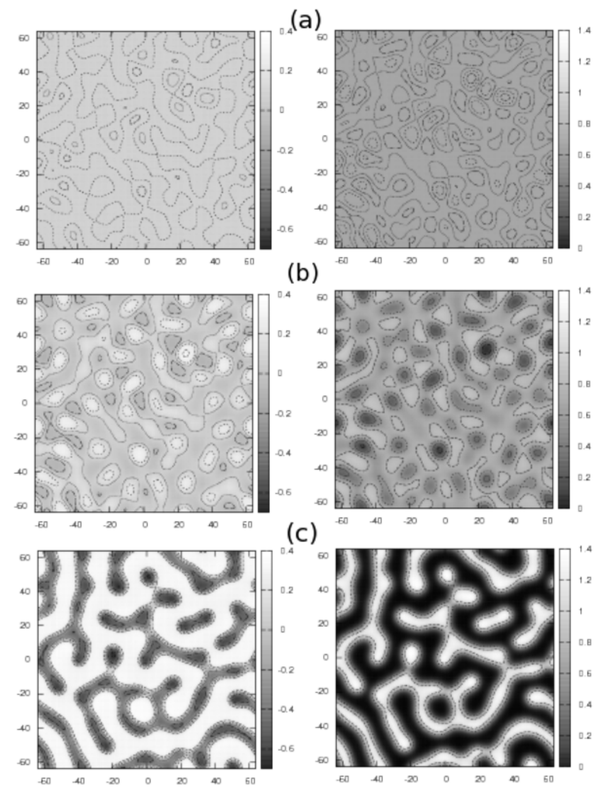
Time evolution (Phase field)

$$\frac{\partial\psi(\xi,\tau)}{\partial\tau} = -\alpha_1\psi + \psi^2 - \alpha_3\psi^3 - \psi\rho + D\frac{\partial^2\psi(\xi,\tau)}{\partial\xi^2}$$
$$\frac{\partial\rho(\xi,\tau)}{\partial\tau} = \frac{1}{2}\frac{\partial^2\psi^2(\xi,\tau)}{\partial\xi^2} + \frac{\partial^2\rho(\xi,\tau)}{\partial\xi^2}$$



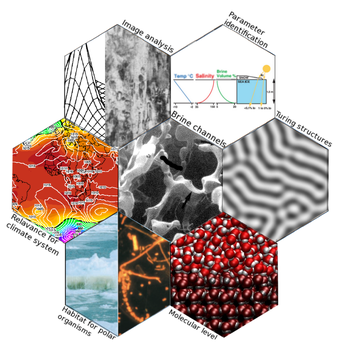
Structure formation for 3 time steps $\tau = 0, 175, 500$ (from top to bottom, a-c) for the order parameter Ψ (left) and the salinity ρ (right). The parameters are $\alpha_1 = 0.1$, $\alpha_3 = 1$, $D = 0.5$ with the initial condition $\rho(\tau = 0) = 0.1 \pm 0.001N(0,1)$ and periodic boundary conditions

Comparision between both models

Turing-Ginzburg-Landau	Phase field
salinity is not preserved	salinity is preserved (conservative quantity)
brine channel formation is a result of the kinetic nonlinear feedback	brine channel formation is a consequence of a exact free energy functional and the conservation condition of salinity

Summary

1. reaction diffusion system which connects the basic ideas both of Ginzburg and of Turing can describe the formation of brine channels with realistic parameters
2. phase separation derived from a variation of the free energy functional with regard to the conservation of salinity
3. morphology of sea ice is one criterion for the choice of an appropriate kinetics for the genesis of sea ice
4. to simulate different structure sizes and textures, we can modify the dispersion relation by varying the parameters α_1, α_2 resp. α_3 and D or by a modified kinetics
5. phase field model (Cahn-Hilliard-Equation) seems to be more realistic



Link of the brine channels to the eco- and climate system

B. Kutschan, K. Morawetz, S. Gemming: *Modeling the morphogenesis of brine channels in sea ice*, Phys. Rev. E 81 (2010) 036106-1-10