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KARST FAULTS: MECHANISM OF EVOLUTION AND ITS MODELLING

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MAIN DIFFICULTY OF KARST PROCESSES MATHEMATICAL SIMULATION

- KARST PROCESSES SIMULATION = SOLUTION OF COMBINATION OF A NUMBER OF NONLINEAR PROBLEMS

MAIN NONLINEAR PROBLEMS:

- Chemical dissolution of rock fractures walls
- Hydrodynamics of flow in multi-scale fractured media
- Underground erosion of over-fractured rocks (suffosion – from lat. suffosio)

KARST TYPS:

- Carbonate karst (dissolution of limestone)
- Sulfate karst (dissolution of gypsum)
- Salt karst (dissolution of halite)

We’ll be concentrated only with carbonate karst (like most widely occurring).

Mathematical model of rock dissolution process

Governing equations:

$$\frac{\partial}{\partial t}(nC_i)+\nabla \vec{J}_i = n\sigma_i^{(v)} + S_u\sigma_i^{(s)}, (i=1,...,N) \qquad (1)$$

$$\vec{V} = -\frac{k}{\eta}(\nabla p + \rho \vec{g}); \quad \mathrm{div}\vec{V} = 0 \qquad (2)$$

$$\sum_{i=1}^{l}\nu_i^{(a)}A_i \leftrightarrow \sum_{i=1}^{m}\nu_i^{(b)}B_i \qquad (3)$$

$$\frac{\partial \xi^{(k)}}{\partial t} = k_d\prod_{i=1}^{l}[A_i]^{\nu_i^{(a)}} - k_r\prod_{i=1}^{m}[B_i]^{\nu_i^{(b)}}, \quad \sigma_i = \nu_i^{(k)}\frac{\partial \xi^{(k)}}{\partial t} \qquad (4)$$

Dissolution rate

Calcite dissolution rate (White, 1977)

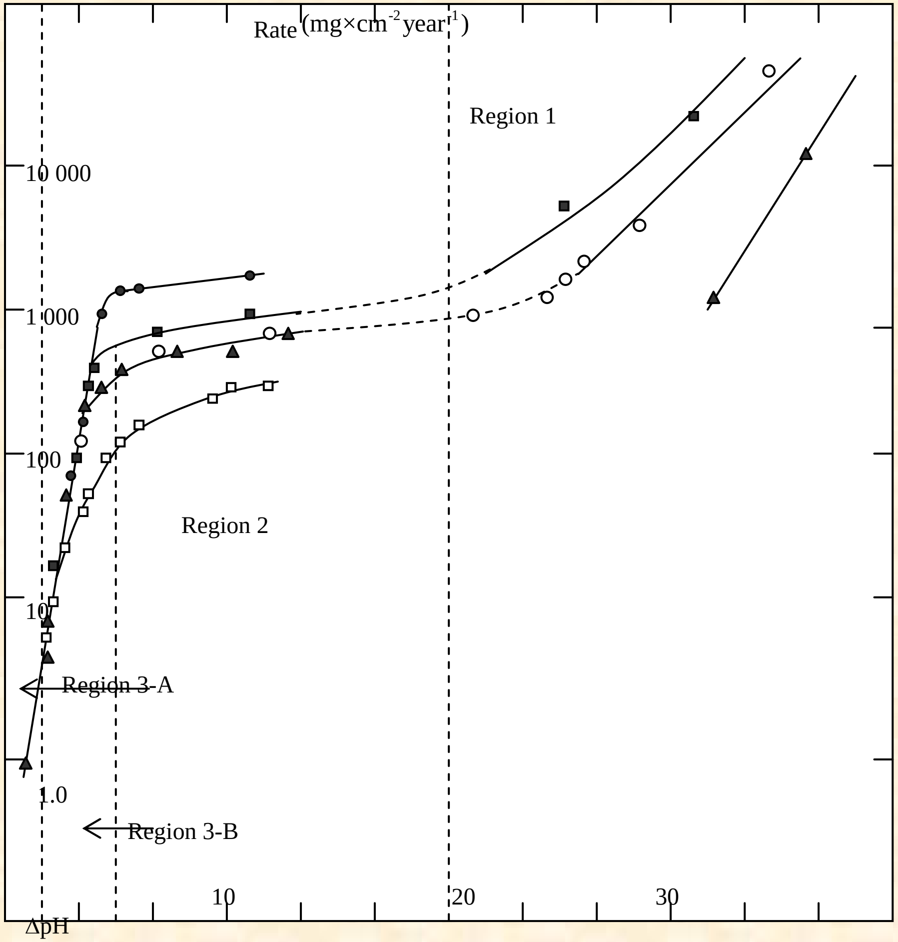
● $\lg P_{CO_2} = 0.0$

■ $\lg P_{CO_2} = -1.5$

▲ $\lg P_{CO_2} = -2.0$

○ $\lg P_{CO_2} = -2.5$

□ $\lg P_{CO_2} = -2.6$



Local equilibrium approach

- Reaction is very fast: $$\prod_{i=1}^{l}[A_i]^{\nu_i^{(a)}} \Big/ \prod_{i=1}^{m}[B_i]^{\nu_i^{(b)}} = K_r$$

- Chemistry:

$$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$$

$$HCO_3^- \leftrightarrow H^+ + HCO_3^{2-}$$

$$(CaCO_3)_S \leftrightarrow Ca^{2+} + CO_3^{2-}$$

- Definitions: $[Ca^{2+}] = C,\ \ [H^+] = x,\ \ [HCO_3^-] = y,\ \ [CO_3^{2-}] = r,\ \ [H_2CO_3] = m$

Diffusion limited model

- Equilibrium constants: $a_1 = 10^{-6,35}/(\gamma_x \gamma_y), \bar{a}_1 = 10^{-6,35}/(\bar{\gamma}_x \bar{\gamma}_y), a_2 = 10^{-10,31}\gamma_y/(\gamma_x \gamma_r),$

  $\bar{a}_2 = 10^{-10,31}\bar{\gamma}_y/(\bar{\gamma}_x \bar{\gamma}_r)$ $\qquad \bar{a}_3 = 10^{-8,5}/(\bar{\gamma}_C \bar{\gamma}_r)$

- Governing equations: $n\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial z} = \sigma_C^*$ $\quad n\frac{\partial x}{\partial t} + v\frac{\partial x}{\partial z} = \sigma_x^* + \sigma_x$ $\quad n\frac{\partial m}{\partial t} + v\frac{\partial m}{\partial z} = \sigma_m^* + \sigma_m$

  $n\frac{\partial y}{\partial t} + v\frac{\partial y}{\partial z} = \sigma_y^* + \sigma_y$ $\quad n\frac{\partial r}{\partial t} + v\frac{\partial r}{\partial z} = \sigma_r^* + \sigma_r$

  $\sigma_i^* = \beta_i(\bar{C}_i - C_i)$ $\quad \beta_i = D_i S_u / h_i$

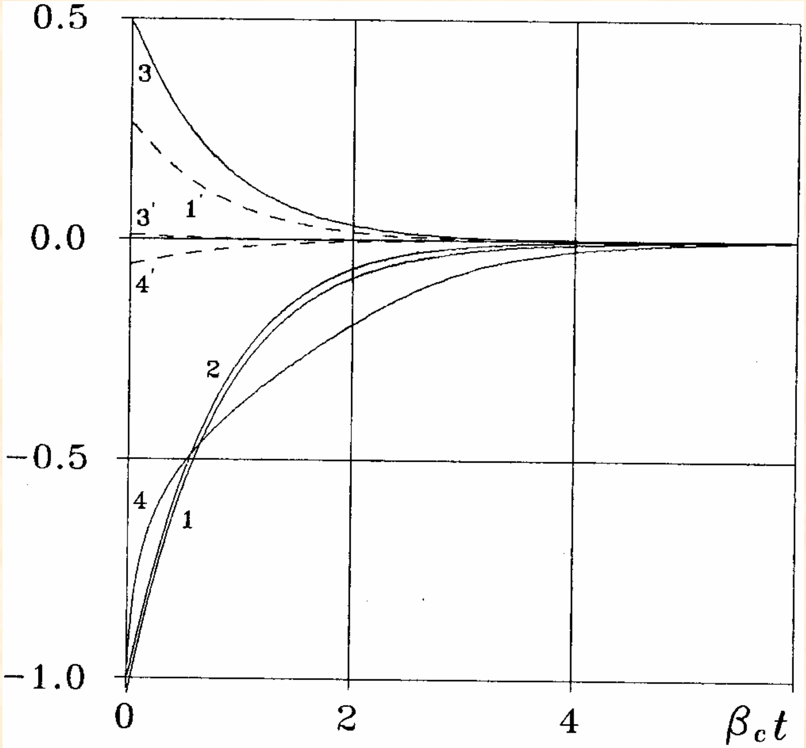
- Balance conditions: $\sigma_C^* = \sigma_r^* + \sigma_y^* + \sigma_m^*$ $\quad \sigma_r + \sigma_y + \sigma_m = 0$
- Solution: $n\frac{\partial \Phi}{\partial t} + v\frac{\partial \Phi}{\partial z} = 0, \quad \Phi = C - (r + y + m)$ $\quad \Rightarrow C - C_0 = r + y + m - S_0$

Boundary conditions: $C_0 = C\big|_{z=0} = 0, w_0 = 0, m_0 = m\big|_{z=0} = 10^{-1.47} P_{CO_2}$

- Dimensionless concentrations and pH versus time
- Denotings:

$$C_p = \frac{C - C_\infty}{|y_0 - y_\infty|}, y_p = \frac{y - y_\infty}{|y_0 - y_\infty|}, r_p = \frac{r - r_\infty}{|y_0 - y_\infty|}, m_p = \frac{m - m_\infty}{|m_0 - m_\infty|}$$

$$\bar{C}_p = \frac{\bar{C} - C_\infty}{|y_0 - y_\infty|}, \bar{y}_p = \frac{\bar{y} - y_\infty}{|y_0 - y_\infty|}, \bar{r}_p = \frac{\bar{r} - r_\infty}{|y_0 - y_\infty|}, \bar{m}_p = \frac{\bar{m} - m_\infty}{|y_0 - y_\infty|}$$



$1 - 2C_p; 1' - \bar{y}_p, 2\bar{C}_p; 2 - y_p; 3 - m_p; 3' - \bar{m}_p; 4 - pH_p; 4' - \overline{pH_p}$

Electro-diffusion model (Khramchenkov, 1998)

- Impact of electrical forces in ion's diffusion

$$\frac{\partial (nC_i)}{\partial t} + \nabla(\vec{V}C_i) = \nabla(\alpha \nabla C_i) + j_i + n\sigma_i^{(v)}, \qquad \vec{V} = \frac{k}{\eta}(\nabla p + \rho \vec{g}), \qquad \mathrm{div}\vec{V} = 0,$$

$$\frac{\partial (\overline{n}\overline{C}_i)}{\partial t} + j_i = \overline{n}\overline{\sigma}_i^{(v)} + S_u \overline{\sigma}_i^{(s)}, \quad j_i = \beta_i(\overline{C}_i - C_i + \frac{z_i C_i F}{RT}\delta\varphi), \quad \sum_i z_i C_i = 0, \quad I = \sum_i z_i j_i = 0.$$

- Chemical reactions:

$$H_2O + CO_2 \leftrightarrow H^+ + HCO_3^-$$

$$CaCO_3 + H^+ \leftrightarrow Ca^{2+} + HCO_3^-$$

- Near the chemical equilibrium:

$$CaCO_3 + H_2O \leftrightarrow Ca^{2+} + HCO_3^- + OH^-$$

Dissolution rate (Dreybrodt, 1988)

- Measured dissolution rate as a function of

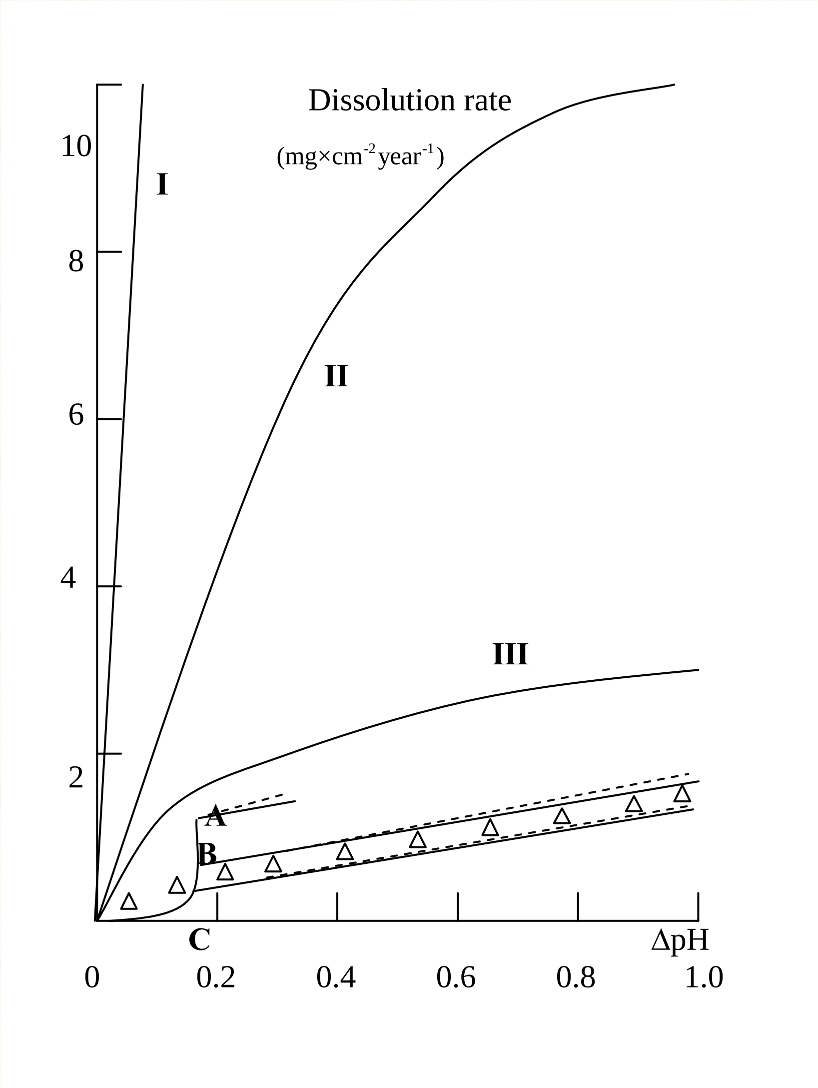
  ΔpH

- Measured curves:

A: $\lg P_{CO_2} = 0.0$

B: $\lg P_{CO_2} = -1.5$

C: $\lg P_{CO_2} = -2.0$



Pure kinetics model

- Chemical reactions:

$$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$$

$$HCO_3^- \leftrightarrow H^+ + HCO_3^{2-}$$

$$(CaCO_3)_S \leftrightarrow Ca^{2+} + CO_3^{2-}$$

$$(CaCO_3)_S + H^+ \leftrightarrow Ca^{2+} + HCO_3^-$$

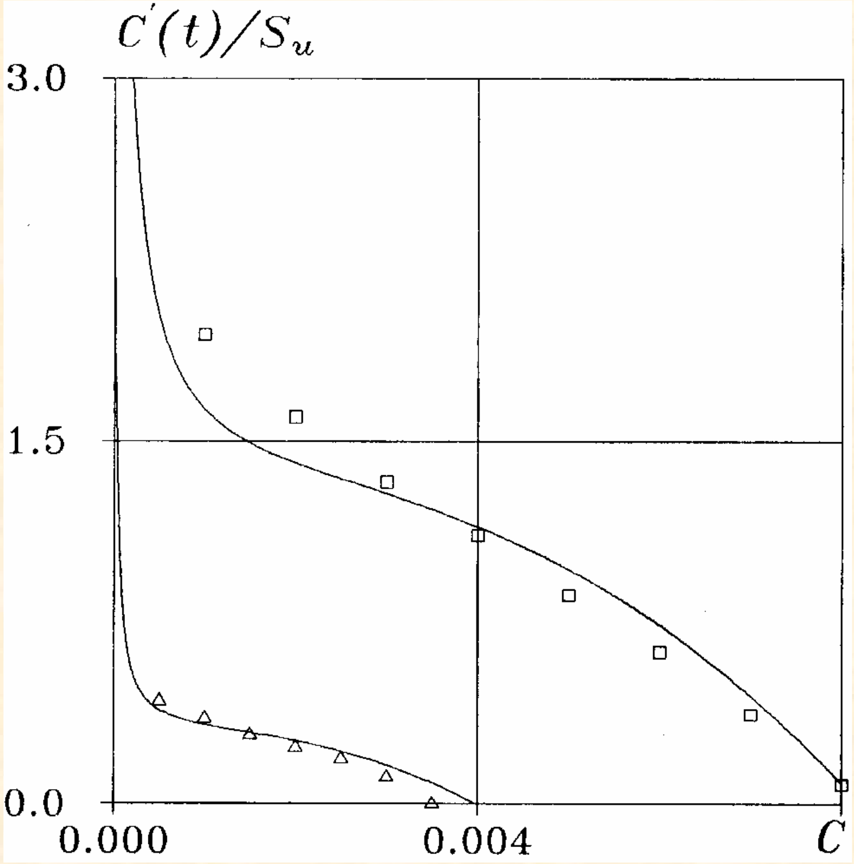
$$(CaCO_3)_S + H_2CO_3 \leftrightarrow Ca^{2+} + 2HCO_3^-$$

- Dissolution rate equation (modified Plummer – Wigley kinetics):

$$\frac{1}{S_u}\frac{dC}{dt} = (k_1 x + k_3)\left[1 - \left(\frac{a_2}{a_3}\right)\frac{Cy}{x}\right] + k_2 m\left[1 - \left(\frac{a_2}{a_3 a_1}\right)\frac{Cy^2}{m}\right], C\big|_{t=0} = C_0$$

Comparison with experimental data of Erga, Terjesen, 1956:

Plot of complex $S_u dC / dt$ versus C:



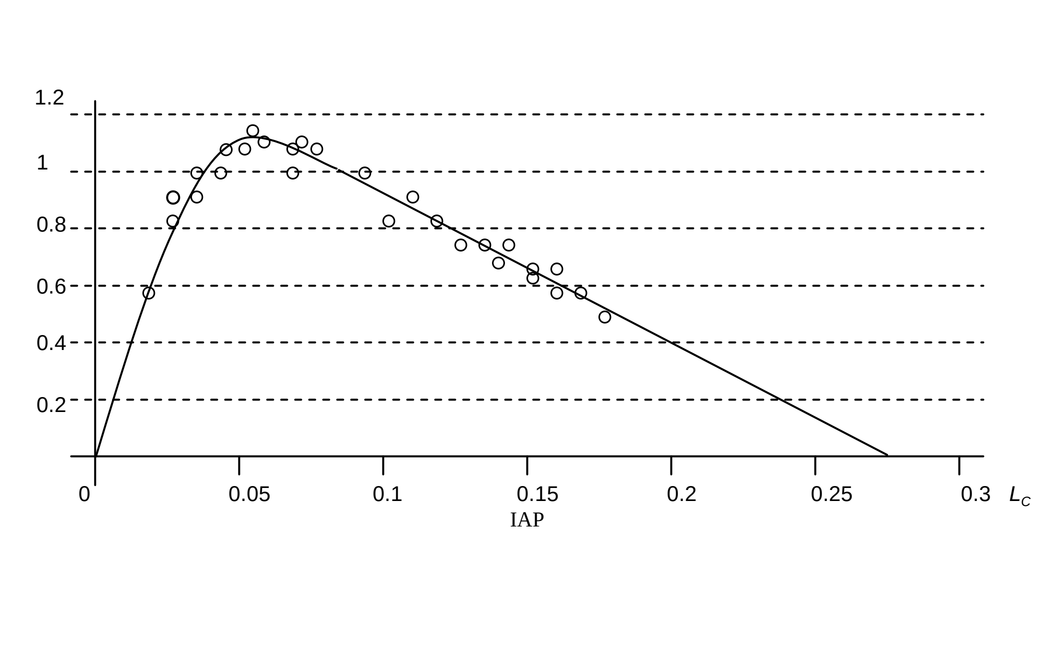
Denoting:

□ $-\ P_{CO_2} = 0{,}0952$ MPa

△ $-P_{CO_2} = 0{,}0135$ MPa

Comparison with experimental data of Lekhov et al., 1974

- Plot of complex $R/[H^+]$ versus IAP

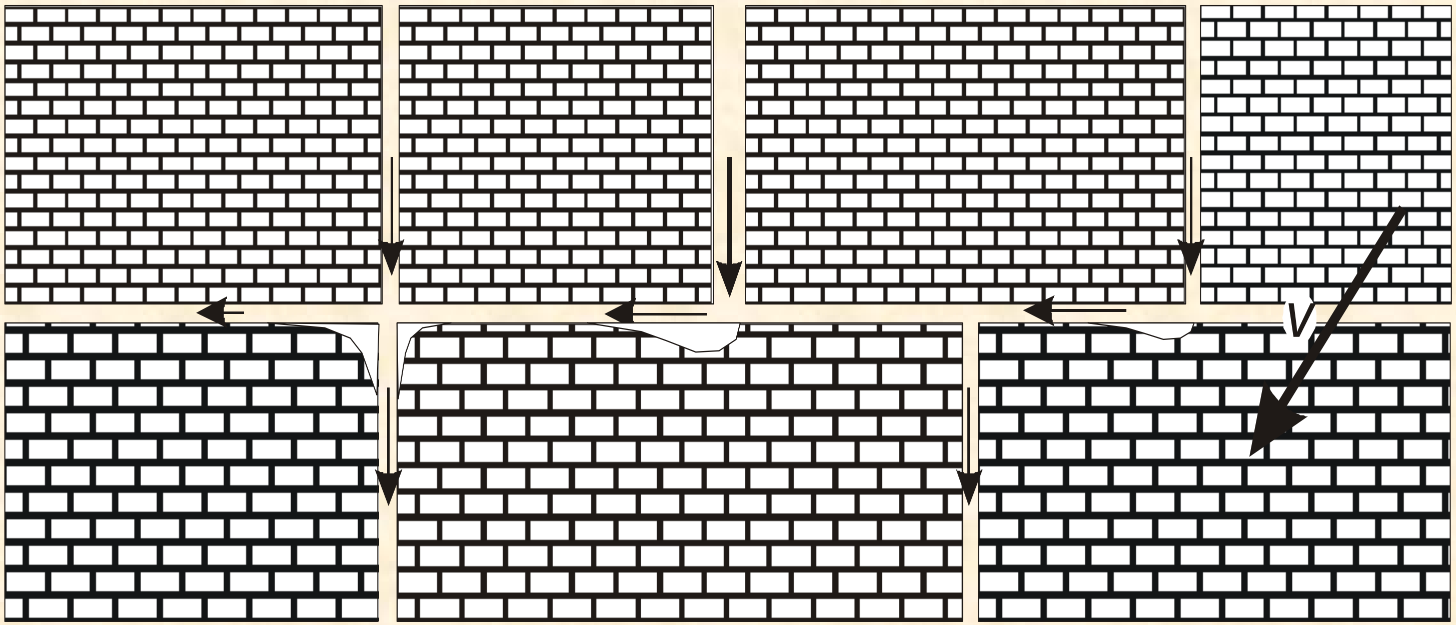


Conclusions ("chemical" part):

- Principal problems are solved
- Some problems are waiting for solution (construction of universal chemical and hydro-mechanical model)

Hydrodynamics of flow in multi-scale fractured media

- **Main problem:** transformation of fissured media into conduit media (media with domination of relatively small number of transport fractures)



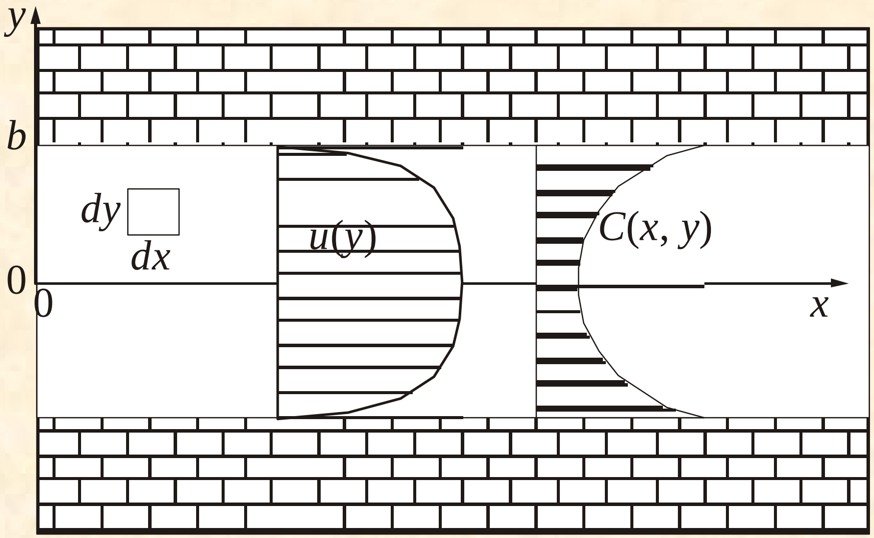
Evolution of transport fractures in consequence of fracture wall dissolution

Hydrodynamics of flow in multi-scale fractured media

- **Main publications (**karst fracture's evolution models):

  Bauer et al. (2003), Baedke & Krothe (2001), Birket et al. (2003), Dreybrodt,(1988, 2000), Jeannin (2001), Kaufmann & Braun (1999, 2000), Kaufmann (2003), Liedl et al. (2003).

Simplest model: dissolution of single fracture



Hydrodynamics of flow in multi-scale fractured media

- **Governing equations:**

$$D\frac{\partial^2 C}{\partial y^2} = u(y)\frac{\partial C}{\partial x} \quad (5)$$

$$u(y) = 1.5u_b\left[1-(y/b)^2\right] \quad (6)$$

- **Boundary condition:**

$$C(0,y) = C_0$$

- **Symmetrical condition:**

$$\frac{\partial C(x,0)}{\partial y} = 0$$

- **Wall's dissolution**

$$D\frac{\partial C(x,b)}{\partial y} = -\rho_s\frac{db}{dt}$$

Approach: integral correlations

$$(5)\times(y-b),\ \int_h^b (5)(y-b),\ h: C(b)=0,\ \frac{\partial C}{\partial y}(b)=0,\ b\geq 0$$

Characteristic point x^*:

$$h = 0 \Rightarrow x^* = gb^4/(40D\nu)$$

Hydrodynamics of flow in multi-scale fractured media

Equation for fracture's size distribution: $\frac{db}{dt}\frac{\partial f}{\partial b} = -k_e sf\,,\; 0 \le s \le 1 \quad (7)$

First case: x^* **small**

Normal distribution with variance $\sigma = \sqrt{\frac{DC_0 \exp[-\chi(x-x^*)]}{ks\rho_s}},\; \chi = 60\nu D/(11gb^4)$

Second case: χ^* **large**

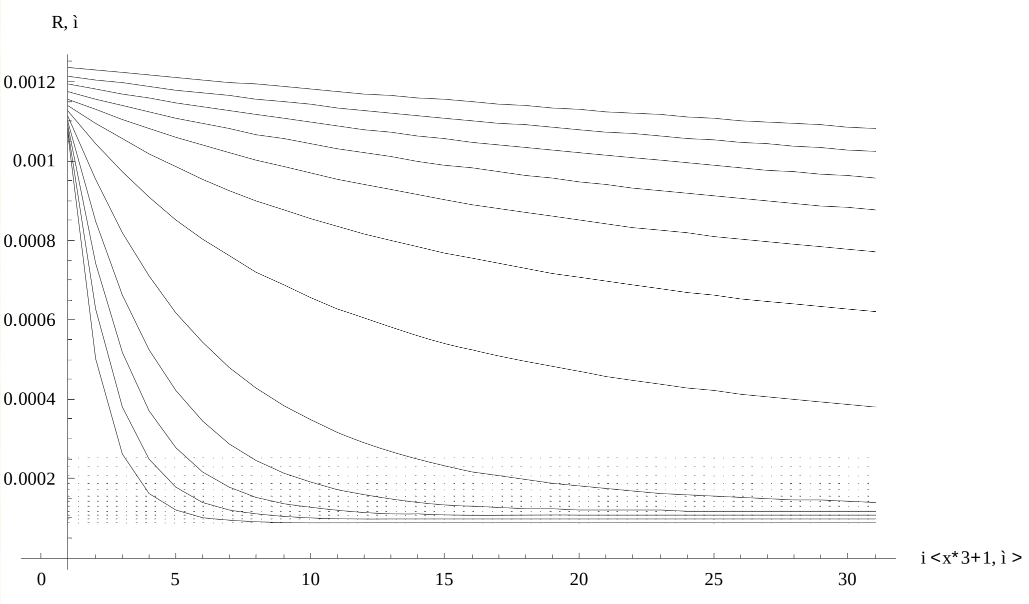
Normal distribution with variance $\sigma = \sqrt{\frac{DC_0}{ks\rho_s \sqrt[3]{(x/x^*)}}}$

Turbulent regime of flow – normal distribution transforms in log-normal distribution

Hydrodynamics of flow in multi-scale fractured media

Numerical simulation

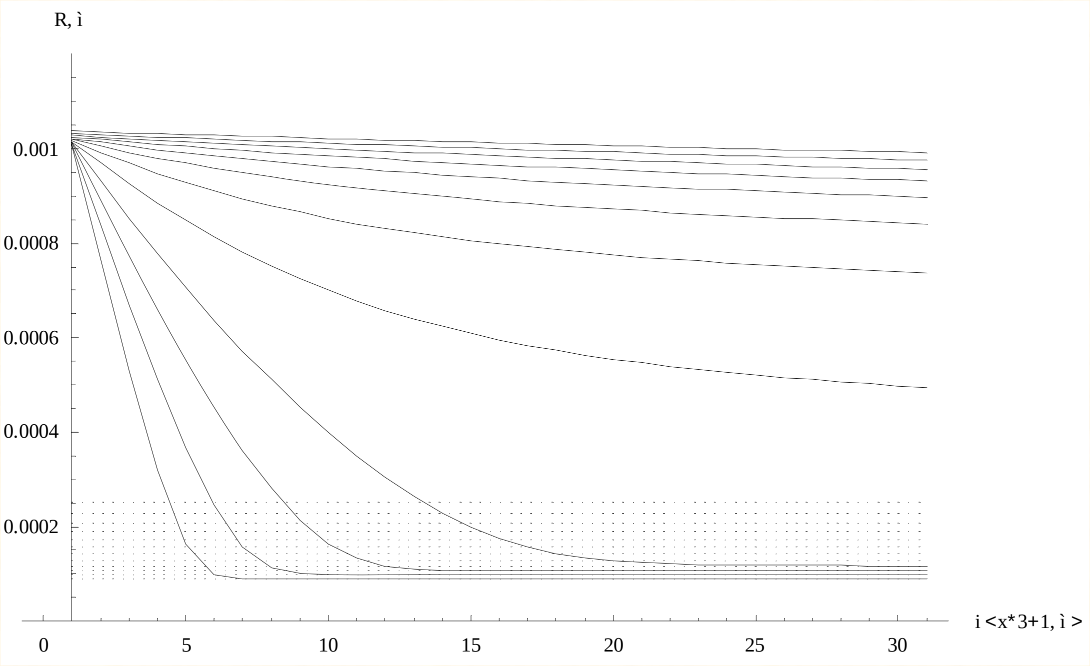
1. Kinetic regime of dissolution, laminar flow – moderate competition between fractures with different size (finish of calculations – an increase of total discharge by two order).



Hydrodynamics of flow in multi-scale fractured media

Numerical simulation

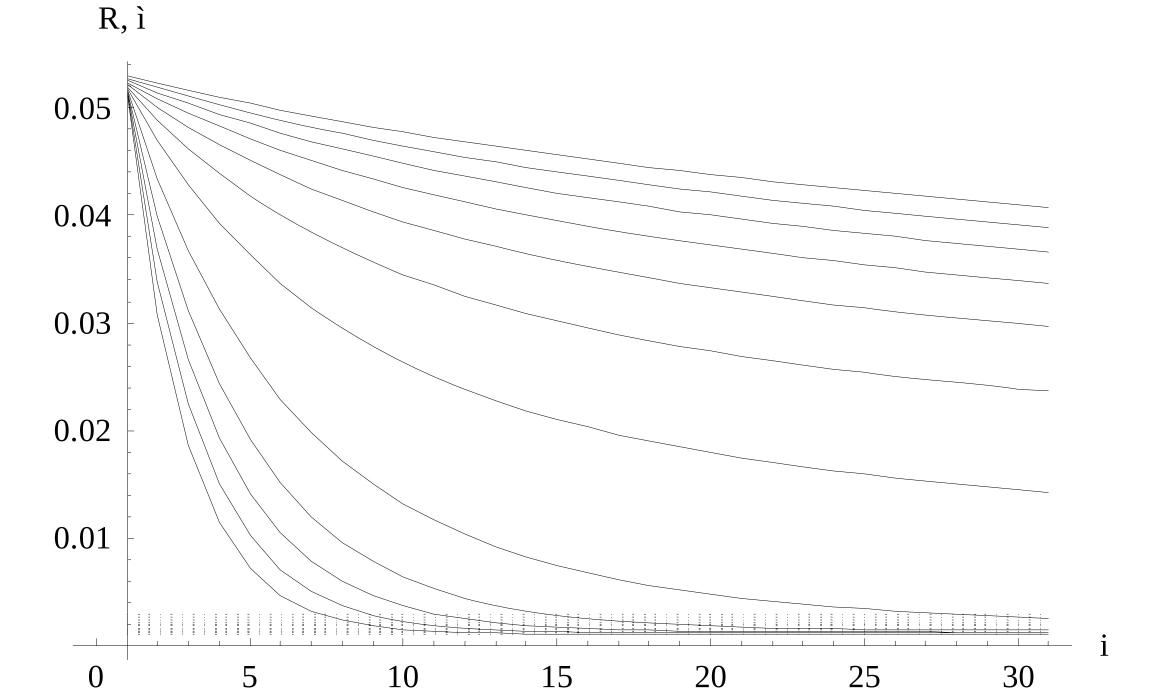
2. Diffusion regime of dissolution, laminar flow – more high competition between fractures with different size.



Hydrodynamics of flow in multi-scale fractured media

Numerical simulation

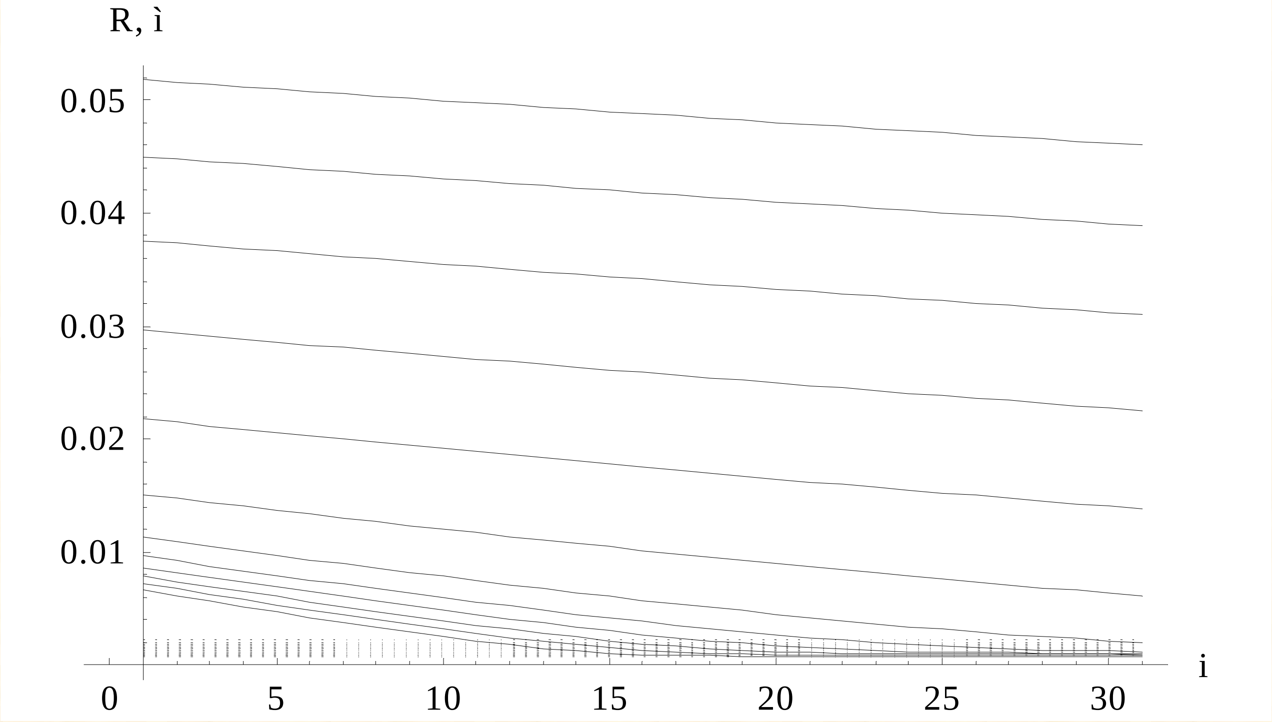
3. Kinetic regime of dissolution, turbulent flow – moderate competition between fractures with different size.



Hydrodynamics of flow in multi-scale fractured media

Numerical simulation

4. Diffusion regime of dissolution, turbulent flow – more high competition between fractures with different size.



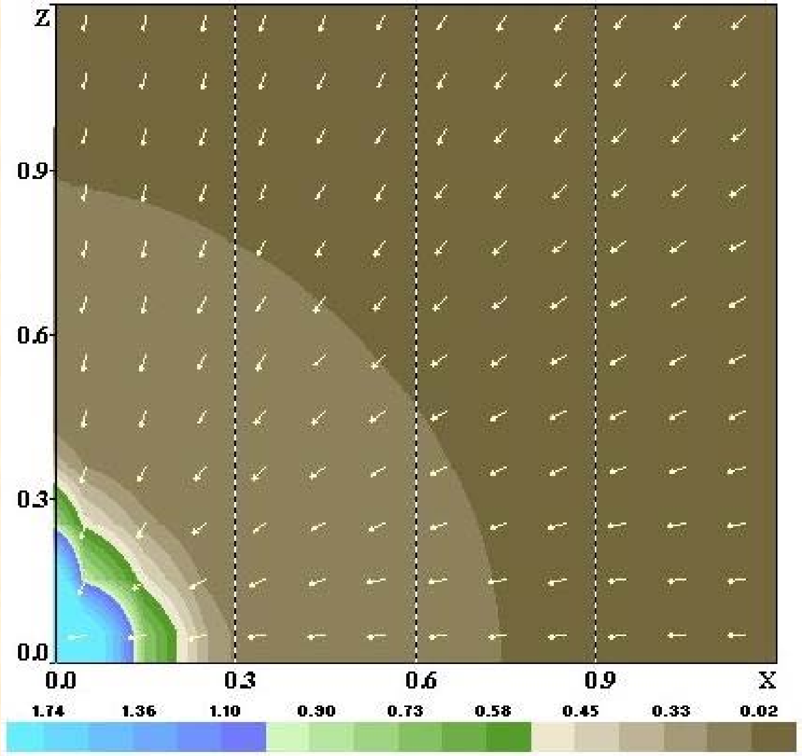
Conclusions ("hydrodynamics" part):

Character of karst fractures growth depends on:

- **Regime of flow (laminar or turbulent);**
- **Regime of dissolution (kinetic or diffusion);**
- **Correlation between discharge, aperture and length of fracture.**

KARST FAULTS

- Karst fractures drain the water from over-fractured rocks
- Simulation of suffosion: suufosion starts when the head of gradient stays more then critical meaning



Distribution of the head of gradient and flow velocity near the point of contact fractured and over fractured rocks (point of initial erosion)

KARST FAULTS

Equation of suffosion (Khramchenkov et al., 2006):

$$\partial N / \partial t = -\Psi(N, |\nabla H| - I_0(N)) \quad (8)$$

We find Ψ , if we solve the integral $\int_{N(t)}^{N_0} \frac{dN}{\Psi} = t$ (9)

Realistic view of Ψ is $\Psi = \gamma \sqrt{N} (|\nabla H| - I_0), \ |\nabla H| > I_0, N > 0$ (10)

Variation of *N* is

$$\frac{N(t)}{N_0} = \begin{cases} 1, & |\nabla H| \le I_0 \\ (1 - Bt)^2, & |\nabla H| > I_0, \ 0 < t < 1/B \\ 0, & |\nabla H| > I_0, \ t > 1/B \end{cases}$$

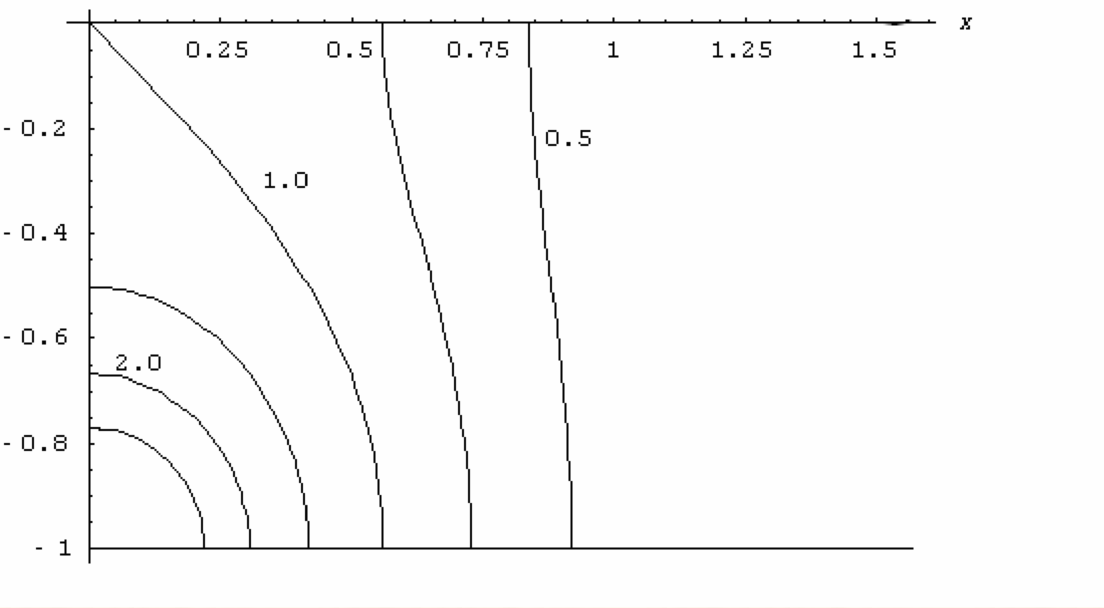
$$B = \gamma (|\nabla H| - I_0) / (2\sqrt{N_0})$$

N - volume fraction of substance of the ground, capable to suffosion

KARST FAULTS

Analytical solution

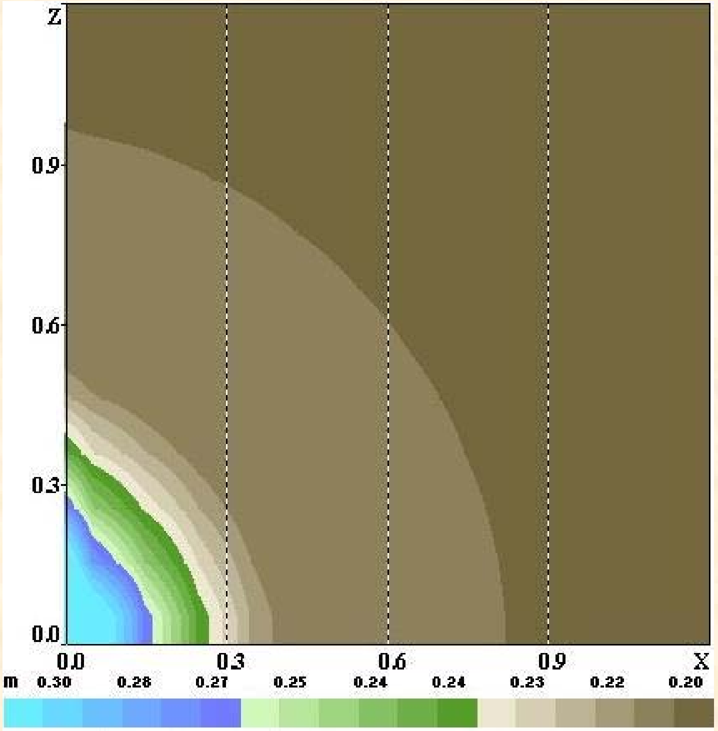
$$x(\theta)=\frac{2T}{\pi}\mathrm{Re}\left(\ \mathrm{ar\,sch}(\frac{2kTI}{Q})\cdot e^{i\theta}\right),\ y(\theta)=\frac{2T}{\pi}\mathrm{Im}\left(\ \mathrm{ar\,sch}(\frac{2kTI}{Q})\cdot e^{i\theta}\right).$$



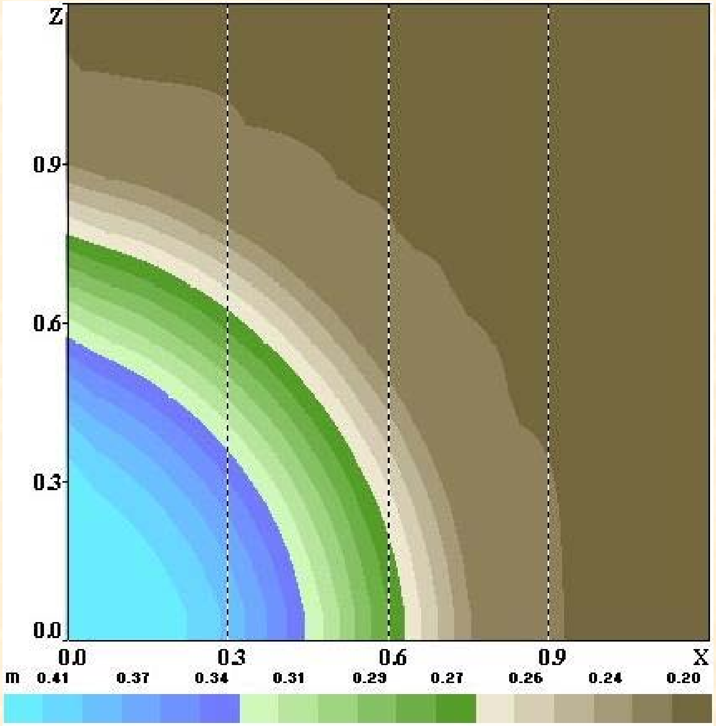
Bounds of suffosion zone for different $2kI_0T$

KARST FAULTS

Numerical simulation: dynamics of porosity changing near the point of initial erosion for different time: a – d - = 1, 20, 140, 950 c. u.

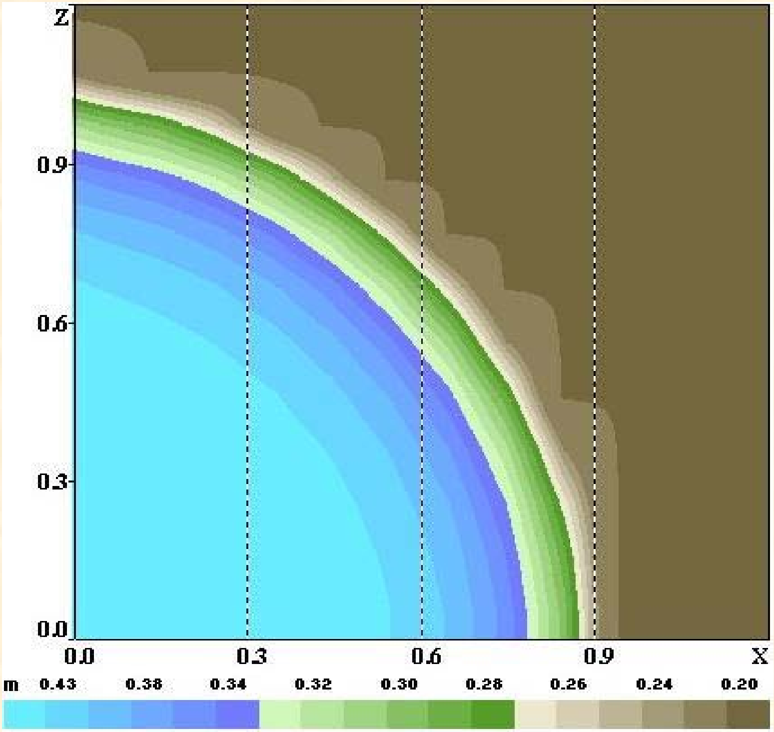


a

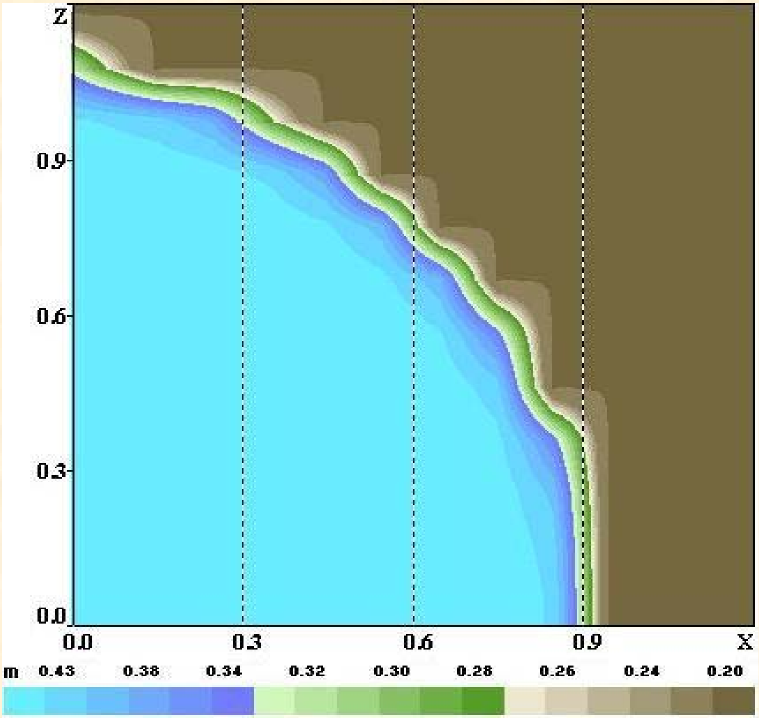


b

KARST FAULTS



c

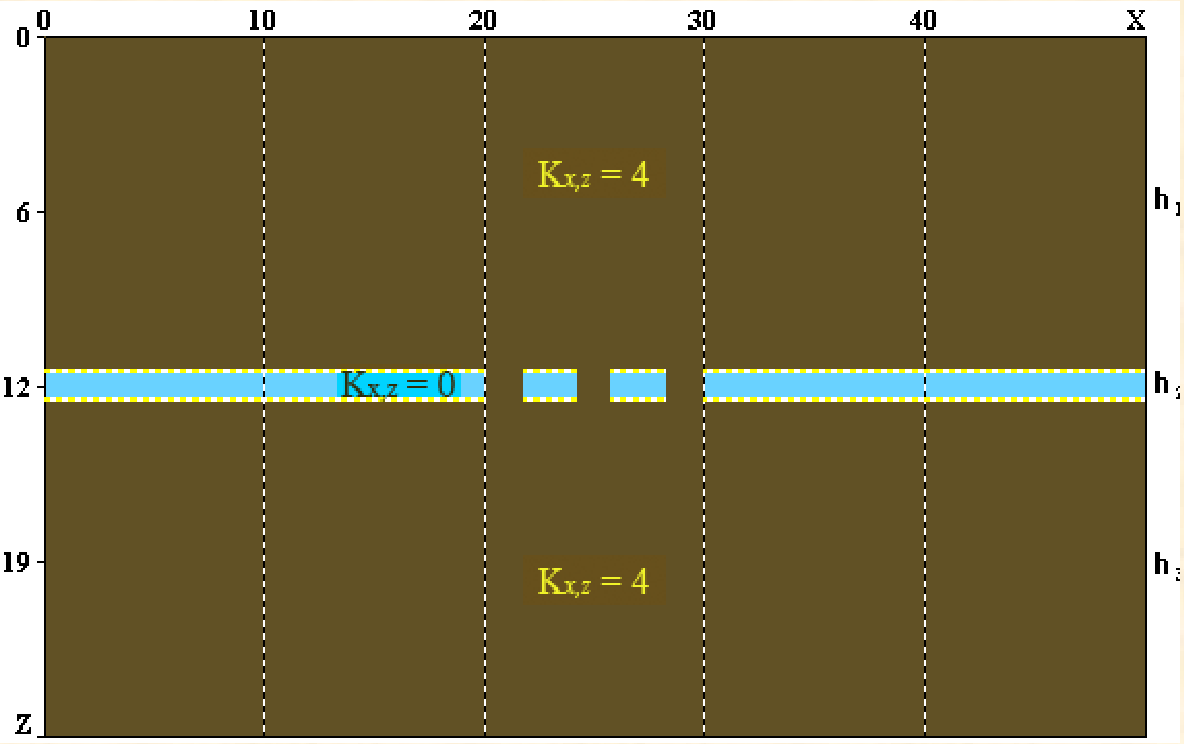


d

KARST FAULTS

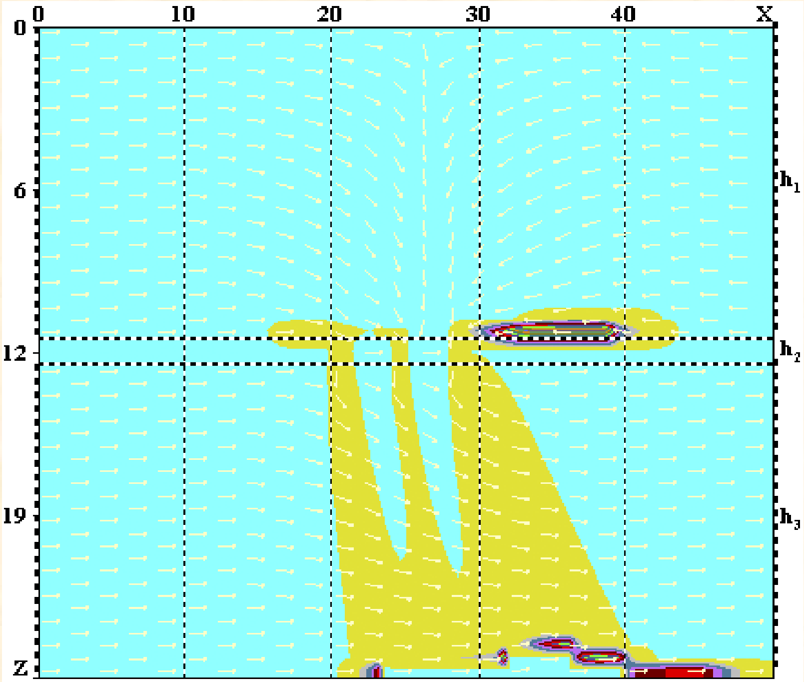
Numerical simulation for the number of points of initial erosion:

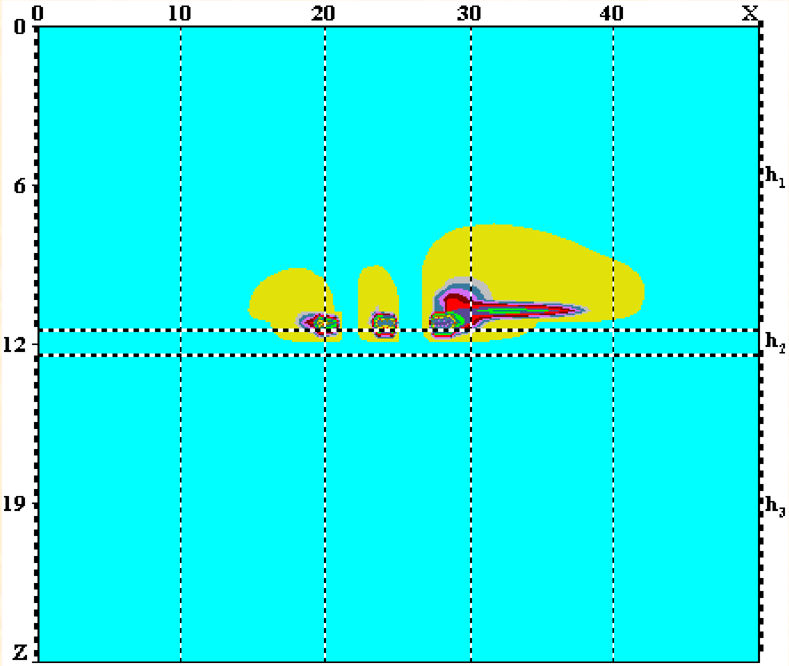
a) isotropic case



KARST FAULTS

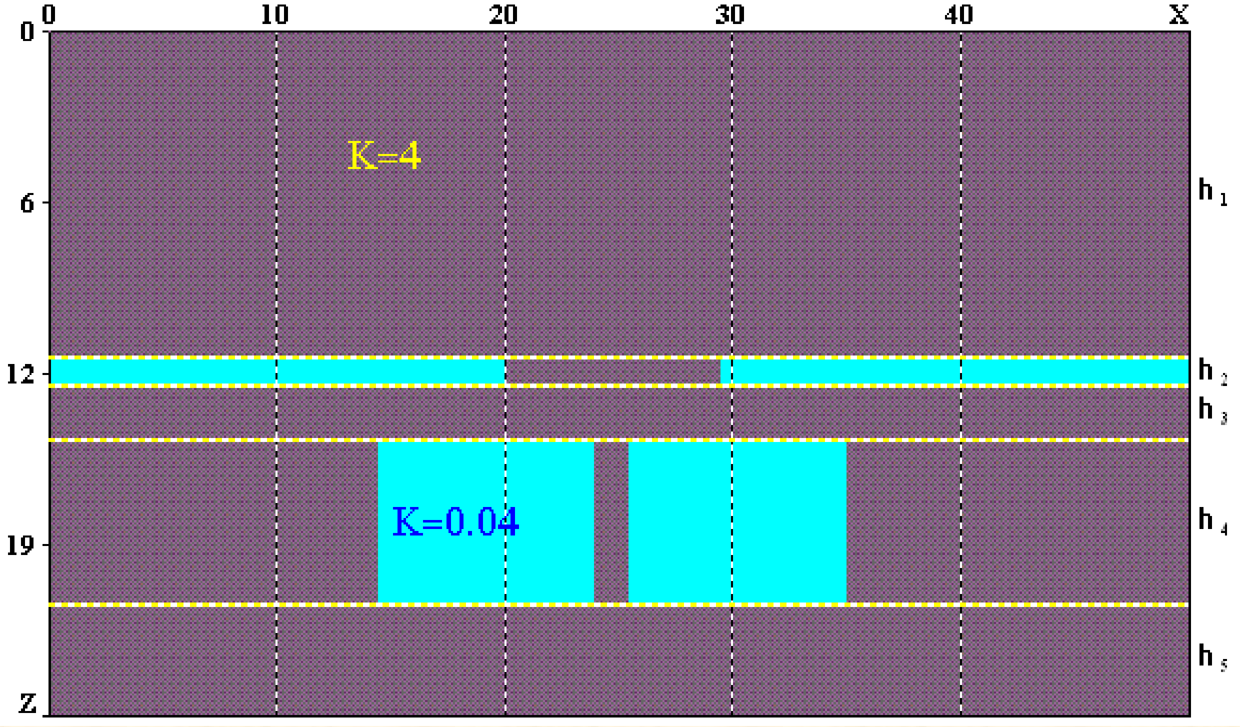
Distribution of mobile particles saturation *s* and porosity *m* for density difference $\rho_{\text{s-w}} = 0,05$



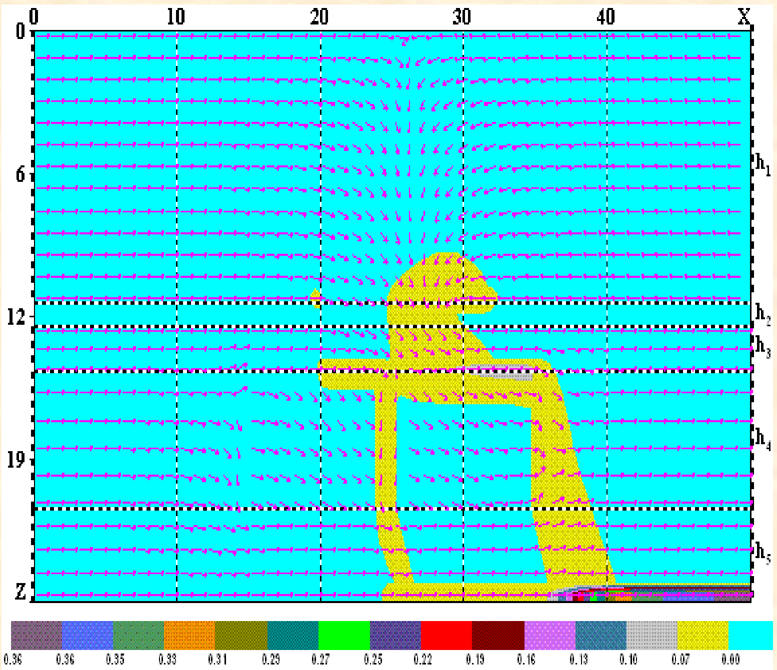


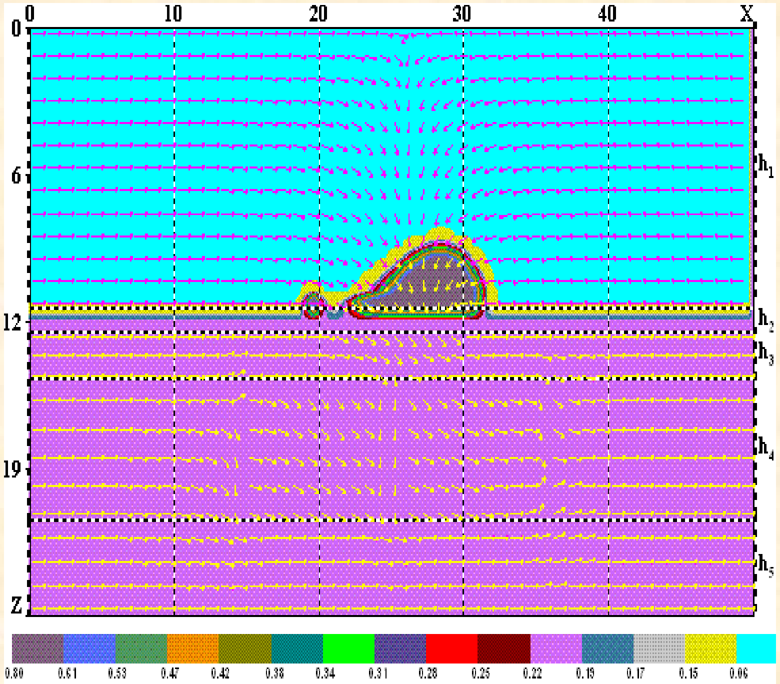
KARST FAULTS

b) anisotropic case



KARST FAULTS





Arrows – field of fluid velocity **V**

Conclusions:

In conclusion I should like to say that mathematical simulation is useful addition to classical methods of karst investigation, but…

really I just like to do it!

Thank You for Your attention!

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