

COLLOQUE ANNUEL DU GDR HYDROGEMM - 2024
MODÉLISATION NUMÉRIQUE DES « SYSTÈMES HYDROGÈNE »

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INTRODUCTION - NATURAL H₂ EXPLORATION

- New challenges for basin geologists: significant differences between H₂ systems and petroleum systems

- Multiple sources, poorly known

- Migration:

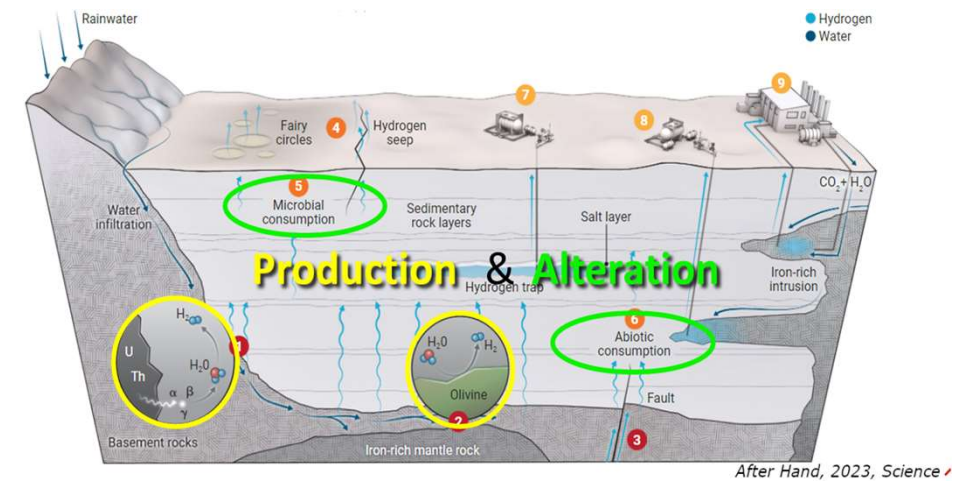
- **Dissolved flow**

Advection as a component of a mixture of dissolved gases:
H₂, He, CH₄, N₂

- Possible **transition to free-gas flow**

- Diffusion

- **Alteration**

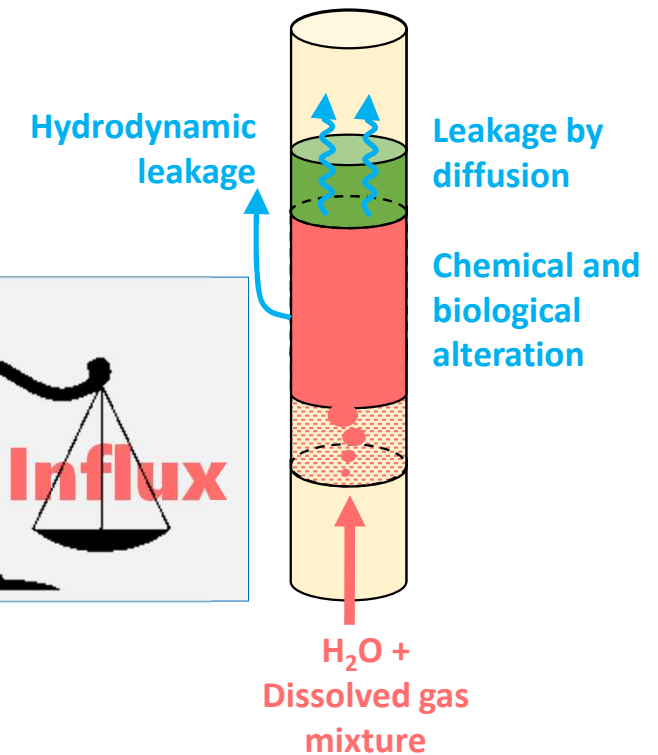
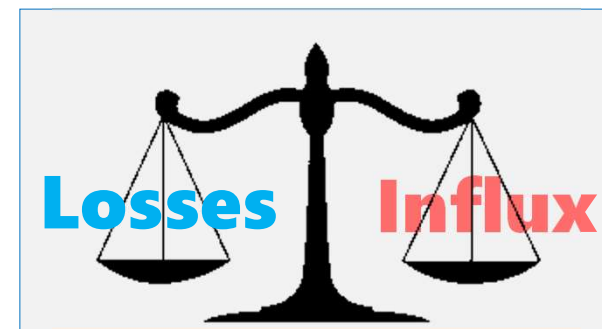


THE EXAMPLE OF NATURAL H₂ EXPLORATION

● What differences between H₂ systems and petroleum systems?

● Accumulation:

- Need a better cap rock
- Chemical and biological alteration
- Most probably **dynamic accumulations**:
 - Leakage balanced by influx
 - **Recharge rate needs to be considered**



FOCUS ON USEFUL FUNCTIONNALITIES

● Water ⇌ Vapor exchange

H₂ solubility from an analytic model calibrated with Sorreide & Whitson

$$\text{solubility} = e^{(a1.m^2+a2.m)}. \left(b1.PT + b2.\frac{P}{T} + b3.P + b4 * P^2 \right)$$

● Diffusion

$$\vec{j} = -D_{eff} \vec{\nabla} c \quad \text{with} \quad D_{eff} = D_0(T) \cdot \varphi \cdot \frac{1}{\tau}$$

Only in water;

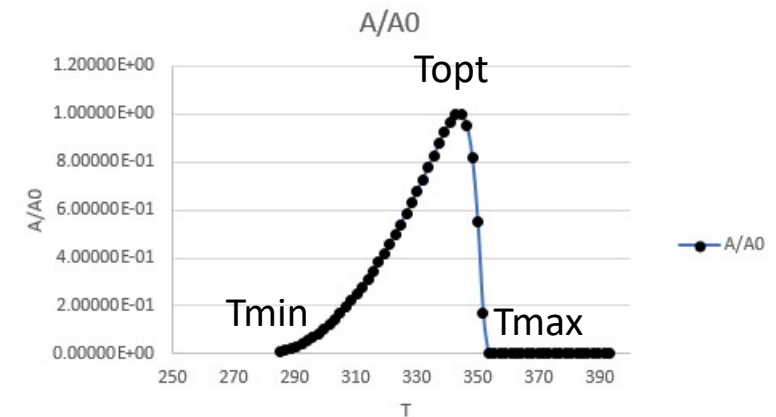
low solubility & low D_0 ➔ limited flux

● Alteration

$$\frac{dx_{H2}}{dt} = -A x_{H2}$$

with

$$A = A_0 * \left\{ \frac{T - T_{min}}{T_{opt} - T_{min}} \cdot \frac{(1 - e^{c(T-T_{opt})})}{(1 - e^{c(T_{opt}-T_{max})})} \right\}^2$$

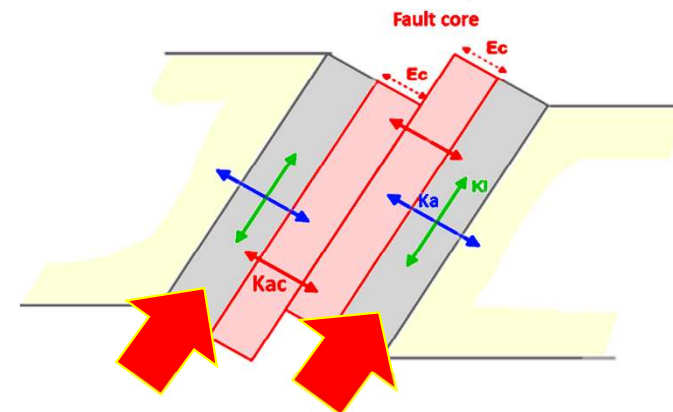
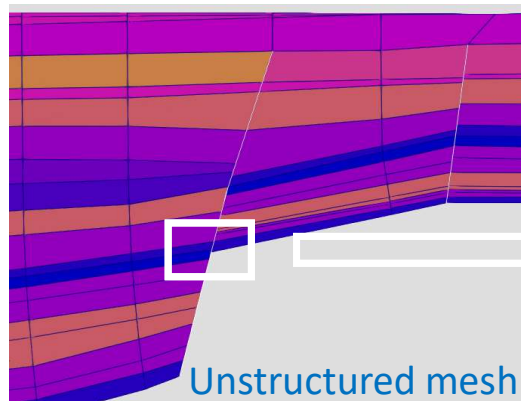


FOCUS ON USEFUL FUNCTIONNALITIES

● Source terms:

- Thermogenic
- Imposed concentration
- Imposed input gas rate (kg/Myrs)
- Imposed input flow rate with imposed concentration

● Fault flow modeling:

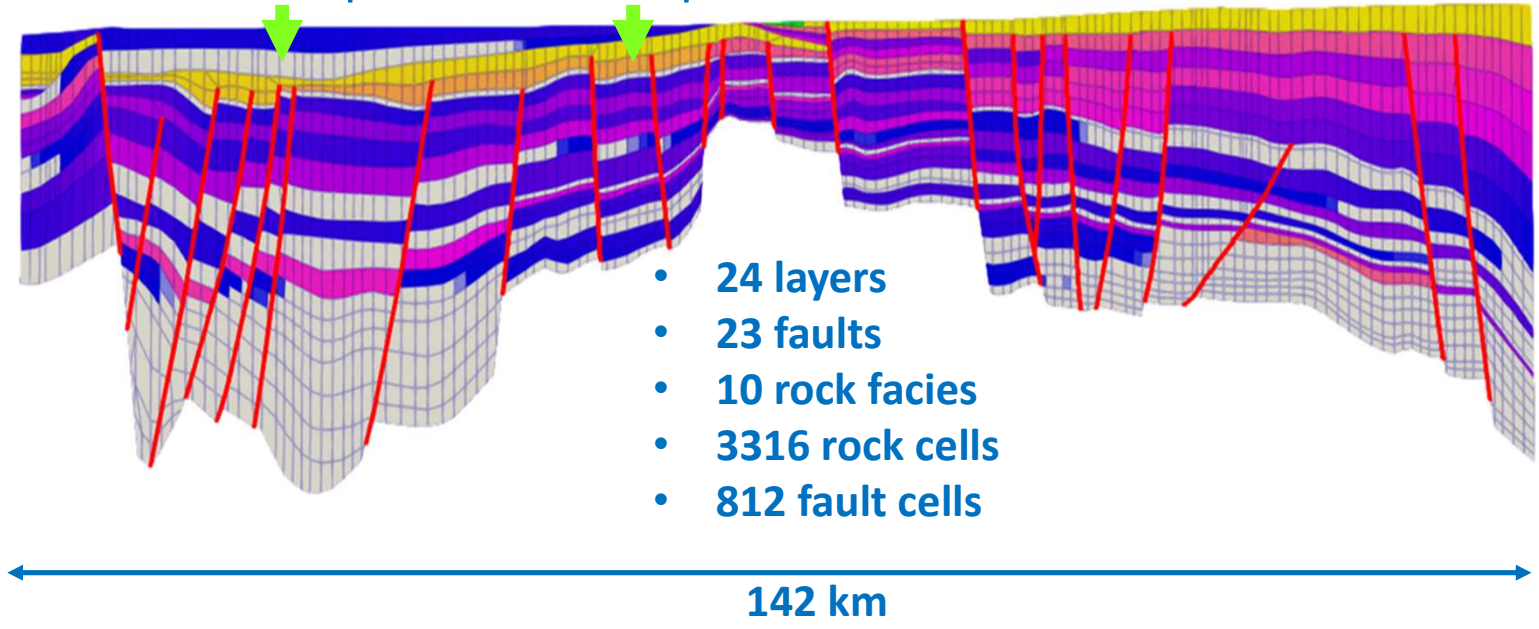


Imposed input flow rate with
imposed concentration

APPLICATION EXAMPLE

7000 m

Potential cap rock Aquifer



- 24 layers
- 23 faults
- 10 rock facies
- 3316 rock cells
- 812 fault cells

142 km

Permeability (Darcys)



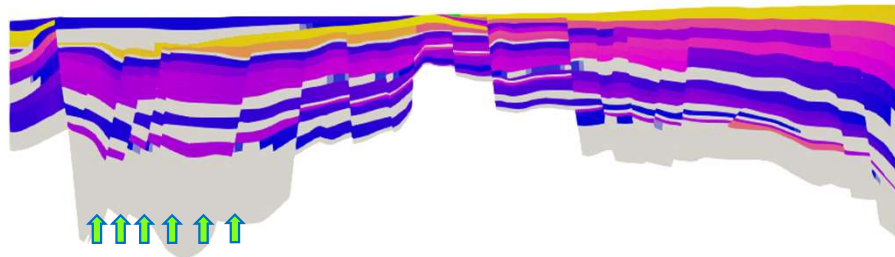
K	Ages	Geological Units/Horizons
24	0.0000	Top_Semmering
		Top_2nd
23	10.0000	Poni_Jurassic
22	15.0000	Yarragadee_1
21	20.0000	Yarragadee_2
20	25.0000	Yarragadee_3
19	30.0000	Yarragadee_4
18	35.0000	Yarragadee_5
17	40.0000	Yarragadee_6
16	45.0000	Top_Catalpa
15	50.0000	Top_Cattamarra_1
14	55.0000	Cattamarra_2
13	60.0000	Top_Eneabba
12	65.0000	Eneabba_2
11	70.0000	Eneabba_3
10	75.0000	Top_Lesueur
9	80.0000	Top_Woodside_1
8	85.0000	Woodside_2
7	90.0000	Top_Kockatea_1
6	95.0000	Kockatea_2
5	100.0000	Kockatea_3
4	105.0000	Base_Kockatea_1
3	110.0000	Base_Kockatea_2
2	115.0000	Top_IRCM_1
1	120.0000	IRCM_2
	150.0000	Top_Basement

Present

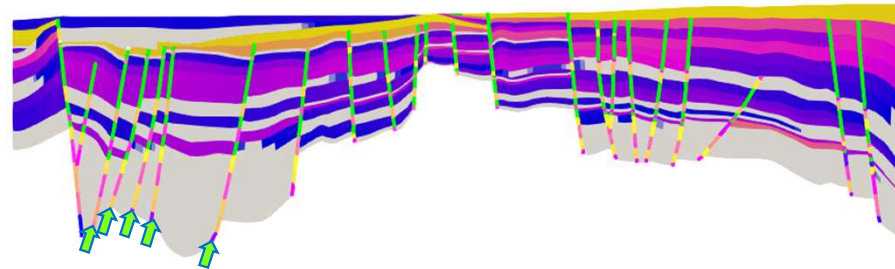
150 Myrs

3 SCENARIOS

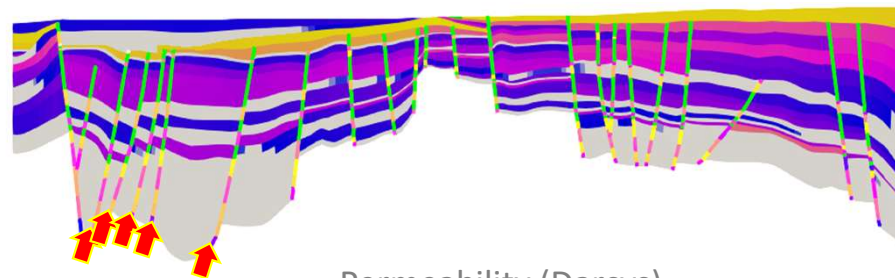
NEW ENERGIES



- A geologic-time-scale system
- **Neutral faults**
- Injection rate = 800l/year, 90ppm, starts at 50 Myrs



- Same as above, but **enhanced permeability faults**
- $K_{\text{faults}} = K_{\text{facies}} \times 10000$
- Fluid is injected at fault roots

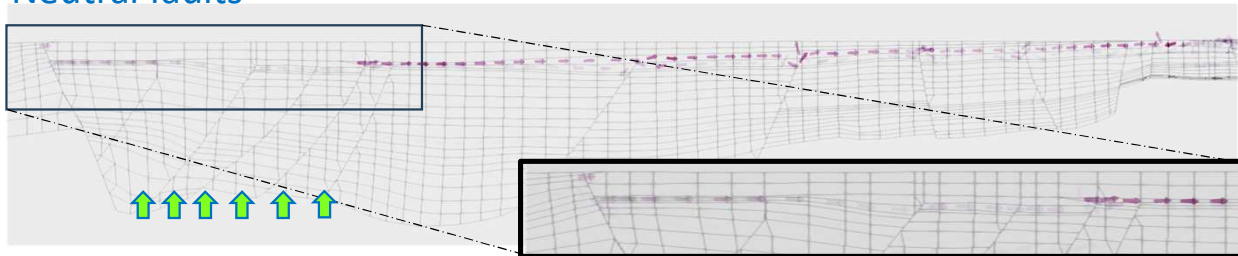


- Same as above but a **dynamic system**
- Injection rate = 800 m³/year, 10 ppm (160 kg H₂/year), starts at 1 Myr

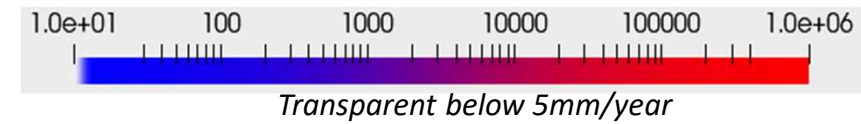


REGIONAL HYDRODYNAMISM, WATER VELOCITY

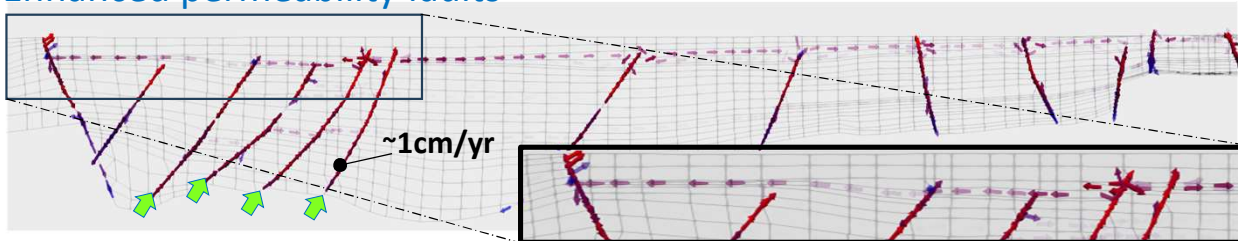
Neutral faults



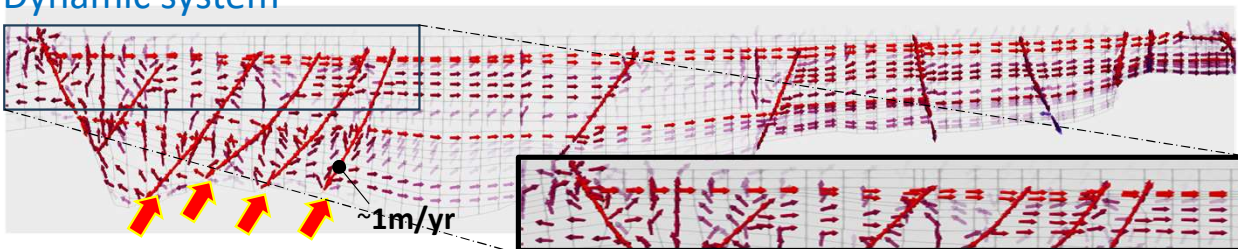
Water Darcy velocity (m/Myrs)



Enhanced permeability faults

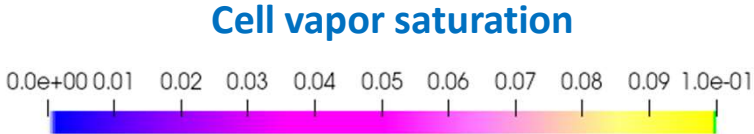
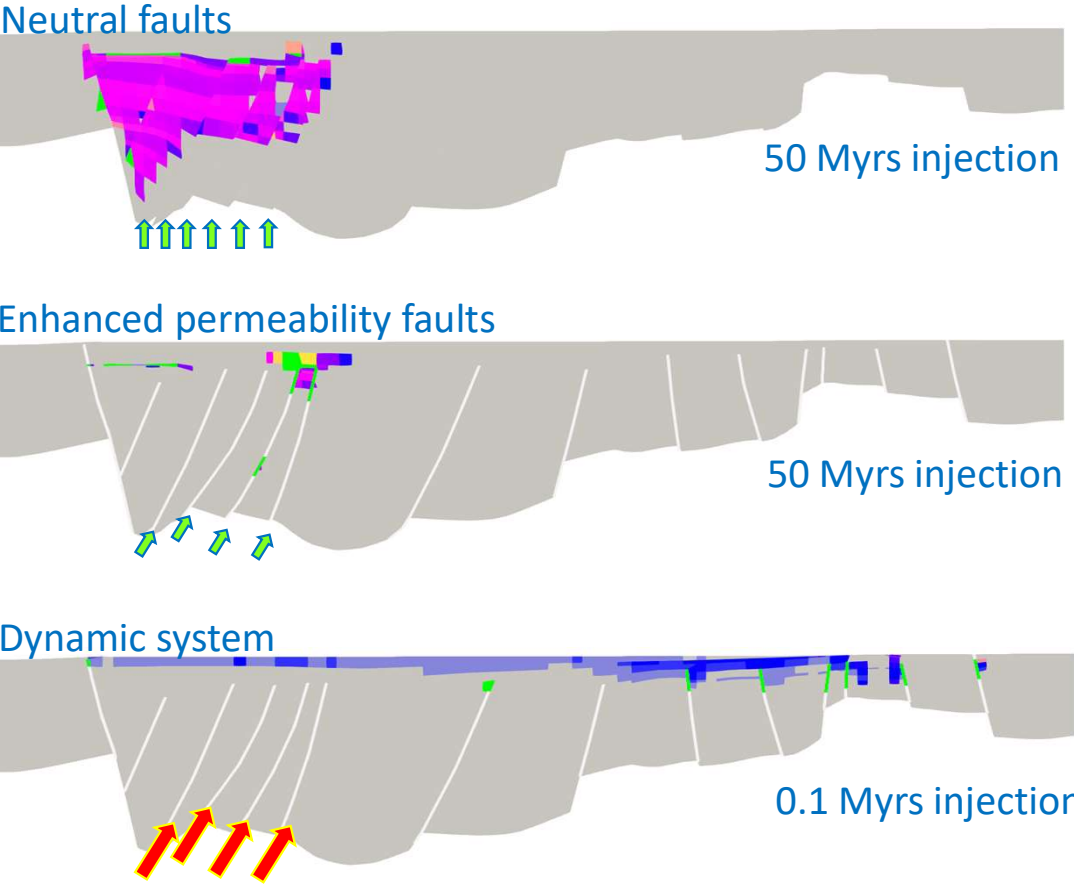


Dynamic system



- Regional hydrodynamism is **very sensitive to faults properties**
- Regional hydrodynamism is **very sensitive to the hydrothermal influx**, even if it is very small at 1st glance

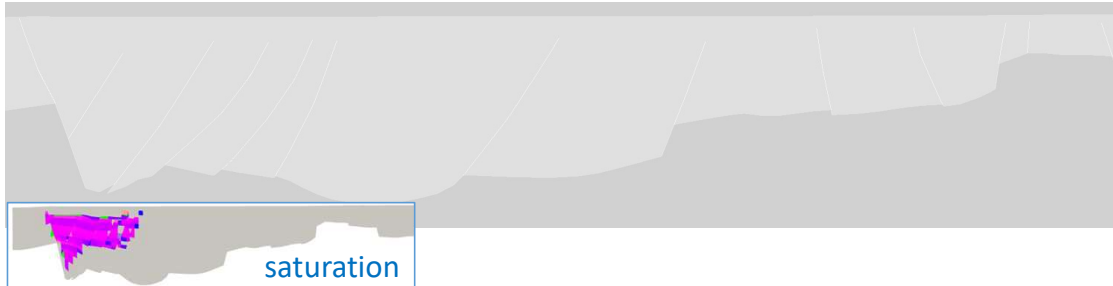
FREE-PHASE HYDROGEN SATURATION



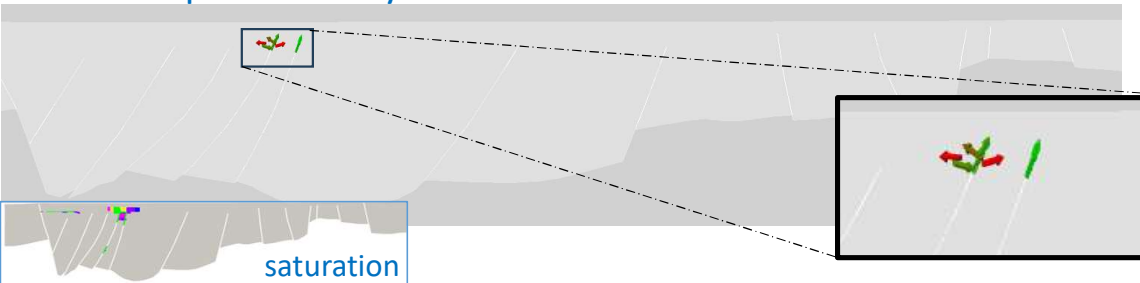
- Vapor accumulates below the cap rock in the geologic time scale scenarios
- High vapor saturations observed only at fault terminations in the dynamic system
- **Very different vapor-phase hydrogen distributions** in the 2 systems

FREE PHASE FLOW RATE

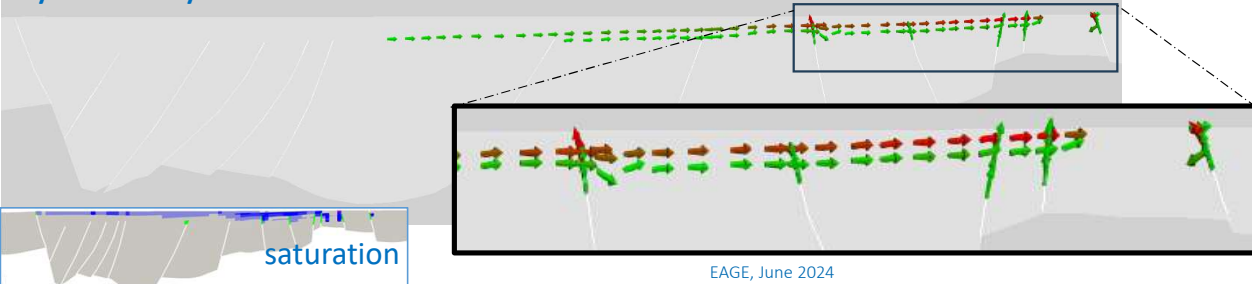
Neutral faults



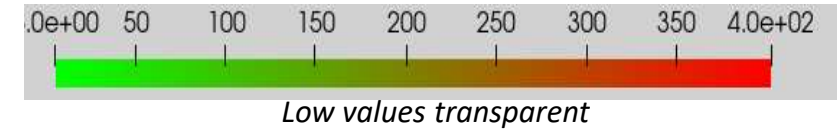
Enhanced permeability faults



Dynamic system



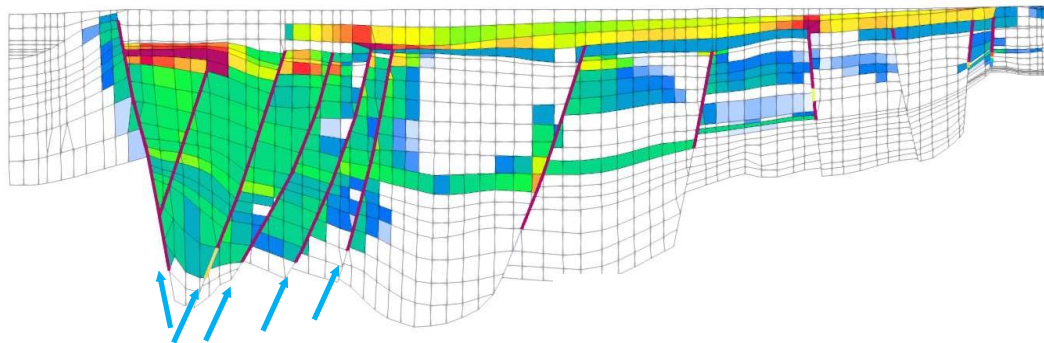
Flux of H₂ vapor (g/m²/year)



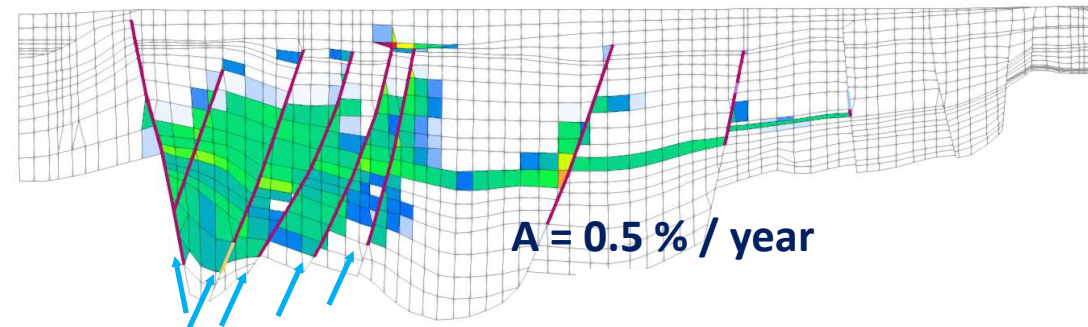
- Diffuse and very low vapor flux with neutral faults
- No significant vapor flux in the western reservoir in scenario #2
- The dynamic scenario gives significant **vapor-phase hydrogen flux above 400g/m²/year**

MICROBIAL DEGRADATION

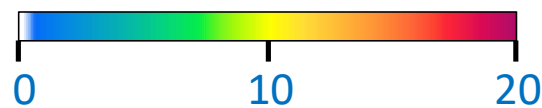
Dynamic system with an increased hydrogen supply, **no microbial degradation**



with microbial degradation



Free gas saturation in %



- No more free gas in the biotic interval with a degradation rate $> 0.5\%$ per year

- H₂ migration is very different from HC migration
- It is more difficult to have an intuition of the migration paths:
 - Very sensitive to the water « plumbing system », especially fault flow properties
 - May migrate over long distances by « dissolved flow »
 - Transition from « dissolved flow » to vapor flow controlled by gas concentration in the water, pressure, temperature and salinity
- Basin simulation is a tool which integrates all these parameters and physical processes
- Although not yet predictive, it is a **useful tool to assess different hypotheses about H₂ sources, migration paths, H₂ accumulations and recharge rate**

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