

# Do we grow old before fluid inclusions leak measurable amounts of substance? or how to play with diffusion models

Reference: Bakker RJ (2009) Reequilibration of fluid inclusions: Bulk-diffusion. Lithos, doi:10.1016/j.lithos.2009.03.006

Ronald J. Bakker

Department of Applied Geosciences and Geophysics  
Mineralogy and Petrology  
University of Leoben, Austria



<http://fluids.unileoben.ac.at>

Perfect Diffusion = Matter is transported from one part of a system to another as a result of „random“ molecular motions. In a dilute solution each molecule behaves independently of the others and is constantly undergoing collision with the solvent molecules. As a result it moves without preferred direction („random walk“). There is a net transfer from the higher to the lower concentration side as a result of this „random walk“

Fick's laws 
$$J = -D \frac{\partial C}{\partial x}$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

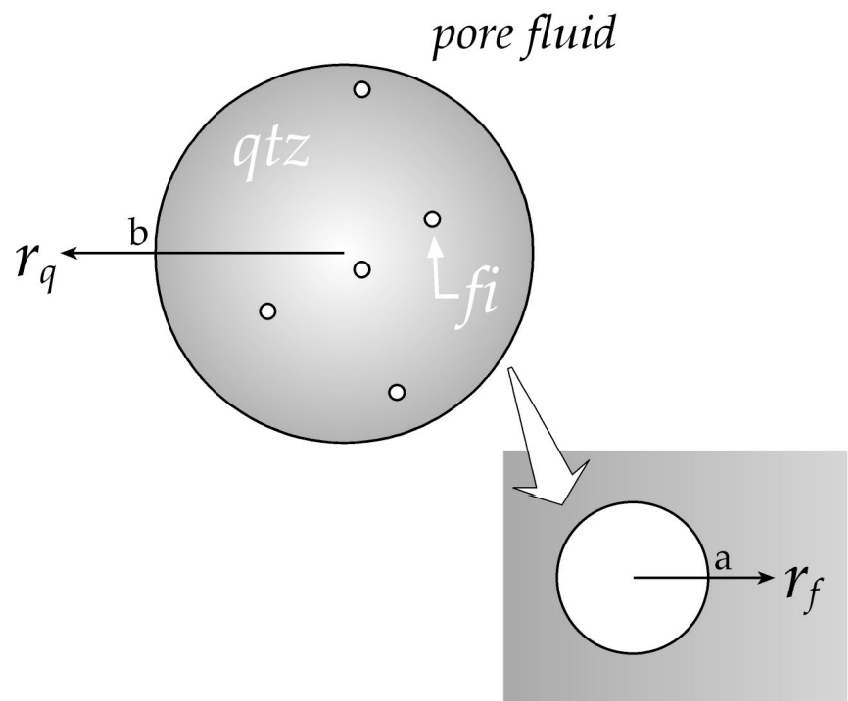
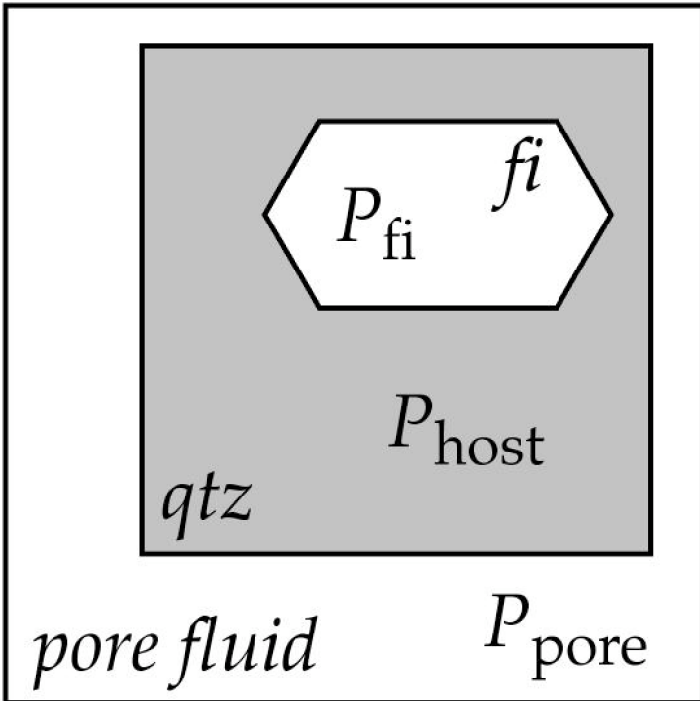
J = flux  
D = diffusion constant  
C = concentration  
x = direction, distance  
t = time

Not-so-perfect Diffusion = Heterogeneous system: diffusing material is a fluid phase and diffusion medium is a solid phase, connecting two fluid reservoirs

Even-less-perfect Diffusion = unknown identity of the diffusing species  
unknown solubility of fluid phase in diffusion medium

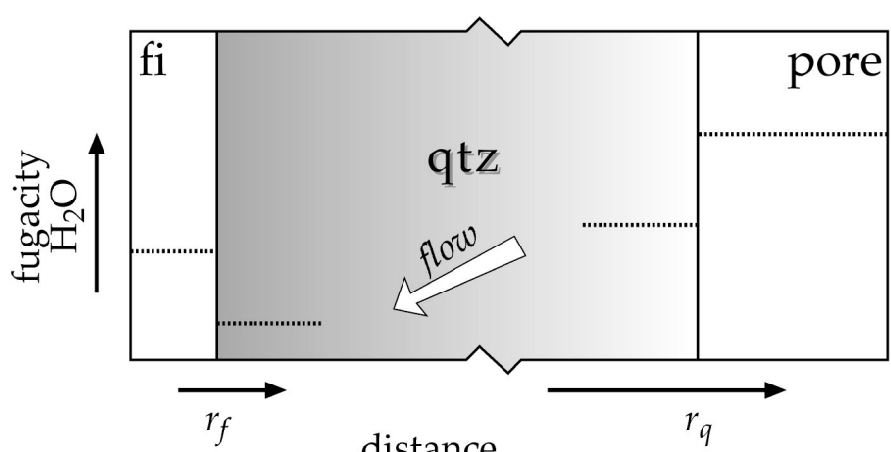
## Fluid Inclusions

System Definition

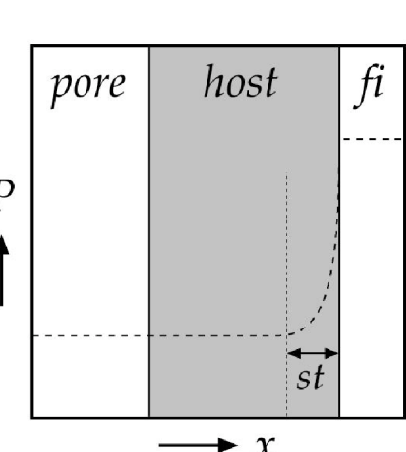


Can we measure diffusional loss / gain of fluid („H<sub>2</sub>O“) from fluid inclusions in quartz?

Fugacity gradient



Additional gradient: Pressure

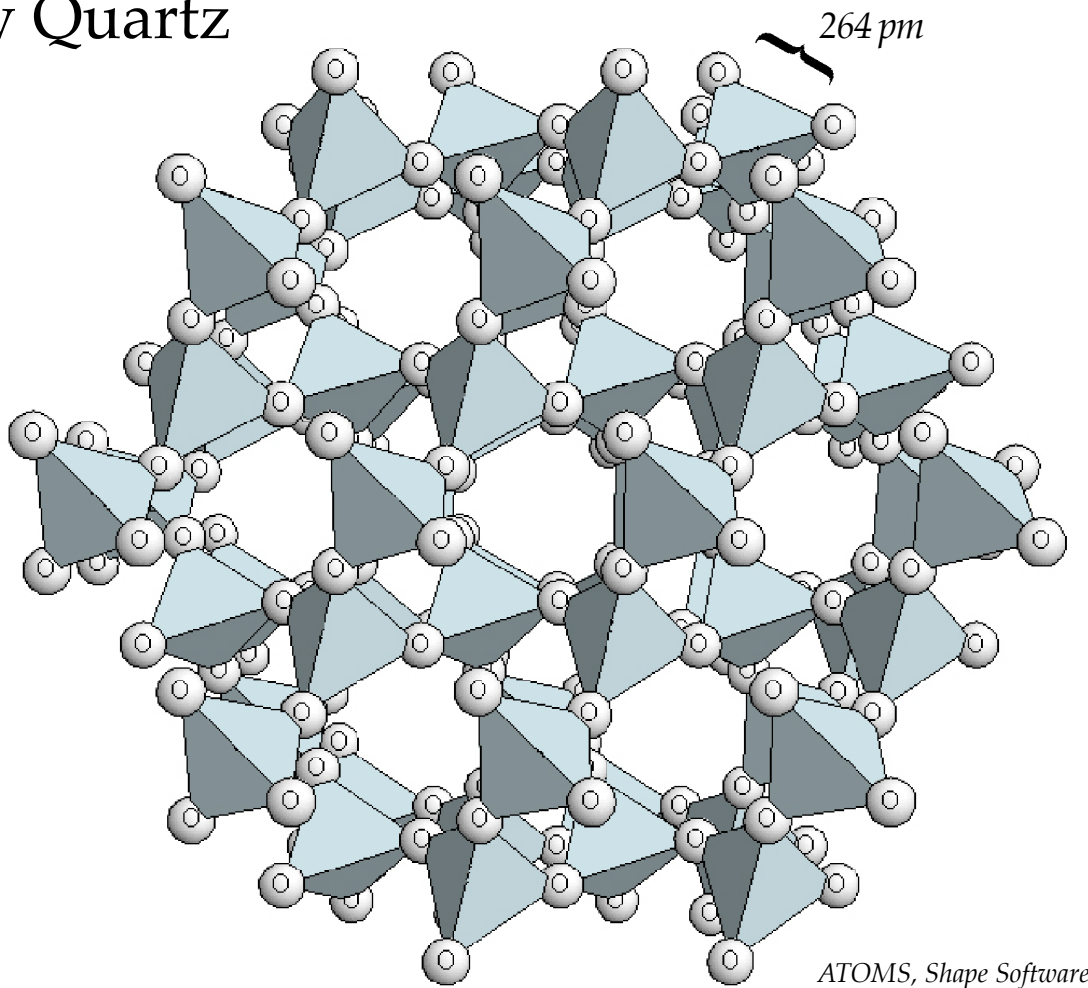


Solubility (i.e. concentration) of „H<sub>2</sub>O“ in quartz also depends on pressure. Pressure gradients in quartz result in variable solubility

Concentration of „H<sub>2</sub>O“ in quartz depends on the fugacity in the adjacent reservoir, as long as quartz is undersaturated in „H<sub>2</sub>O“

## Diffusing Species

Low Quartz



Interstitial Impurities possible candidates:

	H <sub>2</sub>	neutral
	H <sub>2</sub> O	
	O <sub>2</sub>	
	H <sup>+</sup>	
	OH <sup>-</sup>	charged

slower

Substitutional impurities are not diffusing species, because they are fixed in the crystal lattice. However, they provide the only possibility to estimate diffusion coefficients because their concentrations can be measured after experimentation.

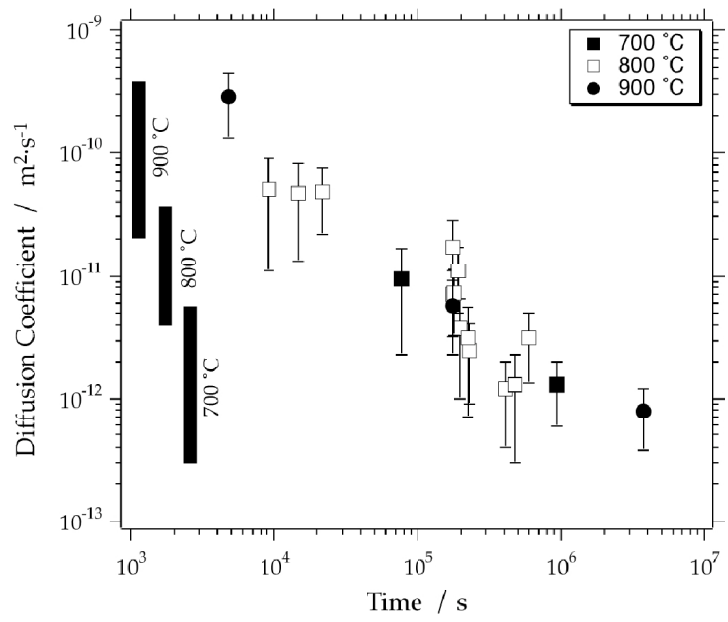
## Diffusion Coefficient

What is the value of D for H<sub>2</sub>O in quartz?

Diffusion of H<sub>2</sub>O in natural quartz is too slow within the limits of experimentation to provide “hydrolytic weakening” (Kronenberg et al., 1986; Gerretsen et al., 1989).

Experimental estimations of “water-related” species diffusion from Kronenberg et al. (1986):

1. no clear temperature-pressure dependence
2. incorrect diffusion model (i.e. time-dependent value of D)



Most likely value of D = 10<sup>-12</sup> m²·s<sup>-1</sup> (or less)

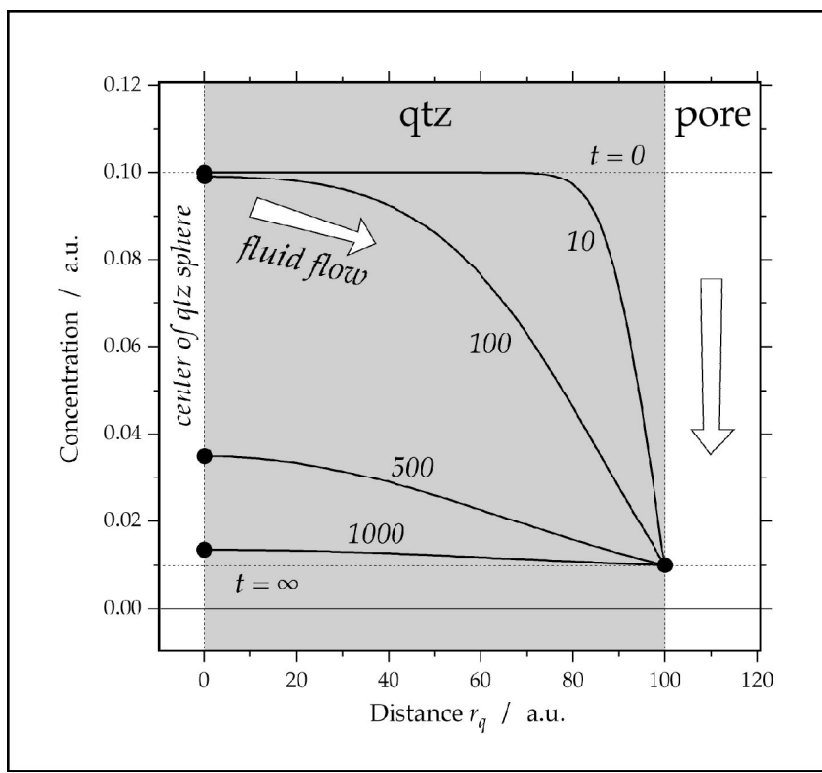
## New 3D Diffusion Model

Concentration profile of H<sub>2</sub>O in spherical quartz grain:

$$c_{H_2O}^{gr}(r_g, t) = (c_i - c_0) \left[ 1 + \frac{2b}{\pi \cdot r_g} \sum_{n=1}^{\infty} \left( \frac{(-1)^n}{n} \sin \left( \frac{n\pi \cdot r_g}{b} \right) \exp \left( \frac{-n^2 \pi^2 D \cdot t}{b^2} \right) \right) \right] + c_0$$

initial concentration of H<sub>2</sub>O in quartz:  $c_0 = c_{H_2O}^{gr}(r, 0)$

concentration obtained from f(H<sub>2</sub>O) in pores:  $c_i = c_{H_2O}^{gr}(b, t)$

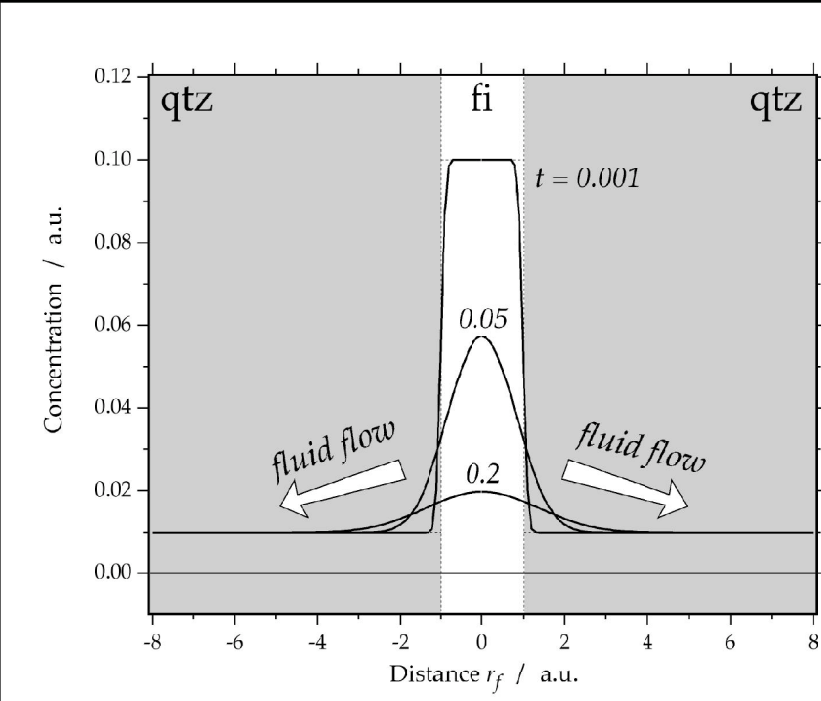


Concentration profile of H<sub>2</sub>O around spherical fluid inclusion:

$$c_{H_2O}^{gr}(r_f, t) = c_0 + \frac{(c_i - c_0)}{2} \left[ \operatorname{erf} \left( \frac{a + r_f}{2\sqrt{D \cdot t}} \right) + \operatorname{erf} \left( \frac{a - r_f}{2\sqrt{D \cdot t}} \right) \right] - \frac{(c_i - c_0)}{r_f} \sqrt{\frac{D \cdot t}{\pi}} \left[ \exp \left( \frac{-(a - r_f)^2}{4 \cdot D \cdot t} \right) - \exp \left( \frac{-(a + r_f)^2}{4 \cdot D \cdot t} \right) \right]$$

$c_0$  = background concentration in quartz obtained from first equation

concentration obtained from f(H<sub>2</sub>O) in inclusion:  $c_i = c_{H_2O}^{gr}(a, 0)$



## Package “Fluids”: computer program ReqDif

New software for calculating the fluid composition/fugacity and density of inclusions, that have been affected by bulk-diffusion processes

Fugacity calculation according to highly accurate equations of state (mainly modified Helmholtz energy functions)

Fluid mixtures: H<sub>2</sub>O - CO<sub>2</sub> - CH<sub>4</sub> - NaCl. Specification possibility of both fluid inclusions and pore fluids

Selection possibilities:

- variable sizes and positions of fluid inclusions in grain
- variable grain size
- diffusion coefficient for each fluid component
- partitioning coefficient of fluid components and direct calculation of the corresponding solubility in quartz
- time

Compositions can be expressed in mass%, amount-of-substance% (as), or molality (as per kg H<sub>2</sub>O)

Fugacity gradients and pressure gradients that have resulted from diffusion are calculated in the program

Free download <http://fluids.unileoben.ac.at/Computer.html>

