

## Vapour phase oxidation of trichloroethylene, ethanol and toluene by solid potassium permanganate: Kinetic study

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### 21g. Process-based reactive transport modelling of aquifer remediation and natural attenuation

Volatile organic compounds may cause major contamination problems in groundwater and soil. Their presence in air can create a hazard to public health. However, limited remedial options exist in controlling the vapour transport of these compounds in the unsaturated zone.

In this study, batch experiments were carried out to investigate the oxidation of TCE, ethanol, and toluene vapour in air by potassium permanganate. For each compound, three experiments with different combinations of vapour concentration and mass of potassium permanganate grains were performed. The objectives of these batch tests were (1) to evaluate the ability of solid potassium permanganate to transform contaminants in the gas phase to harmless compounds and (2) to determine the kinetic parameters. Experimental results have revealed that solid potassium permanganate is able to remove these harmful compounds from the vapour phase. We found that the removal efficiency for TCE and ethanol oxidation is higher than for toluene.

To obtain kinetic parameters, the reaction rate was assumed to be related nonlinearly to the concentration of the targets compounds and the amount of permanganate:

$$\frac{dC}{dt} = kA C^{\alpha} M^{\beta}$$

where  $k$  denotes the rate constant ( $\text{mol}^{1-\alpha} \text{L}^{3\alpha+3\beta-5} \text{M}^{-\beta+1} \text{T}^{-1}$ ),  $A$  is the specific surface area of potassium permanganate ( $\text{L}^2 \text{M}^{-1}$ ),  $C$  is the vapour concentration of the compound ( $\text{mol L}^{-1}$ ),  $M$  is the mass of potassium permanganate per volume of gas ( $\text{M L}^{-3}$ ),  $\alpha$  and  $\beta$  are constant parameters. We made sure that  $\text{KMnO}_4$  was abundantly present so it was assumed that its consumption did not affect the reaction rate. This equation was fitted to experimental data in order to determine  $k$ ,  $\alpha$ ,  $\beta$  for each compound. Results of the simulations are given in table 1.

Compound	$\alpha$	$\beta$	$k(\text{mol}^{1-\alpha} \text{L}^{3\alpha+3\beta-5} \text{M}^{-\beta+1} \text{T}^{-1})$	$R^2$
TCE	0.9	1	$6.92 \times 10^{-7}$	0.99
Ethanol	1.09	1	$5.68 \times 10^{-7}$	0.99
Toluene	0.94	1	$2.99 \times 10^{-8}$	0.99

**Table 1:** kinetic parameters for target compounds

### Conclusion

This study shows that TCE and ethanol in vapour phase can be rapidly oxidized by solid potassium permanganate. Toluene, however, is degraded much slower. A nonlinear reaction formula simulates results of experiment satisfactory. While, potassium permanganate shows promise for the remediation of TCE and ethanol vapour, further investigation of its applicability for toluene is needed.

## Evaluation of Zr in rutile geothermometry for pelitic rocks from the Mica Creek area, British Columbia.

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### ABSTRACT

Rutile occurs both as inclusions in garnet crystals and in the matrices of Late Precambrian metapelitic rocks in the Mica Creek area, British Columbia. Zr contents of these rutile crystals have been analyzed by electron microprobe. The Zr detection limit is 25 ppm (20 samples). Metamorphic grade ranges from staurolite-kyanite zone to K-feldspar-sillimanite zone. Temperatures are based upon experimental calibrations. Temperature (T) estimates for rutile inclusions in garnet range from 555 to 705°C (calculated at 7 kbar). T's for groundmass rutile range from <475 to 700°C. There is no apparent correlation of T with the metamorphic grade. In most samples there is no statistical difference between T's from inclusions and T's from matrix rutile. Many of these inclusion T's are similar to those obtained from garnet-biotite geothermometry. Isoleths for garnet in isochemical phase diagram sections when compared to core garnet compositions yield T's which are much lower than those from Zr geothermometry. The isochemical phase diagram sections also suggest that garnet and rutile are not stable together except at high P-T. T's based upon Zr geothermometry for inclusions appear to be too high for the equilibrium growth of garnet at lower metamorphic grade. A study of Ti in quartz geothermometry for four samples (inclusions in garnet) yielded T's ranging from 417 to 553°C. Zr in rutile has been analyzed on two different microprobes and by laser ablation ICP-MS with consistent results. Other workers have found reasonable correlation between Zr T's and those based upon other methods. For the Mica Creek samples disequilibrium is a possibility but would require metastable growth of rutile with higher Zr contents. Most scenarios would predict T's which are too low rather than too high. Exchange of Zr between garnet and rutile inclusions during subsequent heating does not appear to be plausible. We suggest equilibrium at higher P-T between garnet and rutile inclusions than those suggested from garnet isopleths.