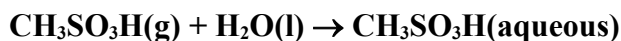


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet VI.A1.9 HET\_H2OL\_9

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### Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Accommodation coefficient: <math>\alpha_b</math></i>			
$0.15 \pm 0.01$	264	De Bruyn et al., 1994	DT (a)
$0.11 \pm 0.02$	279		
$0.16 \pm 0.04$	261	Schweitzer et al., 1998	DT-MS (b)
$0.11 \pm 0.01$	283		
$0.89 \pm 0.04$ (7 - 15 wt% H <sub>2</sub> SO <sub>4</sub> )	296	Hanson, 2005	AFT-CIMS (c)

### Comments

- (a) Monodispersed droplets of 50 to 200  $\mu\text{m}$  in diameter Uptake coefficients were corrected for gas phase diffusion using  $D_g=0.066 \text{ atm cm}^2 \text{ s}^{-1}$  in H<sub>2</sub>O and  $0.299 \text{ atm cm}^2 \text{ s}^{-1}$  in He. The measured uptake coefficients were independent of *pH* adjusted with NaOH or HCl and independent of NaCl content up to 3.5 M. Since the observed uptake coefficient were time-independent, uptake was considered limited by bulk accommodation.
- (b) Monodispersed droplets of 80 to 150  $\mu\text{m}$  in diameter CH<sub>3</sub>SO<sub>3</sub>H was admitted to the reactor at  $10^{13} \text{ cm}^{-3}$ ; its concentration at the reactor exit was measured by an ion-trap mass spectrometer. Uptake coefficients were corrected for gas phase diffusion using  $D_g=0.13 \text{ cm}^2 \text{ s}^{-1}$  in H<sub>2</sub>O and  $0.37 \text{ cm}^2 \text{ s}^{-1}$  in He and assuming the T dependence following  $T^{1.75}$ . The corrected uptake coefficients were independent of time and NaCl content up to 2 M. It was considered limited by bulk accommodation in all cases.
- (c) Uptake to sulphuric acid aerosol was studied in a laminar flow reactor coupled to CIMS detection using HNO<sub>3</sub> as source of primary ions. Sulfuric acid particles were generated by homogeneous nucleation from supersaturated vapour leading to a lognormal particle size distribution within 50-120 nm, with a few  $10^4$  particles per  $\text{cm}^3$ , characterised by a differential mobility analyzer. Concentrations of CH<sub>3</sub>SO<sub>3</sub>H were  $3 \times 10^{10} \text{ cm}^{-3}$  in the flow tube. The measured uptake coefficients were corrected for gas phase diffusion using the Fuchs-Sutugin correction factor. The diffusion coefficient was directly measured based on the observed wall loss rates in absence of aerosol particles. It did not significantly depend on humidity. Its average value was  $0.0786 \text{ atm cm}^2 \text{ s}^{-1}$ .

### Preferred Values

Parameter	Value	T/K
$\alpha_b$	1	260 – 300
Reliability		
$\Delta \log(\alpha_s)$	0.3	260 – 290

### *Comments on Preferred Values*

The two droplet train studies studying uptake of  $\text{CH}_3\text{SO}_3\text{H}$  to water and dilute aqueous solutions agree very well and report a bulk accommodation coefficient around 0.1. However, the aerosol flow tube study by Hanson (2005) found a value for  $\alpha_b$  not different from 1. Since this experiment was much less affected by gas phase diffusion, we adopt this result for our recommendation for  $\alpha_b$ . Solubility of  $\text{CH}_3\text{SO}_3\text{H}$  is high enough to allow bulk accommodation limited uptake into the droplets over the experimental gas – particle interaction times of all studies. While  $\alpha_b$  was apparently independent of pH and NaCl concentration, Schweitzer et al. (1998) and De Bruyn et al. (1994) found a temperature dependence, which they interpreted in terms of nucleation of a critical cluster as rate limiting step for the solvation rate leading to an average cluster of  $\text{CH}_3\text{SO}_3\text{H} \times 0.5 \text{ H}_2\text{O}$ . This would, however, indicate a quite low ability of this very soluble species ( $H = 8.7 \times 10^{11} \text{ M/atm}$ , Brimblecombe and Clegg, 1988) and strong acid ( $\text{p}K_a = -2$ , Serjeant and Dempsey, 1979) to hydrogen bond to water.

### **References**

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