The Effect of Characteristics of Porous Silica within a Cigarette Filter on Volatile Organic Compounds Reduction

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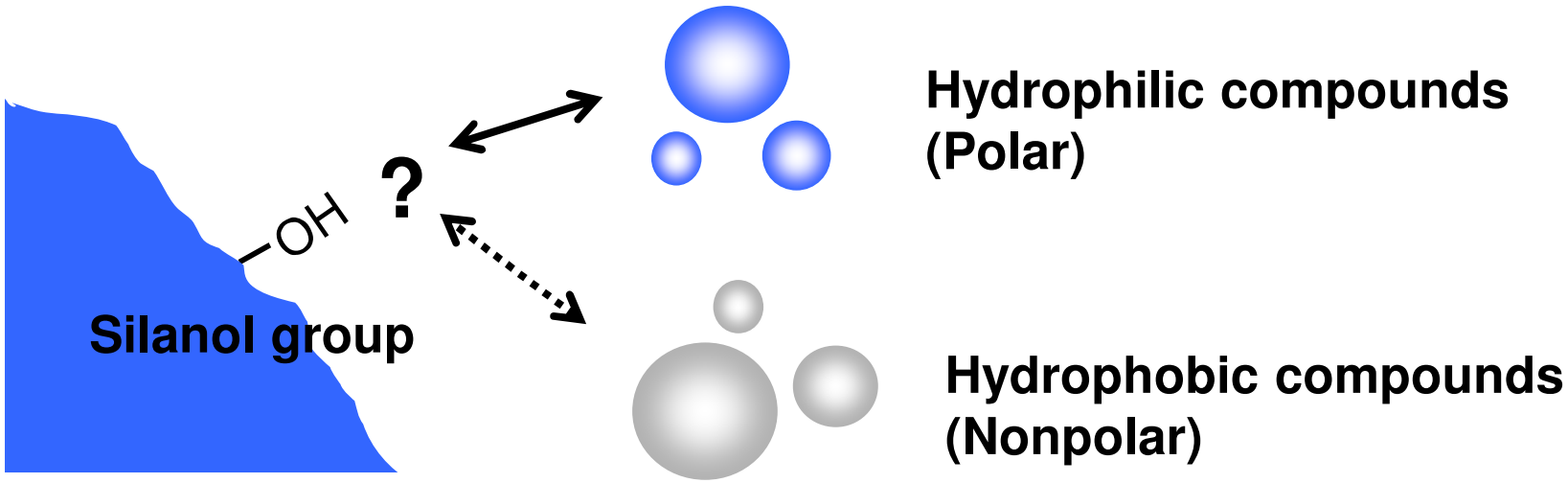
Introduction

- Adsorbent is one of the most effective technologies applied to remove volatile organic compounds (VOCs) in cigarette smoke.
- Silica gel selectively adsorbs polar VOCs in cigarette smoke (Xue et al., 2002).
- Generally, porous silica with silanol groups adsorbs polar compounds.



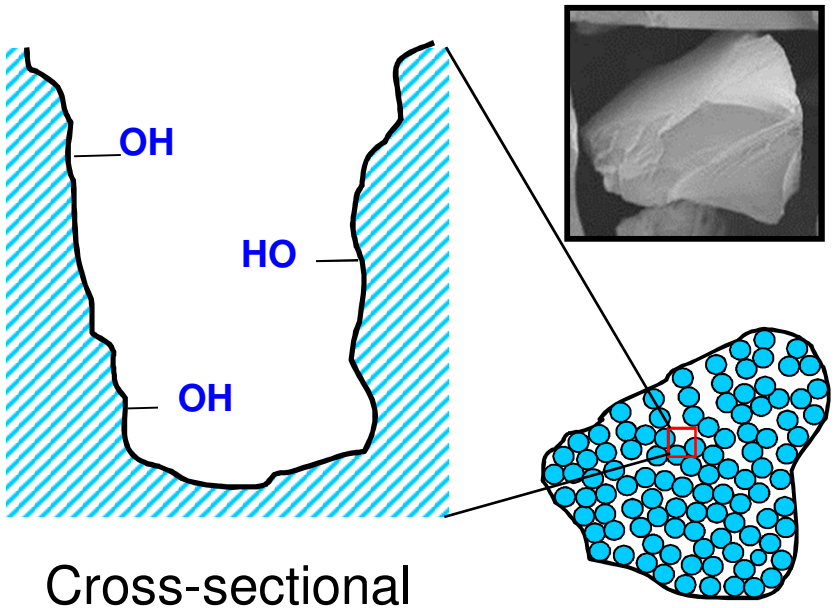
Introduction

- Images of pore structure

Porous silica

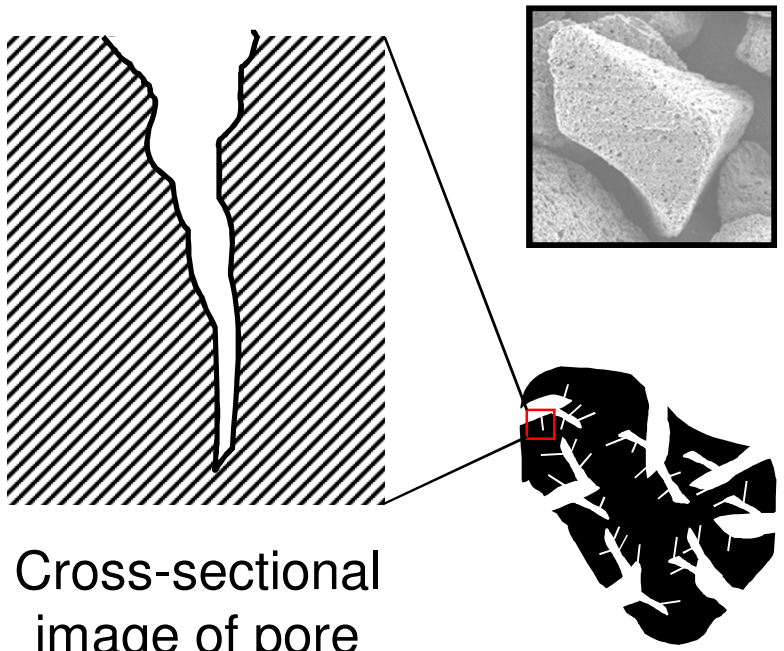
Activated carbon

Hydrophilic surface (OH group)



Cross-sectional image of pore

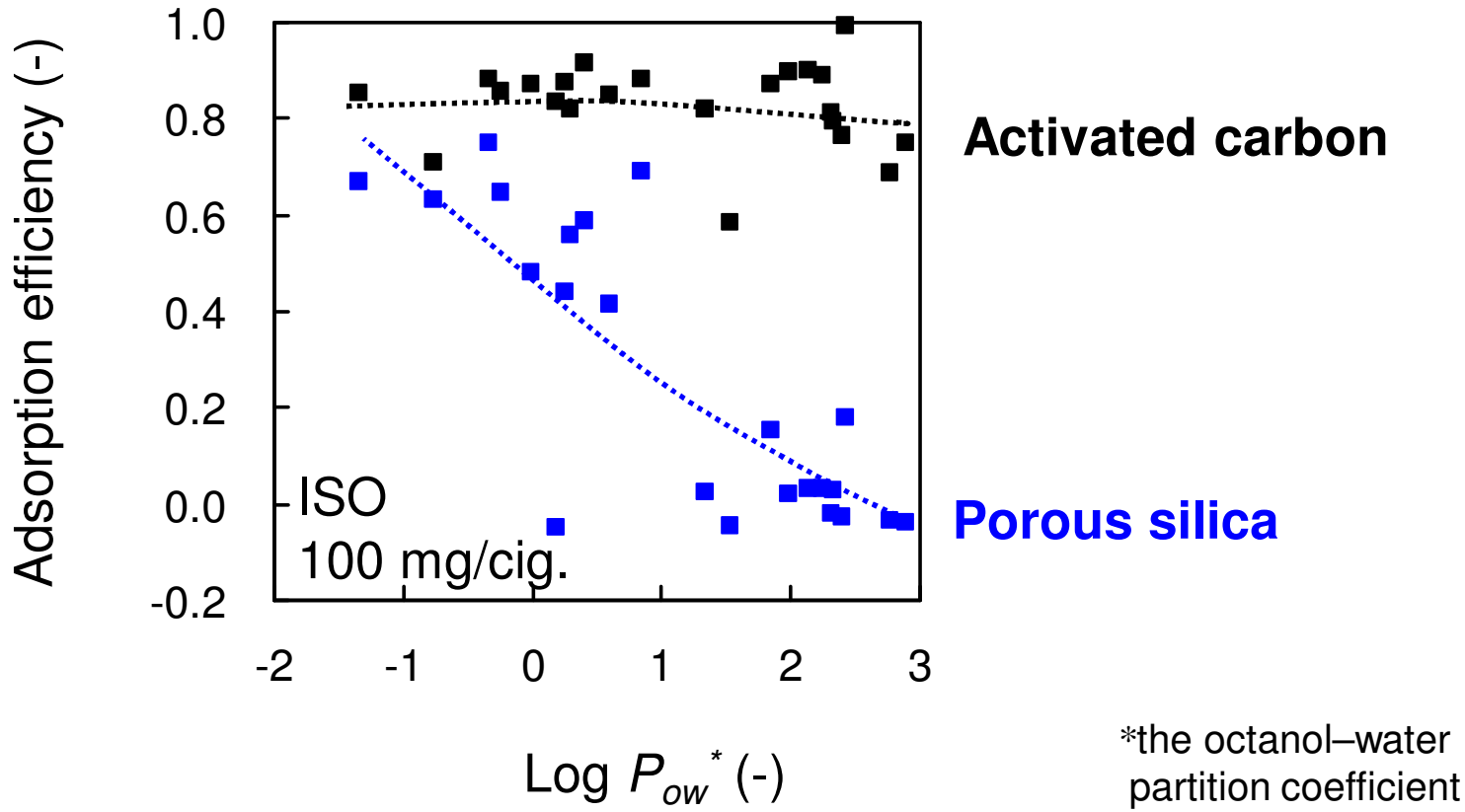
Hydrophobic surface (few OH group)



Cross-sectional image of pore

Introduction

- Comparison of adsorption behaviors between porous silica and activated carbon for VOCs in cigarette smoke

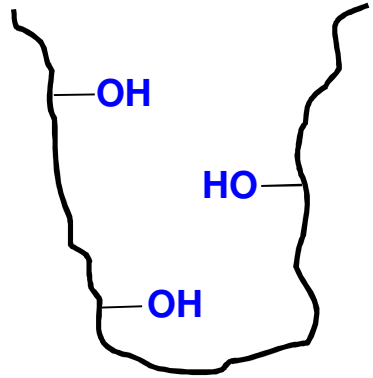


Porous silica selectively adsorbed hydrophilic VOCs.

Objective

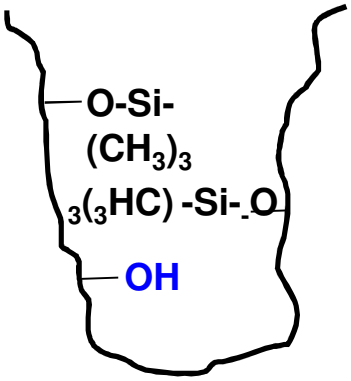
Clarify the effect of silanol groups of porous silica on VOCs reduction in cigarette smoke

Approaches in this work



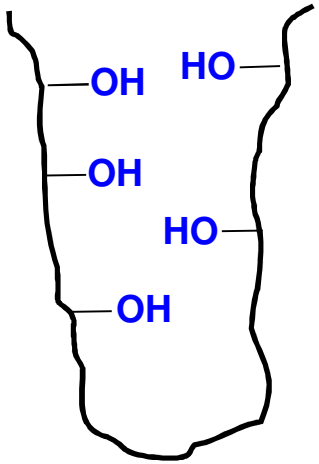
Porous silica

Reduce the number of Si-OH



Modified porous silica

Increase the number of Si-OH



Various unmodified porous silicas

Experimental Methods

Porous silicas and those characterizations

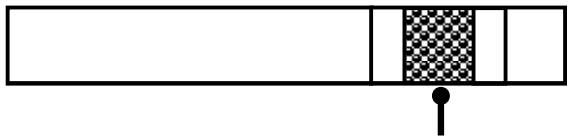
- **Porous silicas**
  - Silica gel
  - Trimethylsilyl-modified silica gel
  - Mesoporous silica

- **Characterizations**
  - Number of silanol groups (Titration of methyllithium)
  - Absorption intensity of Si-OH (FT-IR)
  - Carbon content of trimethylsilyl-modified silica gel (Elemental analysis)
  - Pore structure parameters (N_2 Adsorption)

Smoke analysis and test sample

- **Smoke analysis**
  - GC-FID for VOCs

- **Test sample**
  - Tobacco : Japanese domestic brand (Tar 6mg)
  - Filter configuration : Plug-space-plug, no ventilation holes
  - Adsorbent size : 28 x 70 mesh (212-600 um)



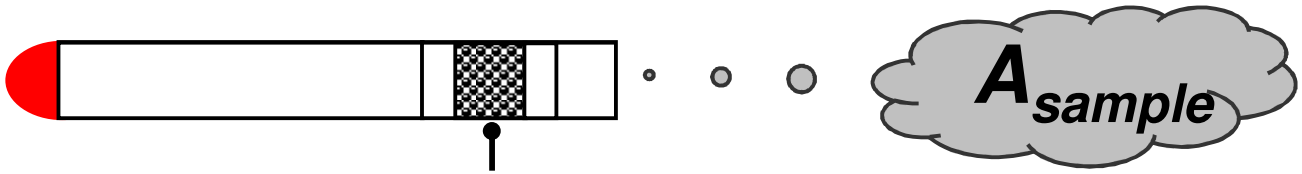
- **Smoking regime**
  - ISO 4387

Calculation of adsorption efficiency

$$Adsorption\ efficiency = \frac{[\ A_{reference}\ ] - [\ A_{sample}\ ]}{[\ A_{reference}\ ]}$$

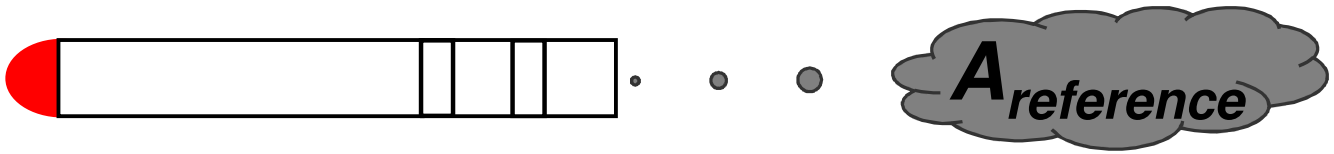
A : GC Peak Area of each VOC / GC Peak Area of ISTD
$sample$: Adsorbent in filter
$reference$: No adsorbent in filter

Sample



Adsorbent

Reference



No adsorbent

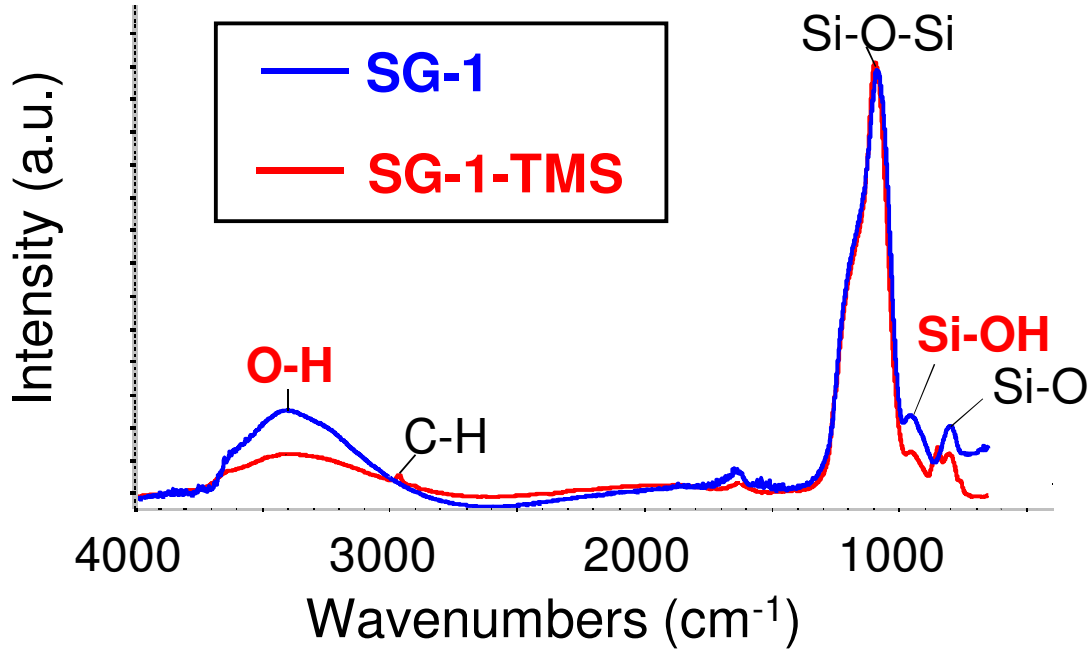
Results and Discussions

Reduce the number of Si-OH

- Physical properties

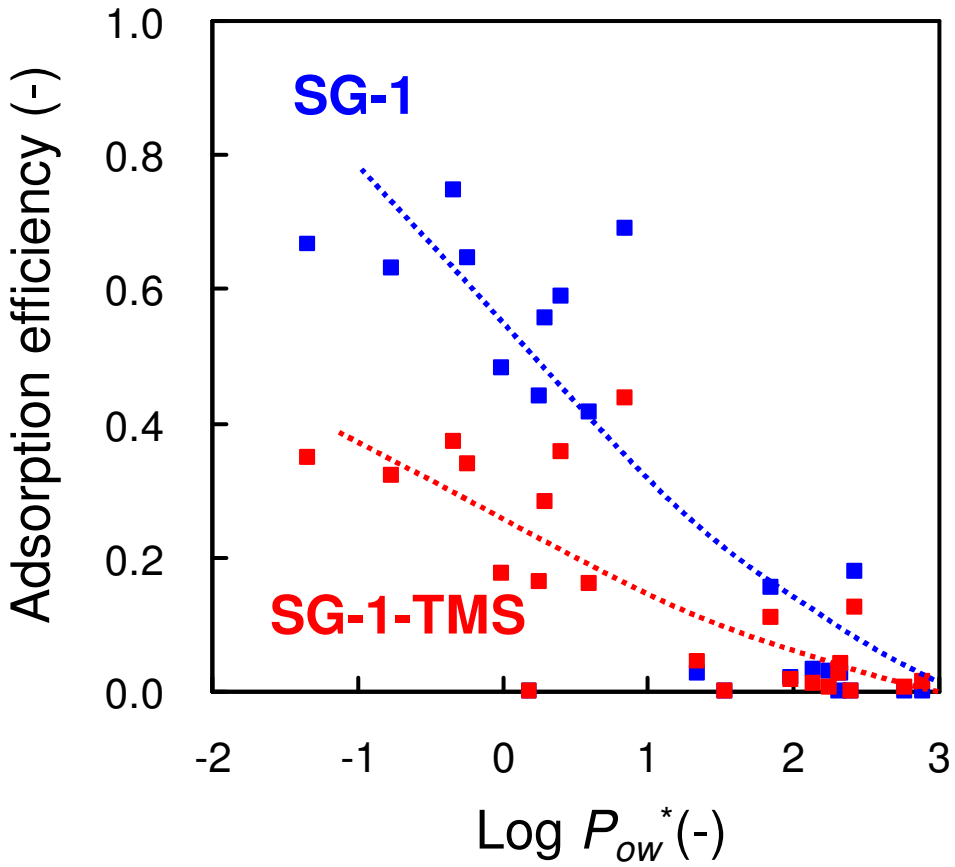
Sample		***Carbon content*** ***(wt%)***	BET Relative surface area ($m^2\ g^{-1}$)	Average pore diameter (nm)
Silica gel	**SG-1**	***0.0***	428	8.3
Silica gel modified with trimethylsilyl groups	**SG-1-TMS**	***3.4***	365	8.1

- FT-IR spectra



Reduce the number of Si-OH

• Comparison of adsorption efficiencies between SG-1 and SG-1-TMS for VOCs in cigarette smoke



Same relative surface area (43 m²/cig.)

*the octanol–water partition coefficient

Silanol groups play an important role in adsorption of VOCs.

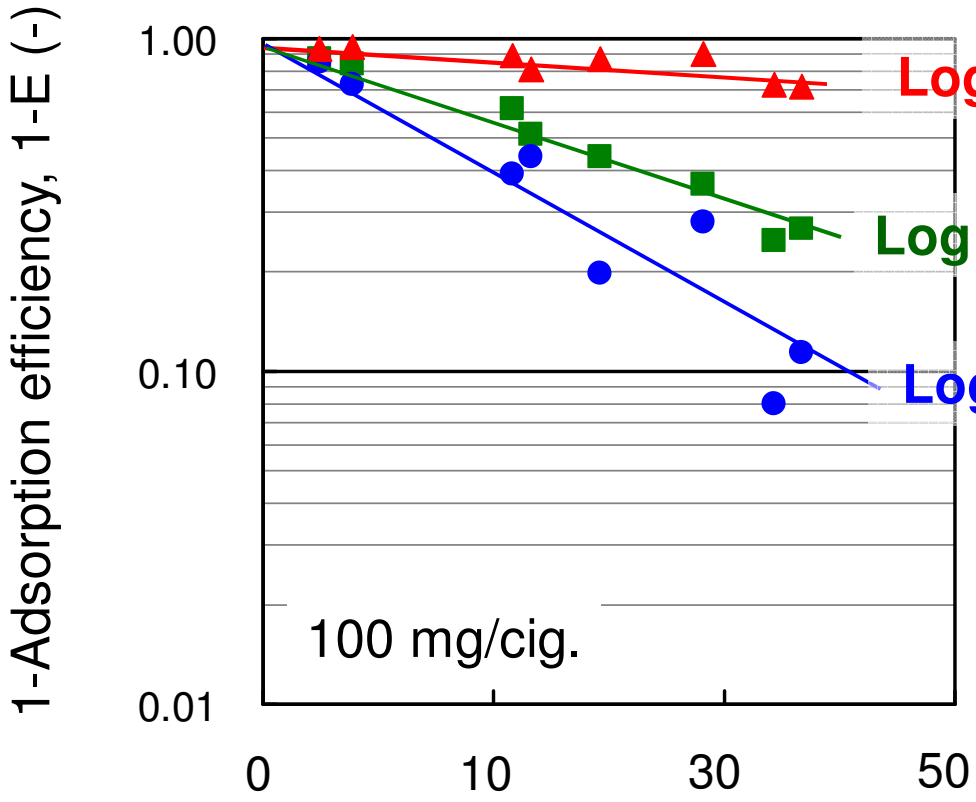
Increase the number of Si-OH

- Physical properties of porous silicas

Sample		**Number of silanol groups** **(x10^{20} g^{-1})**	BET Relative surface area (m^2 g^{-1})	Average pore diameter (nm)
Silica gel	SG-2	**5**	71	62
	SG-3	**8**	118	36
	SG-4	**22**	346	13
	SG-5	**23**	371	7
Mesoporous silica	MS-1	**29**	468	7
	MS-2	**38**	615	6
	MS-3	**44**	713	5
	MS-4	**47**	753	5

Increase the number of Si-OH

• Relationship between adsorption efficiency of each VOC and the number of silanol groups



$$Ln(1-E) = -kn$$

E : Adsorption efficiency
k : the adsorption coefficient
n : the number of silanol groups

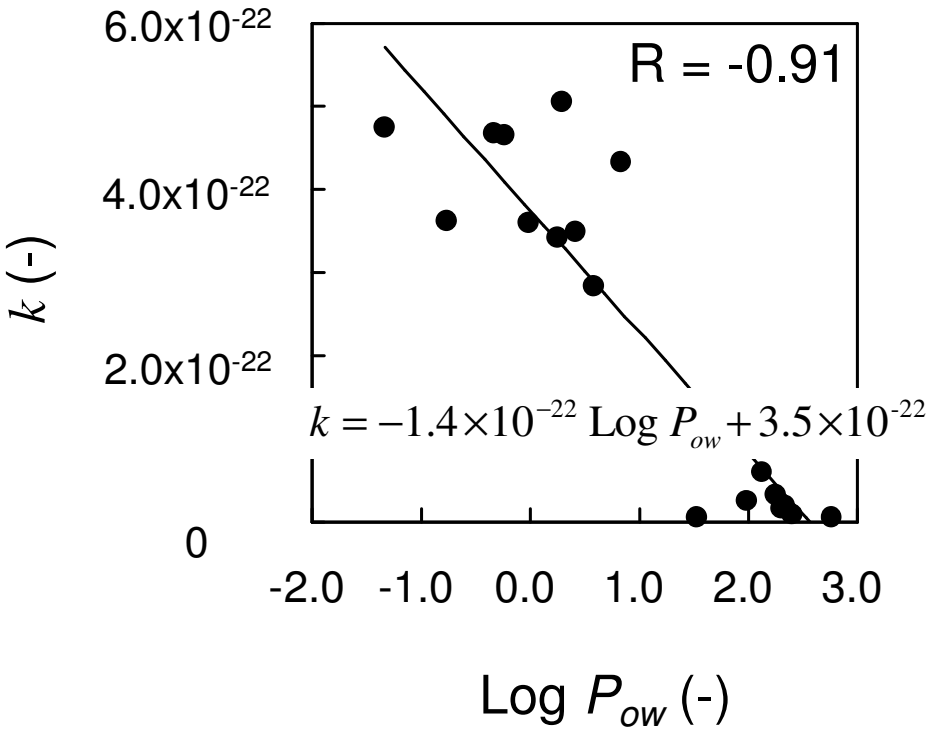
The number of silanol groups decides the adsorption efficiency of each VOC.

Conclusion

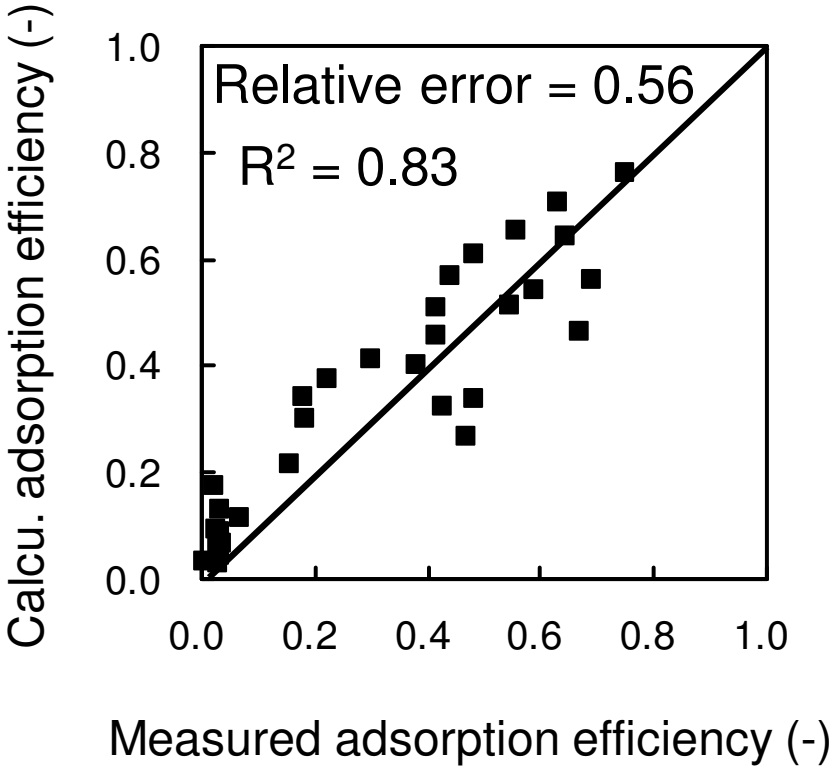
The number of silanol groups of porous silica is the dominant factor in VOCs reduction in cigarette smoke

For practical use
Prediction of adsorption efficiency

- Correlation between k and Log P_{ow} of each VOC



- Comparison calculated and measured adsorption efficiency



k : the adsorption coefficient
Log P_{ow} :the octanol–water partition coefficient

Adsorption efficiency of each VOC could be approximately predicted.