Salt-Induced Diffusiophoresis of a Cationic Micelle in Water Determination of Cross-Diffusion Coefficients FGC Josie (Khanh) Nguyen, Minh Le, and Onofrio Annunziata, Ph.D. **Department of Chemistry and Biochemistry**

Introduction

Enhance oil recovery techniques contribute to approximately 30% of petroleum production. Water flooding in combination with micelles can be employed to improve extraction of hydrocarbons trapped into porous rocks. Micelles, spherical nanoparticles with a hydrophilic outer shell and a hydrophobic core, can encapsulate hydrocarbons. However, a porous rock contains both open and dead-end pores, which are difficult to access. Thus, it is important to identify novel approaches that favor micelle insertion into dead-end pores.¹ Introducing a salt concentration gradient into the micelle-water mixture can generate an internal electric field, propelling cationic micelles into dead-end pores as shown in Fig. 1.2-4 This can enhance hydrocarbon extraction from porous materials. This phenomenon is known as salt-induced diffusiophoresis.



FIG 1. (A) Micelles approach pores of rock. (B) Micelles enter pores (C) Micelles extract hydrocarbons (green in figure) from pores.

SALT-INDUCED MICELLE DIFFUSIOPHORESIS



 $\mathbf{v}_{\mathbf{P}} = -\mathbf{D}_{\mathbf{P}} \left(\nabla \mathbf{n} \mathbf{C}_{\mathbf{P}} + \mathbf{d}_{\mathbf{P}} \cdot \frac{\nabla \mu_{\mathbf{S}}}{\mathbf{k} \cdot \mathbf{T}} \right)$

 d_P : diffusiophoresis coefficient of D_P : Brownian mobility

 $v_{\rm P}$: particle net migration rate $\mu_{\rm S}$: salt chemical potential

 C_{P} : micelle concentration K_b: Boltzmann constant T: temperature

FIG 2. Isothermal migration of micelle induced by gradient of salt concentration in water (color contrast in figure).





 $\mathbf{d}_{\mathbf{S}} = -\frac{\Delta \mathbf{C}_{\mathbf{S}}}{\Delta \mathbf{C}_{\mathbf{P}}}$

d_s: salt osmotic diffusion coefficient C_{P} : micelle concentration C_S: salt concentration

FIG 3. Another transport phenomenon associated with diffusiophoresis is salt osmotic diffusion from high to low micelle concentration in water. The salt osmotic diffusion coefficient, d_s, is related to the salt partition coefficient. This is the change in salt concentration, C_{s} , caused by a difference in concentration of micelles, C_P.



Cationic micelles are prepared using the cationic surfactant cetylpyridinium chloride (CPC, Fig. 4). Diffusiophoresis of CPC micelles in the presence of concentration gradients of NaCl or KCl was characterized using Raileigh interferometry (Fig. 5)



FIG 5. Optical setup of Rayleigh interferometry. Two solutions with slightly different salt concentration are vertically positioned one on the top of the other inside an optical cell. Specifically, light from a green laser (435 nm) goes through a double slit before entering the cell. The light transmitted from the cell is focused onto a detector, where a Rayleigh interference pattern is formed.

Results and Discussion

TABLE. Salt osmotic diffusion coefficient, d_s, and diffusiophoresis coefficient, d_{P} , at different salt concentration, C_{S}



FIG 6. Salt osmotic diffusion coefficient, d_s, as a function of salt concentration, C_{S} . (•) NaCl and (•) KCl. $Z_{P} = 19.9$

 $N_w = 710$ molecules per micelle

d _s	d _P
14.3	0.489
18.7	0.485
23.8	0.462
11.9	-0.185

ds: salt osmotic diffusion coefficient V_{P} : molar volume of surfactant N_W: number of water molecules per micelle V_{W} : molar volume of water C_S: salt concentration



and negative with KCI. experimental values of the order of 10%. diffusiophoresis.

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d_P: diffusiophoresis coefficient of micelle σ : electrophoretic coefficient Z_P: micelle charge D : salt diffusion coefficient

FIG 7. Diffusiophresis coefficient, dp, as a function of salt

Conclusion

Diffusiophore of CPC micelles was found to be positive with NaCl

NaCl osmotic diffusion coefficients were used to determine CPC micelle charge of 20. This is 20% of micelle structural charge, consistent with significant counterion adsorption.

The electrophoresis model of diffusiophoresis was used to predict NaCl-induced diffusiophoresis of CPC micelle with deviations from

Diffusiophoresis studies of PCP micelles in the presence of KCI gradients are needed to develop a more accurate model of micelle

References

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