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Fundamental Modeling and Experimental Investigation of Polymer Washing Process ⋆

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Abstract: After polymerization reaction, impurities such as adduct, solvent and catalyst are trapped inside the polymers. These impurities should be removed by a polymer washing process to improve the purity of the polymer products. Also, the optimization of the polymer washing process is essential to reduce the energy, resources and processing time. This work provides theoretical basis for optimization of polymer washing process by proposing a fundamental model and experimental investigation method of the process. The model describes the impurity distribution inside the polymers, mole balance of impurities inside and outside of the polymers, and impurity diffusion rate at polymer surface. The experimental investigation with SPAEK (sulfonated poly(aryl ether ketone)) samples reports the impurity diffusion coefficient at polymer surface of the performed experiments. The computed D(the impurity diffusion coefficient at the polymer surface) shows different values with time as a lumped parameter, including the unmodelled effects for impurity diffusion. However, these values show the same trajectory with the introduction of a dimensionless number Co for each operation. This means unmodelled impurity diffusion factors included in D are only affected by Co. Finally, we validate the prediction performance of the model by comparing the predicted pH changes of validation experiment with the experimental data.

Keywords: Polymer washing process, Moving boundary of diffusion, Pseudo steady state, Sulfonated poly aryl ether ketone

1. INTRODUCTION

A polymerization is a chemical reaction in which molecules combine to form a larger polymer. On the completion of the polymerization, the formed polymer is solidified. In this process, a small amount of impurities, which may include adduct, solvent and catalyst components, are still trapped inside the polymers. Since these impurities have a significant influence on microstructural characteristic of polymer products, they should be removed by a washing process [1,2]. When a polymer washing process is operated at a large scale without any optimization, waste of energy, resources, and processing time will be considerable. Thus a detail theoretical model is essential to optimize such a process. Moreover, such a complex dynamics involving mass transfer in the polymer particulate is difficult to model using an empirical model structure fitted to operational data. However, theoretical research for the polymer washing process has not been reported yet to the best of the authors' knowledge. This work proposes a fundamental model and experimental investigations of a polymer washing process, which can be readily used for optimization of the process.

In polymer washing process, solidified polymers are washed with deionized water in batch several times. Prior to the washing process, impurities are assumed to be uniformly distributed inside the polymers. When washing begins, the impurities inside the polymers are dissolved in water and diffuse toward outside with the concentration gradient. As the washing process proceeds, the impurity concentration inside the polymer decreases and that of the outside increases. When impurity concentrations of the polymer inside and outside reach the equilibrium, the impurity concentrations stop changing. These processes are repeated until the pH of washing water reaching near 7.

This work introduces the concept of moving boundary of diffusion inside the polymers where impurities begin to diffuse toward outside to describe the impurity diffusion inside the polymers [3,4]. In addition, pseudo steady state approximation and Fick's law are employed to describe the impurity distribution inside the polymer and impurity diffusion rate at polymer surface, respectively. In experimental investigation, we perform the operation of polymer washing process with SPAEK sample, and estimate the diffusion coefficient of impurity at polymer surface using the experimental data. A dimensionless number Co, the ratio of impurity concentration outside the polymer to initial

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impurity concentration inside the polymer, is introduced to model temporal change of the diffusion coefficient regardless of the initial concentration of the impurity inside the polymer. Finally, we validate the pH prediction performance of the model by comparing the simulation results with the experimental data. The simulation results are in agreement with the experimental results, and the proposed model and experimental investigation are expected to be useful for optimization of the polymer washing process.

2. MODELING OF POLYMER WASHING PROCESS

A conceptual model of polymer washing process is constructed as follows. The impurity concentration distributions inside the polymers are assumed to be uniform as the initial impurity concentration prior to washing, then the concentration distribution changes with impurity diffusion toward outside due to the concentration gradient as the washing progress. Finally the concentration distribution stops changing at the equilibrium state. After washing, the used water is removed from the batch and a new batch of polymer washing process starts with fresh water.

A concept of moving boundary of diffusion is introduced where the impurity concentration inside the boundary remains as the initial impurity concentration, and the impurities start diffusing at the boundary (see Fig. 1).

2.1 Pseudo steady state approximation of impurity distribution inside the polymer

As the washing process proceeds, the impurities diffuse in radial direction from the diffusion boundary. The radius of diffusion boundary is the same as the polymer radius before washing, and then decreases with the progress of washing. Since most of materials have small molecular diffusion coefficients in water [5], we use pseudo steady state approximation to describe the impurity distribution inside the polymer [6,7].

$$W_{Mr}4\pi r^2|_r - W_{Mr}4\pi r^2|_{r+\Delta r} = 0 \quad (1)$$

W_{Mr} is described by the Fick's law :

$$W_{Mr} = -D_p\frac{dC_{Mr}}{dr} \quad (2)$$

Table 1. Nomenclature

R	Radius of the polymer
R_b	Radius of the diffusion boundary
W_{Mr}	Radial flux of impurities
C_{Mr}	Impurity concentration according to radial distance from the center of polymers
C_{MR}	Impurity concentration at polymer surface = Impurity concentration outside the polymers
C_{M0}	Impurity concentration inside the diffusion boundary = Initial impurity concentration inside the polymer
D_p	Impurity diffusion coefficient inside the polymer
D	Impurity diffusion coefficient at polymer surface
D_v	Impurity diffusion coefficient at polymer surface in the validation experiment
M_{out}	Moles of impurities outside the polymers
ϕ	Volume ratio of water inside the polymer to polymer
m	Mass of polymer pieces in the batch
n	Number of polymer pieces in the batch
V_{out}	Volume of water outside the polymers
V_p	Volume of polymers
V_{in}	Volume of water inside the polymers

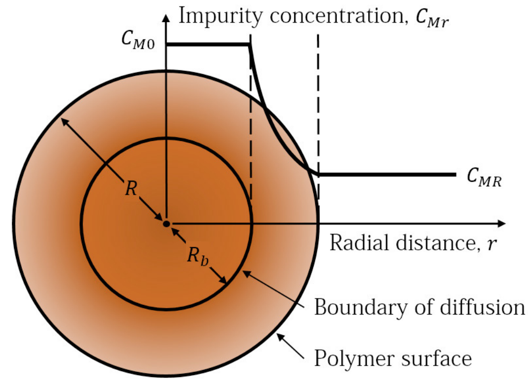

Fig. 1. Distribution of the impurity concentration inside the polymer

Boundary conditions are

$$C_{Mr} = C_{MR} \quad at \quad r = R \quad (3)$$

$$C_{Mr} = C_{M0} \quad at \quad r = R_b \quad (4)$$

Substituting (2) into (1) and integrating with the boundary conditions yields the impurity concentration distribution inside the polymers according to the radial distance from the center of polymer.

$$C_{Mr} = \frac{(C_{M0} - C_{MR})\frac{1}{r} + C_{MR}\frac{1}{R_b} - C_{M0}\frac{1}{R}}{\frac{1}{R_b} - \frac{1}{R}} \quad (5)$$

2.2 Mole balance of impurities inside and outside of the polymers

A mole balance equation of impurities inside and outside of the polymers is derived to obtain a mathematical relationship between the diffusion boundary radius and the impurity concentration outside the polymers. The amount of impurities outside the polymers is the same as the change in the amount of impurities inside the polymers :

$$\frac{M_{out}}{n\phi} = \frac{4}{3}\pi R^3 C_{M0} - \int_0^{R_b} 4\pi r^2 C_{M0}dr - \int_{R_b}^{R} 4\pi r^2 C_{Mr}dr \quad (6)$$

Substituting (5) into (6) and expressing M_{out} as the product of the water volume and impurity concentration outside the polymers yields:

$$V_{out}C_{MR} = \frac{2}{3}\pi(C_{M0} - C_{MR})(2R^3 - RR_b^2 - R^2R_b)n\phi \quad (7)$$

Rearranging (7) by R and C_{MR_0} results in (8) and (9), respectively :

$$R_b = \frac{-R + f(C_{MR})}{2} \quad \left(f(C_{MR}) = \sqrt{9R^2 - \frac{6V_{out}}{\pi n\phi R}\left(\frac{C_{MR}}{C_{M0} - C_{MR}}\right)}\right) \quad (8)$$

$$C_{MR} = \frac{g(R_b)}{3V_{out} + g(R_b)}C_{M0} \quad \left(g(R_b) = 2\pi n\phi(2R^3 - RR_b^2 - R^2R_b)C_{M0}\right) \quad (9)$$