

# Modification of Stokes-Einstein Equation for Diffusivities in Dilute Polymer Solutions

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## Abstract

An improved correlation is presented for the estimation of binary diffusion coefficients in various dilute polymer solutions. The correlation is based on the Stokes-Einstein equation with empirical corrections for the nonroundness and the size ratio of polymer and solvent molecules. These corrections are computed from the UNIQUAC or UNIFAC group contribution  $R$  and  $Q$  parameters. The method works well for various polymer systems. The proposed correlation reduced the average error from 133% to 33%.

**Keywords:** Diffusion coefficient, Dilute polymer solution, Stokes-Einstein Equation.

## Introduction

A knowledge of diffusion coefficients is important for the proper design of some chemical processes, such as distillation, absorption, chemical reactions and polymerization. Diffusion coefficients are needed for the analysis of mass transfer problems, and these processes often are limited by diffusion mechanism [1,2].

There are many methods available for estimating diffusion coefficients in dilute binary liquid mixtures [1,3,4]. However, there is no method that works equally well for all compounds, and there also appears to be very little interest in developing improved correlations. This is somewhat surprising because while the methods presently available have an average relative error of around 12-30%, their maximum errors are much higher, ranging from 45 to 190% [4].

The estimation diffusion coefficients of polymer solutions has been extensively studied. Because of the limitations of the theoretical approaches for estimating

diffusion coefficient, empirical correlation for polymer diffusion coefficients data by physical properties of the polymers has been presented [5]. Here a simple modification of the Stokes-Einstein (SE) equation for diffusion coefficients is proposed that appears to be an improvement over other methods and a step toward the development of more general methods.

## SE Equation

The SE equation for the diffusion of a spherical solute molecule  $i$  in solvent  $j$  is

$$D_{ij}^{SE} = kT_i / 6\pi\eta_j r_i \quad (1)$$

The SE equation was originally derived for the diffusion of large spherical molecules in solvents of low viscosity such as diffusion of spherical polymer molecules in dilute solutions [2]. Unfortunately, for solute molecules  $i$  that are similar in size to the solvent molecules  $j$ , the method predicts diffusivities that are too low [3]. The SE