243a An Efficient Method for Computing Diffusivities in Polymer Nanocomposites

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A modified algorithm for calculating the diffusivities for polymer nanocomposites is preseented. We define the resistance to mass transfer differetlky from Cussler and co-workers and use a series parallel technique to obtain the effective resistance and therefore the diffusivity. A comparisonn is made with both the finite difference solution of the laplace equation and experimental results. It is found that the proposed technique is better than the traditional predictions and the monte-carlo simulation predictions. This is true not only in terms of accuracy but also in terms of computaional efficiency.