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Cost-Efficiency Comparisons of Some Polymer Fractionation Techniques

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NOTE

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Abstract

An expression to permit comparison of various techniques of polymer fractionation in terms of both fractionation efficiency and cost is proposed. Comparisons are made for large-scale gel permeation chromatography at elevated and ambient temperatures, large-scale Baker-Williams fractionation, and narrow distribution unfractionated polymers prepared by anionic polymerization.

There is an ever-increasing need for preparation of narrow molecular weight distribution fractions of polymers for subsequent studies of their solution, mechanical, and rheological properties. A variety of fractionation techniques are well established; see for example Ref. *1*. Usually it is possible to fractionate a polymer by several methods. There appears to be little quantitative information available to aid in choosing the

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optimum method. This is particularly true if the amount of effort required, i.e., the cost, of preparing the fractions is also to be considered.

On the assumption that the objectives are to achieve minimum molecular weight distribution width and cost, a figure of merit, M, to permit numerical comparison is proposed.

$$M = \frac{1}{(\bar{M}_w/\bar{M}_n - 1)^2(C/g)}$$

In this equation $\bar{M}_w$ and $\bar{M}_n$ are the weight- and number-average molecular weights, respectively; C is the cost of preparing the fraction in dollars, and g is the weight of the sample in grams. The figure of merit is completely arbitrary and has no background in theory. Nevertheless it does afford some measure of comparison. The cost figure is particularly difficult to obtain. The figures cited in Table 1 are for solvent-free polymer. Polyethylene and polystyrene are commercially available and the manufacturers' selling price is used as the cost. The polyvinyl chloride and polyisobutylene costs are the average of a number of large-scale fractionations and were calculated from the manpower expended using $10 per hour as an average rate plus the cost of solvents. No allowance was made foi instrument depreciation.

Table 1 gives an estimated figure of merit for room temperature and high temperature large-scale gel permeation chromatography, large-scale chromatography, and for nonfractionated narrow molecular weight distribution polymer produced by anionic polymerization. Even with the uncertainties in the equation it can be concluded that the gel permeation

TABLE 1

Cost Effectiveness Comparison

Fractionation method	Polymer	$\bar{M}_w/\bar{M}_n$	C ($/g)	Figure of merit	Ref.
Gel permeation chromatography, prep scale, ambient temperature	Poly (vinylchloride)	1.1 –1.4	8–24	3– 13	*2*
Gel permeation chromatography, prep scale, high temperature	Polyethylene	1.1	80	1.3	*3*
Baker-Williams column chromatography	Polyisobutylene	1.03–1.2	4–12	21–280	*4, 5*
Not fractionated	*Polystyrene,* anionically polymerized	*1.05*	*1*	*400*	*6*

chromatographic technique as currently employed is relatively inefficient. The column chromatographic method is somewhat more promising although the average M is probably nearer the low end of the range rather than the high figure. The high value was achieved only at relatively low molecular weights. The anionically polymerized polystyrene is by far the most effective method for producing narrow distribution samples at relatively low cost.

It would be useful if reports of large-scale fractionation techniques for polymers included this figure or some other evaluation of cost effectiveness.

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