ESTIMATION OF THE PARTICLE SIZE DISTRIBUTION OF A DILUTE LATEX FROM COMBINED ELASTIC AND DYNAMIC LIGHT SCATTERING MEASUREMENTS. A METHOD BASED ON NEURAL NETWORKS

G.S. STEGMAYER[†], V.D. GONZALEZ[‡], L.M. GUGLIOTTA[‡], O.A. CHIOTTI[†] and J.R. VEGA[†,‡]

[†]*CIDISI (UTN – Facultad Regional Santa Fe), Santa Fe, Argentina*
gstegmayer@santafe-conicet.gov.ar, chiotti@ santafe-conicet.gov.ar, jvega@ santafe-conicet.gov.ar
[‡]*INTEC (UNL – CONICET), Santa Fe, Argentina*
veronikg@ santafe-conicet.gov.ar, lgug@intec.unl.edu.ar

***Abstract*— A method for estimating the particle size distribution (PSD) of a dilute latex from light scattering measurements is presented. The method utilizes a general regression neural network (GRNN), that estimates the PSD from 2 independent sets of measurements carried out at several angles: (i) light intensity measurements, by elastic light scattering (ELS); and (ii) average diameters measurements, by dynamic light scattering. The GRNN was trained with measurements simulated on the basis of typical asymmetric PSDs (unimodal normal-logarithmic distributions of variable mean diameters and variances). First, the ability of the method was tested on the basis of two synthetic examples. Then, the obtained GRNN was used for estimating the PSD of a narrow polystyrene (PS) latex standard of nominal diameter 111 nm. The standard was also characterized by 2 independent techniques: capillary hydrodynamic fractionation, and transmission electron microscopy (TEM). The PSD predicted by the GRNN resulted close to that obtained by TEM. The estimated PSDs were better than those obtained through standard numerical techniques for 'ill-conditioned' inverse problems.**

***Keywords*— Elastic Light Scattering – Dynamic Light Scattering – Particle Size Distribution – Neural Network – Inverse Problems**

I. INTRODUCTION

The particle size distribution (PSD) of a polymer latex is an important morphological characteristic that determines the processability and end-use properties of the material when used as an adhesive, a coating, an ink, or a paint. Transmission electron microscopy (TEM) is the main reference technique for directly observing and measuring the PSD. However, it is experimentally expensive, time-consuming, and difficult, mainly when analyzing soft latexes and/or broad PSDs. Also, the electron beam can produce a sample damage or a size contraction; and the PSD evaluation may involve counting thousands of particles (Llosent *et al*., 1996).

Several fractionation techniques (such as capillary hydrodynamic fractionation -CHDF-, field flow fractionation, hydrodynamic chromatography, and disc centrifugation), are also employed for measuring the PSDs. In particular, CHDF separates the particles according to their size, and employs a turbidity detector for determining the number of particles of each eluted fraction. CHDF is an indirect technique, since it requires a particle diameter calibration usually based on the analysis of narrow standards. Even though it is presented as a high resolution technique, it normally produces broad PSDs, as a consequence of the instrumental broadening that mainly occurs in the capillary tube (Silebi and Dos Ramos, 1989).

The so-called ensemble techniques are based on simultaneously measuring all particles in their media without previous fractionation. They include, acoustic-attenuation spectroscopy and focused-beam reflectance measurements, for concentrated systems (e.g., Scheffold *et al*., 2004; Li and Wilkinson, 2005); and several optical techniques such as turbidimetry, elastic light scattering (ELS), and dynamic light scattering (DLS) (Pecora, 1985; Llosent *et al*., 1996; Vega *et al*., 2003a,b). Particles in the sub-micrometer range are frequently measured by ELS and DLS (Bohren and Huffman, 1983; Chu, 1991). The instruments are similar, and basically consist of a monochromatic laser light falling onto a dilute latex sample. A photometer placed at a given detection angle, θ_r, with respect to the incident light, collects the light scattered by the particles over a small solid angle. In ELS, the light intensity, $I(\theta_r)$, is measured at each θ_r ($r = 1, 2, \ldots, R$). The ELS measurement model is given by:

$$I(\theta_r) = \int_0^\infty C_I(\theta_r, D)\, f(D)\, dD \qquad (1)$$

where $f(D)$ is the (unknown) PSD (represented as number of particles *vs*. diameter (D); and $C_I(\theta_r, D)$ is the light intensity scattered by a particle of diameter D at θ_r, and it is calculated through the Mie scattering theory (Bohren and Huffman, 1983; Glatter *et al*., 1985).

In DLS, a devoted digital correlator measures (at each θ_r) the second-order autocorrelation functions of