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Polyelectrolytes in solutions and dispersions

Habilitation thesis

ABSTRACT

The habilitation thesis entitled "*Polyelectrolytes in aqueous solutions and dispersions*" presents the most important scientific results of the author after defending her PhD thesis at "Petru Poni" Institute of Macromolecular Chemistry (July 1996). This thesis comprises three main parts: Section 1. *Professional and scientific achievements*, Section 2. *Cationic polyelectrolytes in aqueous solutions and dispersions*, Section 3. *Plan of scientific and professional development in the future.*

Polyelectrolytes (PEs) are polymeric materials which have been extensively studied both from theoretical and experimental point of view. The theoretical interest on PE was motivated by their behavior in aqueous solution that differs considerably from that of uncharged macromolecules or low molar mass electrolytes. The high complexity of these systems comes from the combination of properties derived from long-chain molecules with those derived from charge interactions. On the other hands, the investigation of solution properties of PE is of outstanding importance because of their key role in numerous fields, such as biology, medicine, cosmetics, food, textile, papermaking industries, agriculture and wastewater treatment.

In this context, my research activity has been focused mainly on some physico-chemical properties of PE solutions, namely the viscosity and electrolytic conductivity, and their application in solid(liquid)/liquid separation processes (Section 2). Thus, this section begins with an introduction (Chapter 2.1) which includes the definition and classification of PEs, data regarding the chemical structure and characteristics of the

investigated cationic PEs, etc. My scientific achievements have been included in chapters 2.2. and 2.3. In sections 1 and 3 some aspects of my up-to-date research activity (research directions, dissemination), and the plan for my future scientific activity are mentioned. In this regard, I will continue to focus on the polyelectrolytes field with a special attention on ionic polysaccharides, soluble or hydrogel. This thesis ends up with "References" (Section 4), where all the scientific articles, chapters and books used to develop the studies presented in section 2 are listed.

Chapter 2.2. "*Cationic polyelectrolytes in aqueous solutions. Impact of molecular and medium parameters on some transport properties"* focuses the viscosity and electrolytic conductivity of some cationic PEs in aqueous solutions. The macromolecular compounds were of synthetic type (cationic PEs with quaternary ammonium salt groups (*PC*) or with tertiary amine groups and poly(ethylene glycol) in the main chain (*PEGA*)), as well as modified polysaccharides based on dextran and pullulan. The results of these studies allowed:

(*i*) The evaluation of conformational changes of polyelectrolytes in both saltless and salt aqueous solutions, as well as in solvent mixtures (water/methanol and water acetone);

(*ii*) The obtaining of valuable information on solvent-solute and solute-solute interactions by dynamic methods;

(*iii*) Comparative analysis of experimental data with various theoretical models such as Fuoss, Fedors, Wolf, Manning, etc. Thus, Fedors equation, commonly used for describing the viscometric behavior of neutral polymers, has been applied for the first time in my studies to polyelectrolytes. Assessing the viscosity of polyelectrolyte solutions with this equation had a significant impact within the scientific world, this method of analysis being taken over by many other researchers. Likewise, the validity of the Wolf approach for describing the viscometric behavior of some cationic polysaccharides based on dextran in aqueous solution both in the absence and presence of salts as well as in water/methanol mixture was demonstrated for the first time in my papers. The evaluation of conductometric results in terms of Manning's theory for a series of dextran derivatives solutions revealed lower experimental values for both the equivalent conductivity and the interaction parameter than the theoretical ones. Also, it was found that the counterion condensation in the case of these cationic polysaccharides is not a threshold phenomenon,

their association to the charged groups of the polyions taking place regardless of whether the charge density parameter value is higher or lower than the critical value.

Chapter 2.3. *"Cationic polyelectrolytes in aqueous dispersions. Impact of molecular and medium parameters on the solid(liquid)/liquid separation processes"* presents the main results obtained in the destabilization of suspensions and emulsions containing either inorganic (clay, titanium dioxide, zirconium silicate (kreutzonit)), or organic (pesticide formulations: Fastac 10EC, Decis, Dithane M45, karate Zeon, Novadim Progress, etc) contaminants by polysaccharides derivatives based on dextran, pullulan and chitosan. Thus, I have reported for the first time in the field of separation processes several studies on the removal of (*i*) zirconium silicate particles from suspensions prepared in water, (*ii*) titanium dioxide particles from suspensions prepared in both water and water/methanol mixtures, and (*iii*) pesticide formulations by solutions of cationic polysaccharides as flocculants/coagulants. It must be underlined here that all the data reported up to our studies with respect to the treatment of wastewater contaminated with pesticides were mainly focused on the removal of pure active pesticides and not on their complex formulations, as they are used in agriculture.

The analysis of experimental data regarding the properties and applications of the ionic polymers revealed that quite often the results are contradictory, making difficult the development of a comprehensive theory to explain the general dependence of solution properties of PEs on different parameters. In this context, the physico-chemical properties studies on new ionic polymers based on renewable and environmentally friendly products, namely polysaccharides (dextran, pullulan, hydroxyethyl cellulose, hydroxyethyl starch, chitosan, konjac glucomannan) with well-defined structure able to adequately address the removal of a wide spectrum of toxic chemicals (metallic oxides, clays, drugs, dyes, cosmetics, pesticides, etc) from wastewater will be developed. The acquired data will allow the reconsideration of the structure-properties relationships in the context of imperative requirements of materials with multiple applications.