INTRODUCTION TO THE MODELLING AND DESIGN OF PHOTOREACTORS

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ABSTRACT Successful commercial application of photochemical reactions requires not only the scientific insight into the photochemistry of the reactions, but also a rational understanding of the engineering aspects of the photochemical process upon which reliable design can be based. An overview of the important engineering problem of the modelling and design of photoreactors is presented in this introductory paper. Different types of photoreactors are briefly described. The essential model parameters and equations are outlined. The case for systematic design studies is proposed.

I HISTORICAL BACKGROUND

Sixty years ago, photochemistry was just another weapon in the armament of the kineticist(1). It was recognised as a particularly useful tool in the study of reaction kinetics because in many cases the nature of the activating step could be well understood. It also offered a possibility of contributing to our knowledge of the methods by which molecules transfer energy on collision. However, the unique feature of the selectivity of photoreactions and their potential in the production of desired chemicals soon raised the hopes for industrial exploitation of photoprocesses.

By the late fifties and early sixties, photochemistry had already developed into the science of delivering precise amounts of energy, useful for precisely known transformations, some of which became the basis of competitive commercial processes(2). Reactions which showed promise included photo-halogenation,

photo-polymerisation, photo-oxidation for the synthesis of organics and the production of perhalogenated hydrocarbons and cyclohexanone oxime. The photochlorination of aromatic and aliphatic hydrocarbons (3-5) are successful industrial processes which have good yields and enhanced product selectivity.

The last twenty-five years witnessed a great surge towards research on pseudo-homogeneous and heterogeneous photocatalysis where photocatalysts in solid or dispersion form were employed to promote the desired transformations. The shift becomes more apparent when the conversion of solar energy into chemical energy via photochemical routes has been found to be more effective in pseudo-homogeneous and heterogeneous systems. No doubt the study of photocatalysis is fascinating and perhaps even a little controversial. In particular, the success in the use of photocatalysts to achieve the photolysis of water has stirred much excitement in the field of photochemistry, not least because of its implications in solar energy utilisation. A lot of activities have also been focussed on mimicking nature's photosynthesis processes, claiming various degrees of success. Photochemistry is no longer a sideline interest of the kineticist, but has emerged as a full-blown science. The literature on photochemistry and photocatalysis is now voluminous. Furthermore, the patent literature abounds with descriptions of photochemical processes of potential industrial importance which take advantage of the unique selectivity of reactions initiated by electromagnetic radiation.

Despite the attractiveness of photoreactions in their neat way to accomplish the chemical transformation and the enormous amount of research efforts poured into their study, the development of commercial photoprocesses remains rather limited. One major reason for such limited development is because systematic research on photochemical engineering is lagging behind. Successful commercial application of photochemical reactions requires not only the scientific insight into the photochemistry of the reactions but also a rational understanding of the engineering aspects of the photochemical processes, upon which reliable design can be based. To be sure, there exists much engineering know-how within the industrial circle on specific processes, but the information inevitably remains as trade secrecy.

The heart of a photochemical plant is the photoreactor. Obviously the modelling and design of photoreactors are important engineering problems to investigate. The present paper is an introduction to the study of these problems. In the early stage of commercial development of liquid phase photochlorination processes, clear-cut methods for applying physical and kinetic principles to photoreactor design were sought. The problems of