Preface

The science of mathematical modelling and numerical simulation is generally accepted as the third mode of scientific discovery (with the other two modes being experiment and analysis), making this field an integral component of cutting edge scientific and industrial research in most domains. This is especially so in advanced biomaterials such as polymeric hydrogels responsive to biostimuli for a wide range of potential BioMEMS applications, where multiphysics and multiphase are common requirements. *These environmental stimuli-responsive hydrogels are often known as smart hydrogels*. In the published studies on the smart or stimuli-responsive hydrogels, the literature search clearly indicates that the vast majority are experimental based. In particular, although there are a few published books on the smart hydrogels, none is involved in the *modelling* of *smart* hydrogels.

For the few published journal papers that conducted mathematical modelling and numerical simulation, results were far from satisfactory, and showed significant discrepancies when compared with existing experimental data. This has resulted in ad hoc studies of these hydrogel materials mainly conducted by trial and error. This is a very time-consuming and inefficient process, and certain aspects of fundamental knowledge are often missed or overlooked, resulting in off-tangent research directions. Thus it is absolutely necessary to publish a book on the modelling and simulation of the smart hydrogels with real multidisciplinary requirement for establishment of a theoretical platform by developing the correct mathematical models and also the powerful numerical techniques required to solve these challenging highly nonlinear and coupled models.

Polymeric hydrogels are form of matters that possess both the properties of solid and liquid. Their structural framework chains are formed from networks of randomly crosslinked polymers that embody three different phases in general, namely the three-dimensional solid polymeric matrix network, interstitial fluid and ion species. Depending on the component characteristics and synthesis methods, the hydrogels can be designed or tailored to demonstrate the unique property of undergoing discrete or continuous volume transformation in response to infinitesimal changes of external environment stimuli, such as solution pH, electric field, temperature, solvent composition, glucose/carbohydrates, salt concentration/ionic strength, light/photon, pressure, coupled magnetic and electric fields. These magnificent features make the hydrogel better known as smart or stimuli-responsive hydrogels.

Due to their unique properties that include swelling/deswelling behaviour, sorption capacity, mechanical property, permeability and surface property, the hydrogels provide the instrumentation for creating functional materials for broad spectrum of applications as they can sense the environmental changes and eventually induce structural changes without a need for an external power source. Artificial muscle, microfluidic control, sensor/actuator, separation process and chromatographic packing are just few examples of the successful applications of hydrogels. Another exceptional promise of the hydrogels is their biocompatibility and biostability potentials, suggesting that the hydrogels are also an excellent substitution for the human body tissues or biomimetic applications. There are also extensive explorations of the hydrogels in the medical and pharmaceutical applications, such as drug delivery system, articular cartilage, biomaterial scaffold, corneal replacement and tissue engineering. As such, the multi-state characteristics of the smart polymer hydrogels and their wide-range multiphysics applications make the multidisciplinary and multiphase the basic requirements for the mathematical models. For example, these models are required to be highly multi-disciplinary and at least to take into consideration the coupled chemo-electro-mechanical multi-fields and multiphase deformation of polymeric network solid matrices with flow of ions and interstitial fluid. This results in several mathematical challenges, in which usually the models consist of coupled nonlinear partial differential equations with requirements of moving boundary and localized high gradient.

A comprehensive study through modelling and simulation is thus warranted for theoretical understanding of the response behaviour of the smart hydrogels in BioMEMS devices subject to different environmental stimuli, due to the advantages of the material characteristics of the smart polymer hydrogels and their wide range of multiphysics applications. However, as mentioned above, there is a lack of open publications on modelling and simulation of the smart hydrogels, and this monograph is thus written to systematically document the response behaviour of the smart hydrogels to various environmental stimuli. A complete theoretical platform detailing of the fundamental theory for the smart polymer hydrogels is established. It is composed of several novel mathematical models which are already successfully developed. Response of the smart hydrogels to surrounding environment is examined in detail for the basic stimuli within common BioMEMS devices such as solution pH, externally applied electric voltage, temperature, solvent composition, glucose/carbohydrates and salt concentration/ionic strength. The effects of various material properties and environmental conditions on the responsive performance of the smart hydrogels, including Young's modulus, initially fixed charge density, effective crosslink density, ionic strength and valence of bath solution, initial volume fraction of polymeric network, initial geometry, are also investigated in various parametric studies. In addition, an analysis of drug delivery system for the controlled drug release from non-swellable micro-hydrogel particles is presented with consideration of drug dissolution and diffusion through the continuous matrices of spherical micro-hydrogel particles.

This is the first monograph of its kind, which primarily meets the needs of scientists and engineers in the broad areas of polymer materials science, biomaterials engineering, biomedical engineering, sensor/actuator, micro-electro-mechanical system (MEMS) and BioMEMS, physics, chemistry, biophysics, biochemistry and bioengineering. It is especially useful for them as a reference source, and also if they wish to conduct further studies so as to extend their work to practical application. Other important primary readers are postgraduate students in the area of polymer materials science and biomedical engineering, especially those with involvement in the computational aspects such as the modelling and simulation of stimuli-responsive soft materials. Possible secondary readers include undergraduate students taking the advanced mechanical and electric engineering courses which involve sensor or actuator, MEMS and BioMEMS. The chapters on the fundamental theoretical development are especially useful to these students. Correspondingly, the course lecturers will also find this book a good reference source. This book provides both the casual and interested reader with insights into the special features and intricacies of smart polymer hydrogels when environmental stimuli are involved. It is also invaluable to design engineers in the polymer sensor/actuator, MEMS and BioMEMS industry and biomedical engineering, serving as a useful reference source with benchmark results to compare and verify their experimental data against.

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Hua Li, Ph.D.
School of Mechanical & Aerospace Engineering
Nanyang Technological University
Singapore
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