MODELING PH-SENSITIVE HYDROGEL FOR MICROFLUIDIC CONTROL

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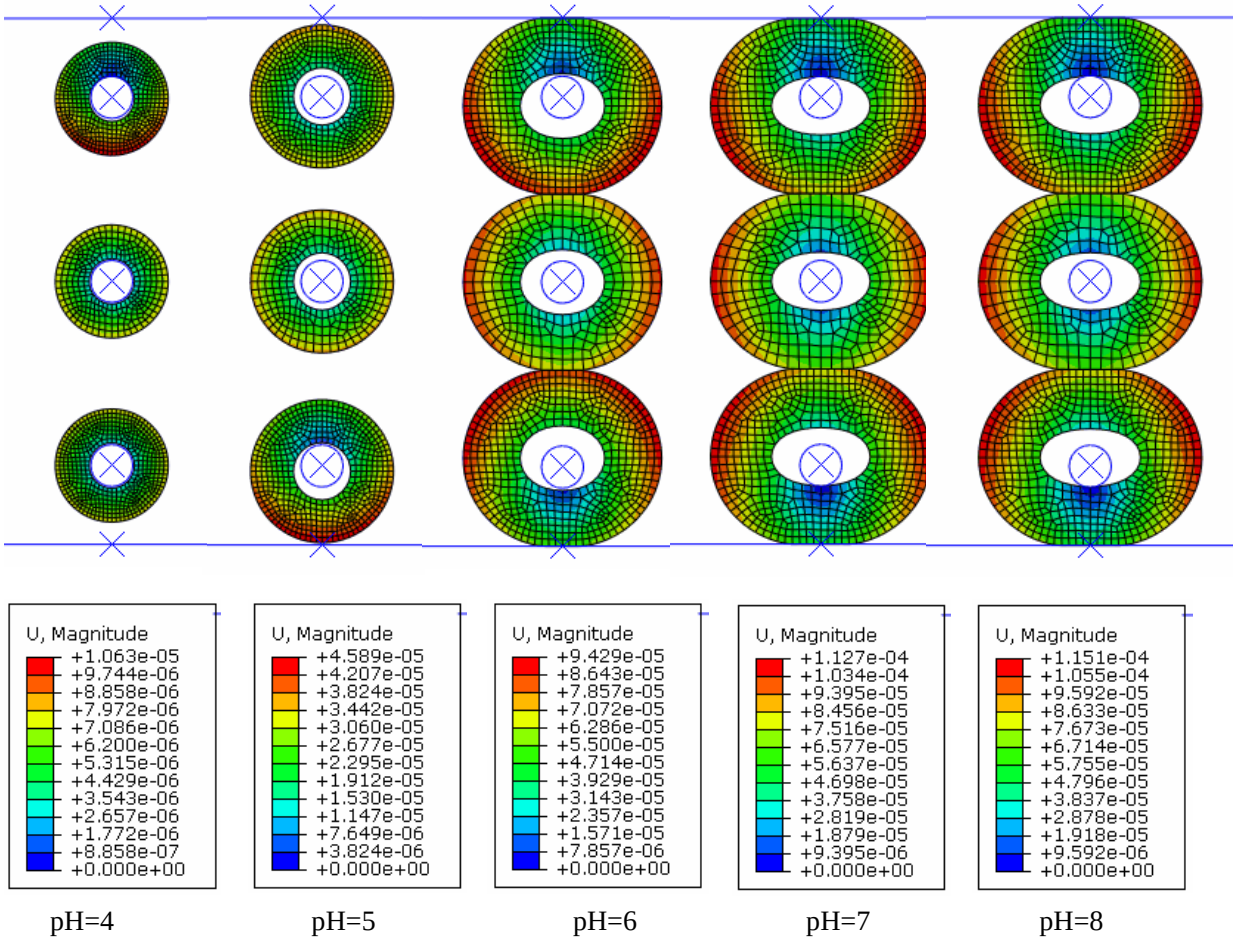
Summary Following a recently developed theory for constrained swelling of pH-sensitive hydrogel and the finite element user-subroutine technique, we modeled deformation and contacts of pH-sensitive hydrogels for real purpose microfluidic flow control systems. A jacket valve consisting of three cylindrical hydrogels coated on three fixed pillars and a hybrid hydrogel/PDMS system are modeled and analyzed in this paper. We present deformation and multiple contacts of the hydrogel based flow control systems when pH of external solution is switched to various values. Also included is the pressure in the contacts, stress distribution, sensitivity of swelling ratio with respect to pH values, and in addition the influence of initial fabrication imperfections. The presented results provide helpful guidance for the design, fabrication and optimization of pH-sensitive hydrogel devices for microfluidic flow control.

MANUSCRIPT PREPARATION

Polymer gels can integrate multiple functions (eg., sensing and actuation) into a single component and perform prescribed tasks through the sensing of local environment information. This makes stimulus-responsive hydrogel an ideal component for sensor, actuator, drug delivery, adaptive microlense, soft robotics, and a tremendous number of bioengineering applications [1]. Among these a wide variety of applications, responsive hydrogel for microfluidic flow control has emerged as a cutting-edge technology.

Following a recent trend in the study of theory of pH-sensitive hydrogel and a subsequent development of ABAQUS user-subroutine [2-3], we modeled two flow control systems: a hydrogel jacket valve consisting of three cylindrical hydrogels with hard posts, and a hybrid hydrogel/PDMS flow control system. The following picture shows the deformations and contacts of the jacket valve subject to variation of pH values.



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The response of swelling ratio to variation of pH of external solution, i.e., the sensitivity of the hydrogel, is another factor of utmost importance. Our study shows that the hydrogels are most sensitive for pH variation from 4 to 6. This is in good agreement with a lot of pH-sensitive hydrogel experiments. This optimal tunable range of pH of external solution should be fully explored in the control of this type of jacket valve.

During real fabrication process, some imperfections are evitable and hydrogels may start to swell from a lightly skewed initial state. We modelled this case by introducing a small imperfection to the middle hydrogel, artificially misalign the middle hydrogel to left a very small distance. The hydrogels are in such a skewed initial state and in equilibrium with an external salt with pH=1. Starting from this initial state, we modeled the swelling of hydrogels as a dynamic problem and solved it by using the Dynamic/implicit solver in ABAQUS.

We then apply the technique to simulate hybrid hydrogel/PDMS flow regulation valve. A piece of a pH-sensitive hydrogel sandwitched between a rigid porous membrane and a soft silicone rubber membrane, constituting a much smaller but more efficient flow control system. The fluid can flow through the upper porous membrane, causing the swelling of the hydrogel. The swelling of the hydrogel deforms the rubber membrane and eventually conceals the orifice below the rubber membrane. We modelled the deformation and contacts of such a hybrid hydrogel/PDMS flow control system when the pH of the external solution is changed from initial value pH=1 to 4, 5, 6, 7. The numerical strategy and the simulation presented herein can aid the design and fabrication of hydrogel-based microfludic flow control devices.

CONCLUSIONS

Hydrogels are soft active meterials which can sense, move and deform in response to external stimuli. Hydrogel-based devices offer promise of autonomous microfluidic flow control, resulting in lap-on-chip systems without the need of external power, control system and complex algorithms. Based on a recently developed theory for constrained swelling of pH-sensitive polyelectrolyte gels and the finite element user-subroutine, we modeled the deformation and contacts of a hydrogel jacket valve and a hybrid hydrogel/PDMS flow control system. Contact pressure profiles and stress distributions of these real-purpose design congigurations, as well as the sensitivities of the volume expansion with respect to variations of pH of external solution, are crucial factors to be determined for such systems, and we explore these factors in details, hopefully to throw some light on the design, fabrication and operation of hydrogel-based microfluidic flow control systems.

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References

[1] Beebe, D. J., Moore, J. S., Bauer, J. M., Yu, Q., Liu, R. H., Devadoss, C. and Jo, B. H.: Functional hydrogel structures for autonomous flow control inside microfluidic channels. *Nature 406:* 588-590, 2000.

[2] Hong, W., Zhao, X., Suo, Z.: Large deformation and electrochemistry of polyelectrolyte gels. *J. Mech. Phys. Solids* 58: 558-577, 2010.

[3] Marcombe, R., Cai, S., Hong, W., Zhao, X., Lapusta, Y., Suo, Z.: A theory of constrained swelling of a pH-sensitive hydrogel. *Soft Matter* 6: 784-793, 2010.

[4] He, T., Li, M, Zhou, J.: Modeling deformation and contacts of pH sensitive hydrogels for microfluidic flow control. *Soft Matter*, in press.