

Área: MAT

The effect of the molecular structure of HPMC on the interaction with water for cryogels prepared with and without calcium peroxide

Camila G. Chiaregato (PG),^{1*} Oigres D. Bernardinelli (PQ),² Amin Shavandi (PQ),³ Edvaldo Sabadini (PQ),⁴ Denise F. S. Petri (PQ).¹

camichiaregato@usp.br

¹Department of Fundamental Chemistry, Institute of Chemistry, USP, São Paulo, Brazil; ² Department of Physics, UFSCar, São Carlos, Brazil; ³ BioMatter Unit, École Polytechnique de Bruxelles, ULB, Brussels, Belgium; ⁴ Department of Physical Chemistry, Institute of Chemistry, UNICAMP, Campinas, Brazil

Keywords: hydroxypropyl methylcellulose, transverse relaxation time, swelling rate, contact angle, CaO₂

Highlights

The incorporation of CaO₂ particles into HPMC cryogel reduced the O₂ release.

The molecular characteristics of HPMC drive the swelling rate and wettability.

Abstract

The interaction between polymers and water is critical for determining the final characteristics of a material. Hydroxypropyl methylcellulose (HPMC) belongs to the cellulose ether family that has both hydrophobic methyl groups (DS) and hydrophilic hydroxypropyl groups (MS) on its chain. The interactions between water molecules and cryogels prepared with different types of HPMC, in the presence and absence of a linear nonionic surfactant (containing a dodecyl chain and a PEG chain) and CaO₂ microparticles, were systematically investigated using sorption experiments and Time-Domain Nuclear Magnetic Resonance (TDNMR). Solutions of HPMC at 3.0 wt% containing 0.3 wt% of citric acid (crosslinker) and 0.15 wt% of sodium hypophosphite (catalyst) were prepared. The surfactant concentration was 0.168 g L⁻¹, and 50 mg of CaO₂ was added to 1.6 g of HPMC solution. Then, the precursor gels were frozen for 24 h and freeze-dried during 10-12 h. The resulting cryogels were oven heated at 165 °C for 5 min to promote the esterification reaction between citric acid and HPMC hydroxyl groups. Regardless of the DS and MS of the HPMC, most water molecules showed transverse relaxation time t_2 typical of intermediate water and a small population of more tightly bound water. HPMC cryogels with the highest DS of 1.9 had the slowest swelling rate ($0.519 \pm 0.053 \text{ g}_{\text{water}}/(\text{g.s})$) and the highest contact angle values ($85.250^\circ \pm 0.004^\circ$), providing the best conditions for a slow reaction between CaO₂ and water. The presence of the surfactant increased swelling rate and decreased contact angle values, likely due to hydrophobic interactions possibly favored the exposition of the surfactant's polar head to the medium. The HPMC with the highest MS had the fastest swelling rate and the lowest contact angle. The initial rate (V_0), calculated from the kinetics of O₂ release, was slower for all cryogels compared with pure CaO₂, avoiding burst release. These findings are relevant for the formulations and reactions, where tuning the swelling kinetics is crucial for the final application, such as biomedical applications and wastewater treatment.

Acknowledgments

The authors thank the São Paulo Research Foundation (FAPESP) (2018/13492-2 and 2022/06284-0) and CNPq (304017/2021-3) for the financial support.