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Дослідження молекулярної динаміки трикомпонентних сумішей вода-NaCl-ДМСО під час заморожування та відігріву

І. Клбік[1,2]
[1]Інститут фізики Словацької академії наук, м. Братислава, Словаччина
[2]Факультет математики, фізики та інформатики, Університет Коменського, м. Братислава, Словаччина

Molecular Dynamics Study of Ternary Water-NaCl-DMSO Mixtures During Freezing and Thawing

I. Klbik[1,2]
[1]Institute of Physics of the Slovak Academy of Sciences, Bratislava, Slovakia
[2]Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovakia

Cryopreservation is crucial for preserving biological materials, but the mechanisms of ice formation and its impact on cell membranes are not fully understood. Ice formation is known to exert mechanical forces on membranes, which can cause damage. A tensodilatometric study (Osetsky 2007). suggests that extracellular ice formation within closed fluid inclusions among ice crystals can increase hydrostatic pressure due to density changes during phase transitions. This study employs fully atomistic molecular dynamics simulations to explore ternary water-NaCl-DMSO mixtures representing cryopreservation media. It examines how DMSO influences temperature-induced density changes and potential pressure buildup during freeze-thaw cycles.

The simulations were carried out across two scenarios: 1) a freeze-thaw cycle from 25 to –125°C at a rate of 0.2°C/ns without spontaneous ice formation, and 2) an isothermic process at –53°C with a seeded ice crystal for 500 ns, followed by cooling to –125°C and reheating to 25°C. Simulations were carried out using GROMACS – molecular dynamics software package (Abraham 2015), applying AMBER force fields (Case, 2023) to describe interaction potential and individual atoms: OPC model for water, GAFF2 model for DMSO, and Li&Merz (12-6 IOD) model for NaCl.

MD simulations identified a second-order phase transition within the range of –72 to –64°C, decreasing with increasing DMSO concentration. Both amorphous and ice-containing scenarios exhibited significant density changes during freeze-thaw cycles. The greatest density difference (amorphous *vs.* ice-containing) was observed near the equilibrium freezing point, suggesting potential stress impacts linked to cryoinjury. Greater supercooling resulted in smaller density changes, potentially reducing stress. DMSO moderated these changes across all temperatures and scenarios, slowed ice crystal growth, and promoted an ice-free fraction. Radial distribution function analysis showed DMSO strong interaction with Na^+ and its reduction of NaCl ion pairing at –53°C, while Cl^- remained primarily solvated by water.

DMSO effectively reduces temperature-induced density variations and differences between amorphous and ice-containing mixtures, mitigating potential volumetric expansion during ice formation. It also slows the kinetics of ice crystal growth, which is beneficial against osmotic shock and 'solution effects' injury. Additionally, DMSO impact on NaCl ion pairing might influence protein stability, highlighting its broader cryoprotective potential and possible role in preventing eutectic NaCl crystallization.

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Врожайність насіння томату залежно від передпосівної обробки

М. Шапко[1], Н. Шевченко[2], Г. Коваленко[2], О. Куц[1]
[1]Інститут овочівництва і баштанництва НААН, с. Селекційне, Харківська обл., Україна
[2]Інститут проблем кріобіології та кріомедицини НАН України, м. Харків, Україна

Tomato Seed Yield Depending on Pre-Sowing Treatment

M. Shapko[1], N. Shevchenko[2], G. Kovalenko[2], O. Kuts[1]
[1]Institute of Vegetable and Melon Growing of the National Academy of Agrarian Sciences of Ukraine, Selektsiine village, Kharkiv region, Ukraine
[2]Institute for Problems of Cryobiology and Cryomedicine of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine

Tomato is currently one of the most economically important crops in Ukraine. In 2019, the gross production of tomato fruits in Ukraine amounted to 9688 thousand tons. Reducing the anthropogenic load on agrobiocenoses, implementation of technologies based on the principles of organic cultivation is actual task. One of the ways is to replace chemical seed treatment with physical methods of reducing seed damage and stimulating the growth processes of vegetable plants at the initial stages of ontogeny.

The aim of this study was to determine the effect of freezing or ozonizing tomato seeds on their germination, biometric parameters of plants and yield.

The experiments were conducted in 2023 on fields located in the left-bank Forest-Steppe of Ukraine, in the Kharkiv region. Seeds were placed in 2 ml cryovials and transferred to a refrigerator (–40 and –80°C) or liquid nitrogen for 4 days. The samples were heated in air at 22°C in the dark. To determine the effect of ozonation, the seeds were treated for 20 minutes with an ozone-air mixture, the ozone concentration was 0.5, 1, 1.5 mg/l. The seeds were sown 4 days after treatment. The control was untreated seeds. Seed germination, such plant biometric parameters as plant height, number of main stem leaves, number of first-order stems, number of main stem bunches of tomato and yield were determined. The data were analyzed using the statistical software PAST 3.

Low-temperature treatment by freezing to –40 and –80ºC or ozonation at all studied ozone concentrations did not affect seed germination. Immersion of samples in liquid nitrogen significantly reduced this index. Field studies have shown that low temperature treatment or ozonation did not change the biometric parameters of plants. The yield increased significantly after treatment at –40°C (by 20%) or ozonation at an ozone concentration of 1.5 mg/l in the ozone-air mixture (by 30%) compared to the control, while other studied methods of pre-sowing treatment did not affect the tomato yield.

Thus, it has been shown that pre-sowing seed treatment by freezing to –40ºC or ozonation at an ozone concentration of 1.5 mg/l in an ozone-air mixture can be used to increase its yield. In order to exclude the influence of weather conditions, it is necessary to conduct the same series of studies over several years.