Detoxifying Nerve Agents Using Functionalized Polymer Nanofiber Membranes

A group of scientists from the National University of Singapore published a study in the May 30th issue of *Nanotechnology*, which developed polymer nanofiber membranes with a synthesized catalyst to detoxify nerve agents.

Research fellow Subramanian Sundarrajan, with the University's Bioengineering Division, and his colleagues wanted a method to detoxify organophosphorus nerve agents, such as Soman, Sarin, and Tabun. "Nerve agents disrupt the human nervous system by inhibiting the actylcholine esterase enzyme," Sundarrajan said.

Currently, protective clothing for OP nerve agents use functionalized activated carbon. Disadvantages to carbon include its heaviness, its ability to hold moisture, and having to dispose of contaminated clothing because of absorption.

An important aspect of the study involved the choice of catalyst. "Literature showed that B-CD (B-cyclodextrin) and IBA (o-iodosobenzoic acid) have a history of hydrolyzing nerve agents. We hypothesized that if we synthesized a CD derivative with IBA functionality, it would have better catalytic properties," Sundarrajan explained.

As a result, Sundarrajan and his group chose 3-carboxy-4-iodosobenzyl oxy-B-CD, which was a CD derivative, as one of the catalysts in the experiment. The team also used other variations of B-CD and IBA. The material for the nanofiber membranes was equally vital; in the past, the scientists had experimented with nanofibers spun from cellulose acetate, but found this material to be too fragile.

Instead, the scientists used PVC polymer for the nanofibers because of its advantages: PVC has a small fiber diameter, is extremely porous, and has a high surface area. "A high surface area helps in obtaining better reactivity with the catalyst," Sundarrajan said.

For the control portion of the experiment, Sundarrajan and his colleagues electrospun one set of PVC polymers into nanofiber membranes without a catalyst. They also electrospun PVC with B-CD, PVC with IBA, PVC with B-CD and IBA and PVC with oxy-B-CD.

All functionalized nanofiber membranes were hydrophilic, with varying static water contact angles: 10 degress for the plain PVC and PVC with IBA, 12 degress for PVC with B-CD, 7 degrees for PVC with B-CD and IBA, and 9 degrees for PVC with the oxy-B-CD.

To test the effectiveness of the functionalized nanofibers, the scientists chose paraxon, a nerve agent stimulant that can be analyzed with UV spectrophotometry. They dipped the nanofiber membranes in three different concentrations of paraxon, 10mM, 25mM, and 50mM, at 25 degrees C, as well as one additional beaker which had unhydrolyzed paraxon for comparison.

Using UV spectrophotometry, Sundarrajan and his peers analyzed the hydrolysis of paraxon and found that the most effective hydrolysis came from oxy-B-CD nanofiber membrane. “The ether group from oxy-B-CD acted as a linker with the benzene ring and optimized the interactions between the catatlyst and the paraxon,” he explained.

The scientists made another startling observation: “As the yield of the oxy-B-CD increased, the extent to which the nerve agent stimulant hydrolyzed also increased,” Sundarrajan said. By manipulating the ether group that is between B-CD and IBA, the scientists could cause this increase in oxy-B-CD.

The oxy-B-CD broke down paraxon into diethyl phosphoric acid and p-nitorphenol, which changed from the acid base to the base form (p-nitorphenolate). “A highly-stable complex between p-nitrophenolate anion and B-CD occurs, possibly from polarizability and resonance delocalization,” Sundarrajan added.

Sundarrajan and his team measured the amount of p-nitrophenol with UV spectrophotometry, finding a maximum at 410 +- 10 nm. In other words, the nanofiber membranes functionalized with oxy-B-CD were effective in decontaminating paraxon.

Furthermore, the team of scientists compared the hydrolysis of paraxon with activated carbon to the hydrolysis with oxy-B-CD, as well as the other types of functionalized PVC polymer nanofiber membranes. The team found that the oxy-B-CD was 11.5 times faster than the activated carbon and that the oxy-B-CD was also faster than B-CD, IBA, and the B-CD and IBA combination nanofibers.

Manufacturers can add oxy-B-CD nanofiber membranes to woven clothing, leading to decontamination of organophosphorous nerve agents, as well as lighter and more breathable clothing. “Next we are trying to develop non-specific catalysts that will decompose both nerve and blister agents,” Sundarrajan says.

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