Mathematical model predicts drug concentration in the brain

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Do medicines arrive in the right amount at the right spot in our brain? By making a model that depicts our brain in small "brain blocks," Ph.D. student Esmée Vendel tries to find an answer to this question. She made

a mathematical model that predicts the concentration of medicines in the brain over time and space.

Target in the brain

"The success of medicines intended for the brain is to this day still limited," says Vendel. Scientists still do not understand enough about the complexity of our brain and how a medicine distributes itself within it. Together with her promoters, Vendel therefore developed a mathematical 3-D model that can predict the drug concentration within the brain. "Our model is new in its kind because it describes the spread of a drug over both time and space. In this way, different processes of drug distribution can be taken into account."

According to Vendel, knowing exactly how and in what quantities a drug spreads in the brain is essential for the development of new drugs. "If a drug is not sufficiently present at the target site, such as a local brain tumor, the desired effect will not occur," she explains. "And if the drug is present in too large quantities, (more) side effects may occur. In addition, there may be local differences within the brain, often as a result of illness. This is difficult because these differences influence the spatial distribution of a drug and thus the effect."

Building blocks

For both practical and ethical reasons, it is difficult to experiment with real brains. Vendel's mathematical model is a safe way to find out more. The model is based on so-called brain blocks. Vendel: "One little brain block is an abstract representation of one piece of brain tissue." It can be regarded as a kind of building block, she explains, in which she mathematically describes the smallest blood vessels in the brain, the cerebral capillaries, and the cerebral fluid outside the cells.

Within such a brain block, a drug divides itself by first crossing the blood-brain barrier from the blood vessels, after which it spreads further through the extracellular brain fluid and binds to its targets. "By linking several of these blocks together like building blocks, you can describe a larger part of the brain," Vendel explains. "And by giving certain brain blocks different properties than others, you can even study the effect of spatial variations within the brain."

Personalised model

The latter is useful because the spatial processes and properties of the brain can differ from one medicine or patient to another and change as a result of disease. By rendering the brain abstract in adaptable building blocks, the model can be made to measure for each patient and situation.

The research builds a bridge between two disciplines, by using mathematical techniques to better understand pharmacological processes. Vendel: "The 3-D brain unit model is the first of its kind and I believe that with our 3-D model we have laid a solid foundation for the description of the spread of medicine within our complex brain."

Provided by Leiden University

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