Chemical microdroplet computers are easier to teach than to design

October 15 2015

These are different spatio-temporal structures that appear in chemical systems can be used for information coding and processing. Credit: IPC PAS, Grzegorz Krzyzewski

Scientists from the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw have developed a simple chemical computer made of microdroplets capable of searching databases. Computer simulations, carried out on databases of malignant tumours, have confirmed the validity of the new design strategy, which opens the door to the popularisation of chemical methods for processing information.

Under the appropriate conditions, oscillating chemical reactions can occur inside a droplet. If there is more than one droplet and they are in contact with each other, the resulting chemical waves can penetrate into neighbouring droplets and disperse throughout the whole complex. This phenomenon is well known, and efforts are underway to use microdroplets for such applications as chemical data processing.

Propagation of information through many droplet systems depends on their geometrical arrangement. Until recently, not much was known about how to design microdroplet complex shapes that could execute specific tasks. Researchers at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) in Warsaw, Poland, have now proposed a novel strategy. Instead of laboriously designing complex systems of microdroplets for a particular purpose, it is better to first produce a system and then try to teach it something useful.

"We adopted a strategy that nature uses with great efficiency. Let's just look at ourselves. For instance, our brains don't evolve to recognise letters. First, the brain grows, and only then does it learn to read and write. Why not approach complex microdroplet systems in a similar manner, since we know that they also process information? Our proposal is therefore as follows: first, let's make a system of chemically interacting microdroplets, and then let's see what it can learn to do," says Prof. Jerzy Gorecki (IPC PAS).

Research on the chemical processing of information by microdroplet systems, funded by the Polish Ministry of Science and Higher Education, the Foundation for Polish Science and the European Union, was carried out using the Belousov-Zhabotinsky oscillating reaction. When the conditions of this reaction are suitably selected, a chemical front wandering in space appears. Oscillation reactions are common in living organisms. In humans, at the stage of embryonic development, they form the beginnings of the spinal vertebrae; in adults, they are responsible for the contractions of heart muscle, among other things.

"In the Belousov-Zhabotinsky reaction, the passing of a chemical front is accompanied by changes in ion concentrations leading to a change in the colour of the solution. When the reaction occurs inside the droplet, clear pulses radiating in all directions can be seen within it under the microscope. The bigger the drop, the more often it pulsates," explains PhD student Konrad Gicycski (IPC PAS).

Chemical pulses in complexes of adjoining droplets spread much like electrical stimulation in nerve fibres. Researchers from IPC PAS used pulse frequencies in individual drops to encode information: A high frequency corresponded to TRUE, a low frequency to FALSE. In order to control the pulses, and thus to input data, the researchers used the sensitivity of the reactions to blue light taking place in the droplets: in droplets illuminated with blue light, the reactions die off completely.

Computer simulations were used to examine the calculating possibilities of a planar array of adjoining microdroplets arranged in a 5x5 square. Within the array, droplets for inputting data and droplets for processing information were distinguished. Data was entered by simulating appropriately long exposure of the input droplets. Learning took place by the selective interruption of reactions taking place in the drops (in a real system, the interruption would also be performed by light). Researchers identified the droplet with oscillations that best matched the correct answer as the droplet giving the answer. The aim of the learning process was to select the light exposure time of all the droplets in the system in such a way as to obtain the highest number of correct answers for all the records in the database.

The simulated array of oscillating microdroplets classified tumours that were in the CANCER database. This database is composed of 699 records, of which 66% correspond to benign tumour cells. This means that on seeing the next entry, if we randomly say, "Don't worry, your tumour is not malignant" there's a 66% chance of giving the right answer.

"Our little chemical computer answered correctly in more than 90% of cases. This is a very good result, and proves the effectiveness of the strategy we adopted. It is not completely unequivocal, but even the classic computer does not have to give the right response to cases outside the database. In any case, we humans also don't always make the right decisions," says Prof. Gorecki.

Microdroplet information processing systems can be built using microfluidic devices. These are usually small plates made of transparent plastic in which a carrier liquid flows through a system of appropriately designed channels, carrying droplets of other liquids immiscible in the carrier. In such systems, it is relatively easy to produce drops of different sizes, substrate concentrations, or even substrates themselves.

"We are able to arrange the microdroplets in a controlled and repeatable manner in space, for example, enclosing many droplets of one liquid within a droplet of another liquid—and in such a way that the selected droplet always has the same neighbours. Furthermore, we also have techniques that allow us to influence the rate of chemical exchange through the membranes of the adjoining droplets," says Prof. Piotr Garstecki (IPC PAS) and gives the example of an arrangement of nine microdroplets enclosed within another droplet, recently constructed at his laboratory.

Systems processing information chemically cannot replace consumer electronics—they are too slow. They have important advantages, however, including parallel processing of information, and the potential possibility of functioning in extreme environments, e.g. at significant pressures and/or high temperatures, in which modern electronics fail. An interesting application is intelligent medicines, which would respond to many factors within the body and which are activated only under specific, strictly defined, circumstances. Theoretically, chemical computers could arise using the phenomenon of self-organization. This suggests such applications as futuristic space probes, capable of independently building key components from materials available on other planets.

Provided by Polish Academy of Sciences