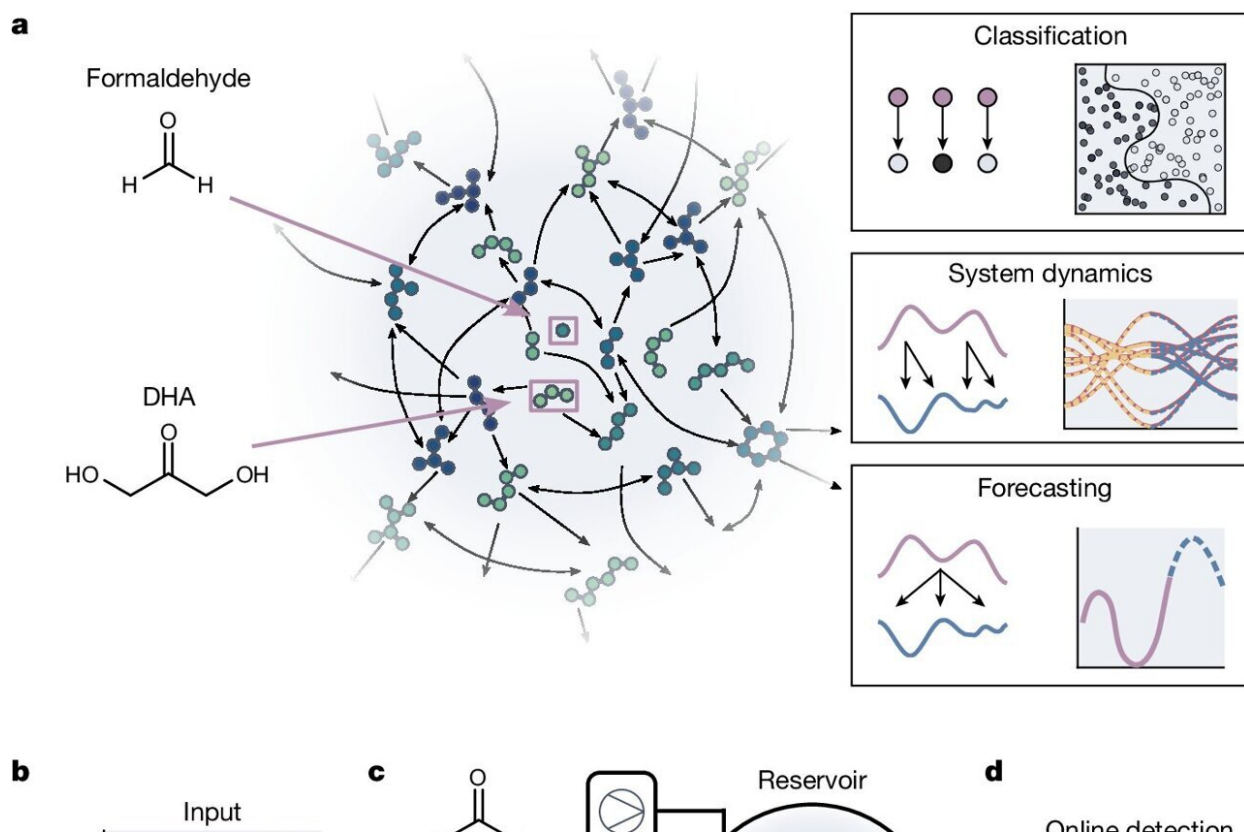# Scientists demonstrate chemical reservoir computation using the formose reaction

July 13 2024, by Tejasri Gururaj

A schematic overview of the formose reservoir computer. Credit: *Nature* (2024). DOI: 10.1038/s41586-024-07567-x

Researchers from the Institute for Molecules and Materials at Radboud University, Netherlands, have demonstrated that a complex self-

organizing chemical reaction network can perform various computational tasks, such as nonlinear classification and complex dynamics prediction.

The field of molecular computing interests researchers who wish to harness the computational power of chemical and biological systems. In these systems, the chemical reactions or molecular processes act as the reservoir computer, transforming inputs into high-dimensional outputs.

The research, published in *Nature*, was led by Prof. Wilhelm Huck from Radboud University.

Researchers have tapped into the potential chemical and biological networks offer due to their complex computing abilities. However, implementing molecular computing presents challenges in terms of engineering and design.

Instead of trying to engineer molecular systems to perform specific computational tasks, Prof. Huck and his team are exploring how naturally complex chemical systems can exhibit emergent computational properties.

"I am very interested in the chemical driving forces that led to the origin of life. In this context, we are looking for mechanisms by which chemical evolution can shape the properties of complex reaction mixtures. This research drove us to consider how molecular systems can process information," he explained to Phys.org.

The formose reaction

The formose reaction is a chemical reaction that synthesizes sugars from formaldehyde in the presence of a catalyst, calcium hydroxide. This reaction was chosen because of its unique properties.

Prof. Huck explained, "Although chemistry might seem complex to outsiders, most reaction sequences are rather linear. The formose reaction is the only example of a self-organizing reaction network with a highly non-linear topology, containing numerous positive and negative feedback loops."

In other words, the reaction isn't straightforward and produces multiple intermediate compounds which react further to form new compounds. These dynamic reactions can result in a diverse set of chemical species and are non-linear in nature.

Additionally, the network includes positive feedback loops which amplify reaction outcomes, and negative feedback loops which dampen reaction outcomes.

The network is known as "self-organizing" because it naturally evolves and reacts to the chemical inputs without the need for external intervention, producing a diverse range of outputs.

The computational capabilities emerge from the network's inherent properties rather than being explicitly programmed, making computation very flexible.
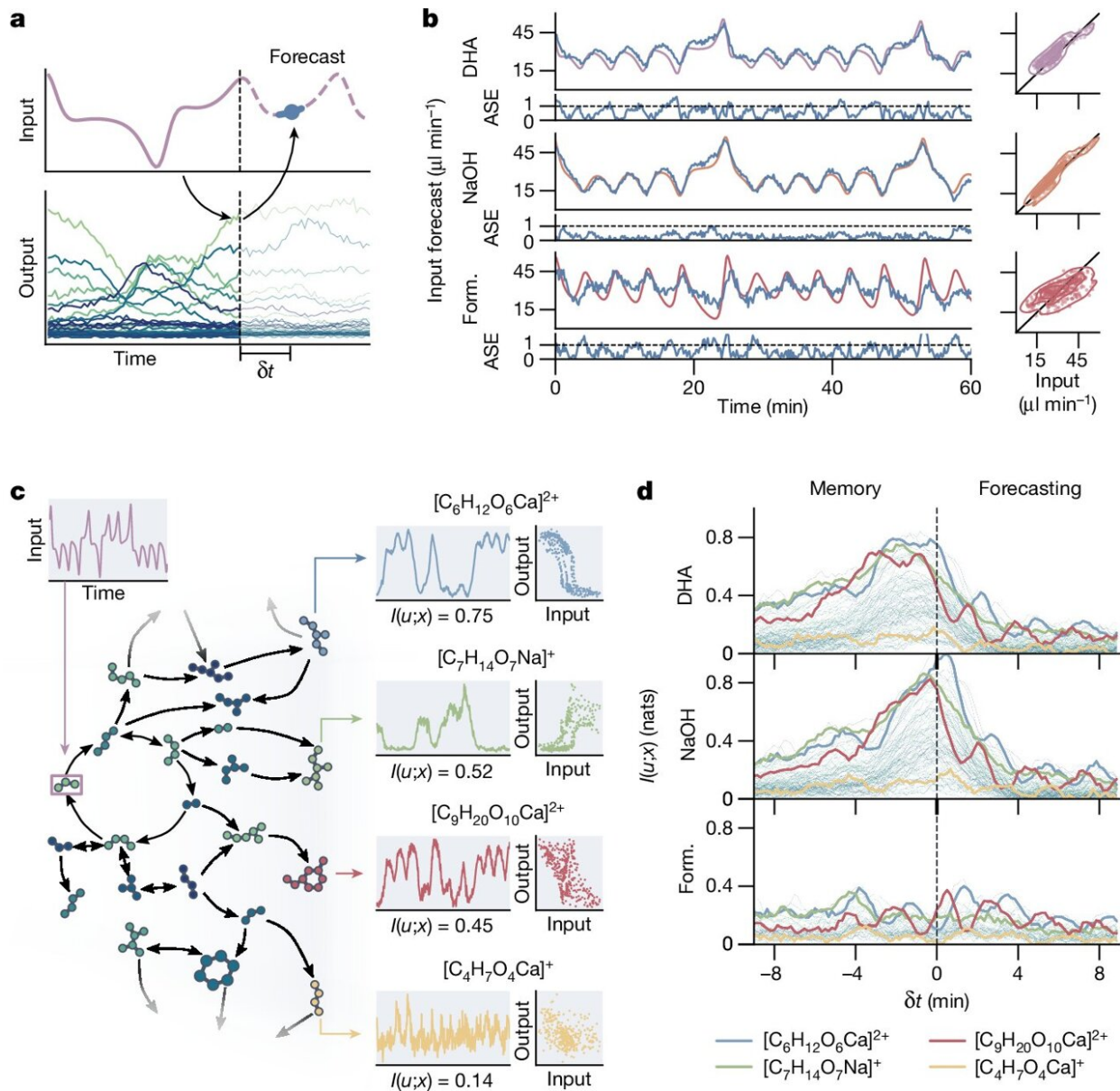
Memory and prediction in the formose reservoir computer. Credit: *Nature* (2024). DOI: 10.1038/s41586-024-07567-x

Implementing the reservoir computer

The researchers used a continuous stirred tank reactor (CSTR) to

implement the formose reaction. The input concentrations of four reactants—formaldehyde, dihydroxyacetone, sodium hydroxide, and calcium chloride—are controlled to modulate the reaction network's behavior.

The output molecule is identified using a mass spectrometer, which allows them to track up to 106 molecules. This setup can be used to do calculations, with the reactant concentrations being the input value to any function that needs to be computed.

But first, the system has to be trained to find the outcome of this computation, which is done using a set of weights.

"We need to find a set of weights that converts the traces in the mass spectrometer to the correct value of the computation. This is a linear regression problem and is computationally simple. Once done, the reservoir computer computes the outcome for this function for any new input," explained Prof. Huck.

The weights are coefficients that determine the influence of each input on the output. This training step is essential as it allows the reservoir to learn and predict how the changes in input affect the output so it can predict the output for a new set of inputs.

Computational capabilities

The researchers used the reservoir computer to do several tasks. The first was doing nonlinear classification tasks. The reservoir computer could emulate all Boolean logic gates and even tackle more complex classifications like XOR, checkers, circles, and sine functions.

The team also showed that it could predict the behavior of a complex metabolic network model of E. coli, accurately capturing both linear and

nonlinear responses to fluctuating inputs across various concentration ranges.

Furthermore, the system demonstrated the ability to forecast future states of a chaotic system (the Lorenz attractor), accurately predicting two out of three input dimensions several hours into the future.

The research team also found that some chemical species in the system exhibit short-term memory, retaining information about past inputs.

They also demonstrated a proof-of-concept for a fully chemical readout using colorimetric reactions, showing how the system's state could be interpreted without electronic measurement devices.

In other words, the system's state could be interpreted using color changes from chemical reactions, eliminating the need for electronic measurement devices.

Origins of life, neuromorphic computing, and beyond

This new approach to molecular computing could bridge the gap between artificial systems and the information processing capabilities of living cells.

It suggests a more scalable and flexible approach to molecular computing, opening up possibilities for creating autonomous chemical systems that can process information and respond to their environment without external electronic control.

Prof. Huck expressed his team's interest in this field, saying, "Can we embed reservoir computing into chemical systems that sense their environment, process this information, and take correct action?

"This would require coupling the reservoir to other elements that can translate the output of the chemical brain to some form of mechanical response or into an interaction with living cells, for example."

The research also has intriguing implications for the origin of life. The emergent computational properties of this relatively simple chemical system might provide insights into how early biological systems could have developed information processing capabilities.

Prof. Huck mentioned that this was his primary motivation for studying reservoir computation.

The research team also sees potential in neuromorphic computing, which mimics the neural structure and functioning of the human brain to improve computational efficiency and power.

"We are very interested in exploring the technological limits of the computing power of the formose reservoir computer—this is ongoing research in collaboration with IBM Zurich. Reservoir computing is an example of neuromorphic computing, which has gathered interest as it is expected to consume less energy than conventional computers," explained Prof. Huck.

More information: Mathieu G. Baltussen et al, Chemical reservoir computation in a self-organizing reaction network, *Nature* (2024). DOI: 10.1038/s41586-024-07567-x