

## Current Science Reports

### Coupled Auto-catalytic Reactions *Travelling waves and spatial patterns*

When the product of a chemical reaction acts as catalyst for the reaction, the rate of reaction goes up. And, when the reaction rate goes above a critical value, strange things happen. The Belousov–Zhabotinsky reaction is a typical well-known auto-catalytic reaction and has attracted a lot of researchers from the last century because of the spatial and temporal patterns that it generates. The patterns form spontaneously by coupling chemical reaction to diffusion.



Image: Stephen Morris via Flickr

What if there were two autocatalytic reactions and what if they were coupled, wondered S. Pushpavanam and team at IIT Madras. What if the product of the reactions acts as catalyst for the other reaction?

The corresponding dynamical equations are coupled differential equations. To understand the chemical kinetics of this system, they adapted singularity theory and bifurcation analysis.

Based on the kinetics of the chemical reactions, the researchers identified two cases that are quadratic and cubic in nature. By carefully analysing those equations, they realised that a well-mixed or homogeneous system can indeed produce a very high concentration of the specific species where only one of its isomers is produced from the precursor.

Additionally, this system, when not mixed, exhibits spatial patterns like travelling waves since the reaction is autocatalytic and diffusive in nature.

In biochemical systems there are many autocatalytic reactions which are mostly coupled to other such reactions. This analysis of coupled chemical reactions may be used to explain compartmentalisation within cells. But more importantly, it gives clues to the pharma industries which often find difficulties in producing a specific isomer with the required biological effects.

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### Groundwater Defluorination *Zirconium-impregnated resin*

Fluoride in groundwater is a major concern as large populations worldwide depend on groundwater for drinking and domestic needs. A high concentration of fluoride is harmful and has adverse health effects. There are several fluoride removal techniques but each with its own limitations. Cost-effective defluorination techniques can play a critical role in high fluoride areas to minimise public health risk.

Polymeric ion exchange resin has been used for fluoride removal. But the defluorination capacity of polymeric ion exchange resin is reduced by other anions such as sulphate, and chloride that may also be present in groundwater.

Fluoride is a highly electronegative ion and electropositive elements-based substances can help remove fluoride from water. Zirconium is a highly electropositive element. So Sanjay Singh and Sanjeev Chaudhari from IIT Mumbai in collaboration with researchers from the US decided to try zirconium impregnated resin for removing fluoride from water.

The researchers impregnated zirconium dioxide nanoparticles on polymeric anion exchange resin. The scanning electron microscopy image of the adsorbent indicated the presence of zirconium on the resin surface. The material had high surface area – more than thirty square metres per gram!

The adsorption isotherm analysis promised that the material had higher fluoride ion adsorption capacity than other commonly used adsorbents. The adsorption was endothermic. So in-

crease in temperature increased adsorption. The researchers realised that an increase in pH and the presence of bicarbonates reduce the resin's adsorption capacity. So they decided to use a weak acid cation exchange resin before the water to be treated enters the zirconium hybrid polymer anion exchange resin.

Using this two-column setup, they conducted batch studies and found that about 60 per cent of fluoride can be removed within 30 minutes, but it takes about three hours to reach equilibrium.

The team then used groundwater samples with more than permissible fluoride concentration from Piraya, Nagpur district, Maharashtra to test defluorination efficiency in a continuous flow type reactor.

The defluorination capacity is much better than that of other fluoride removal adsorbents, say the researchers. According to them, zirconium-impregnated hybrid anion-exchange resin has a very high defluorination capacity of more than 8 milligrams per gram.

The hybrid resin can be regenerated by flushing the fluoride with sodium hydroxide and sodium chloride solution.

Ion exchange-based adsorption techniques are widely accepted and popular for fluoride removal as they are simple to operate and minimum waste is generated in the process. The approach suggested by the scientists removes the excess total dissolved solids from brackish groundwater as well.

Now large-scale field trials need to be done with working modules for providing safe drinking water in fluoride-affected areas. Any takers?

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### Mercury-contaminated Sites *Phytoremediation by Indian mustard*

India produces 180 million tonnes of fly ash. Most of it ends up in dumping sites. Fly ash has significant concentrations of mercury. Various physico-chemical and biological methods

have been used to remediate mercury in fly ash dumping sites. But they generate toxic by-products, require skilled personnel and are expensive.

Scientists from IIT-Dhanbad and the Ural Federal University, Russia propose phytoremediation using Indian mustard, *Brassica juncea*, for fly ash-contaminated sites. The plant easily grows in metal-rich soils with limited nutrients and has been found to remediate lead, cadmium, nickel, and other metals. Researchers have also reported the plant's tolerance to mercury.



Image via Wikimedia Commons

The team collected samples of fly ash from the Chandrapura thermal power plant. The fly ash consisted mostly of the oxides of silica, aluminium and iron. They mixed fly ash with mercury-free garden soil in different proportions and germinated mustard seeds in pots for three months.

In the garden soil, 98% of the seeds germinated. With increasing percentages of fly ash in the soil, the germination potential decreased. In 100% fly ash soil, leaves showed chlorosis after two months and, in three months, the plant perished.

The researchers tested the plant's growth parameters. Root: shoot elongation ratio and dry biomass increased with time and were maximum for soils containing a maximum of 50 per cent fly ash.

The metal accumulated primarily in roots followed by stem and leaves. The amount of mercury taken up increased with time.

The garden soil was acidic and the fly ash soil was alkaline. The team points out that with decrease in pH, the mobility of mercury increases. The amount of organic matter in the soil can also impact mercury uptake.

So, controlling the pH and organic matter can help increase the plant's remediation property.

The scientists suggest that mercury is not a limitation for the growth of *B. juncea*. Indian mustard is an excellent bioaccumulator for phytoremediating fly ash-contaminated soils when grown in equal ratios of fly ash and garden soil, they say.

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### Banana Agrosystem Managing pseudostem weevil

The pseudostem weevil, *Odoiporus longicollis*, plays havoc in the banana agrosystem. Dark weevils of about 3 or 4 centimetres lay eggs in slits made on the pseudostem's leaf sheath. The larvae tunnel through the pseudostem, destroying the plant internally. If not managed, the infestation can destroy the whole crop.

The traditional technique of management uses pesticides. But some pesticides are quite harmful to the environment and toxic to humans.

The pseudostem weevil can be managed by *Metarhizium majus* – a fungus that is pathogenic to insects but not harmful to plants or other animals. Can it be used in conjunction with chemical pesticides? If that can be done, the amount of chemical pesticides used can be reduced and the chances of the pest developing resistance to the chemical pesticide can also be reduced.

T. Sivakumar from Krishi Vigyan Kendra along with T. Jiji and A. Naseema from the Kerala Agricultural University decided to study the interaction between fungus and different agro-chemicals to look for the right combination.

They experimented with twelve pesticides to examine their effect on fungal growth, sporulation and viability. They introduced fungal discs cut from actively growing cultures of *Metarhizium majus* into petri-plates with different pesticides and a control plate with no pesticides.

The growth of the fungi was measured once in two days for 30 days. The researchers found maximum growth on neem soap, followed by thiamethoxam.

Next they studied the effect of pesticides on the fungal spores. They cut the discs from all the plates after 21 days of fungal introduction and mixed the discs in sterile water. Then they counted the fungal spores under a microscope. Total spore count showed maximum spore production with thiamethoxam closely followed by neem soap.

Finally, they checked the effect of pesticides on the viability of spores. For this they allowed the spores to grow on the petri dishes for four days at approximately 28°C. The total spore count is not ideal to estimate the effect of chemicals as the dead spores also get included in the counting. Therefore, they tested the viability of the spores. Spore viability of the fungus was most with thiamethoxam.

Therefore, thiamethoxam or neem soap, in combination with *Metarhizium majus*, can be safely applied for controlling pseudostem weevil in banana cultivation, say the investigators.

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### Intelligent Packaging For chicken and fish

Fish and chicken are perishable. So they are generally packaged and refrigerated. Even when packaged and stored in most hygienic conditions, fish and chicken undergo endogenous enzymatic degradation. And consumers cannot get to know till the package is opened.

Sweetie R. Kanatt from BARC, Mumbai recently reported an intelligent packaging material for fish and chicken that indicates the freshness of the product by change in colour.

She used amaranthus leaf extract for the purpose. The extract contains betalain colour pigments which act as indicators. When the pH goes beyond six, the extract's colour changes to light pink. When the pH is increased further, it turns yellow. Since spoilage of chicken and fish leads to an increase in pH, why not use amaranthus leaf extract as spoilage indicator, she thought.

She washed, dried, and powdered amaranthus leaves. And mixed the powder in distilled water, and

centrifuged and filtered the extract. Then, she made the packaging film with polyvinyl alcohol, gelatin and the extract.

When the extract is incorporated into the film, thickness increases by about sixty micrometres. The film's tensile strength improves and the packaging becomes more resistant to puncturing by sharp objects. Useful properties when food has to be transported.

The opacity of the film also increased when the extract was incorporated. This helps reduce light-induced degradation of food, Sweetie explains. UV light, especially, is more strongly absorbed by the film when the extract is incorporated.

Moreover, swelling due to adsorbed moisture is also reduced when the extract is incorporated – useful for refrigerated food packaging.

The extract has antibacterial and antioxidant properties. Will these properties show up in the packaging? Sweetie examined the bacterial count. While fish and chicken packaged in ordinary film showed an increase in bacterial count by the third day, this was not significant even on the 12th day in fish packaged with film incorporating the extract. The extract-incorporated packaging reduced the oxidative rancidity of the products.

The use of the extract slowed down the increase in the pH of fish from three to 12 days. This was reflected by a change in the packaging's colour.

So we now have packaging that increases shelf life and signals spoilage. If that is not good news for the food packaging industry, what is?

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### **Fighting Obesity-related Disorders** *Calcium-enriched diets*

Obesity is a modern day lifestyle condition which predisposes one to the risk of other diseases. The extra storage of fats hinders the proper functioning of the body, leading to higher risk of hypertension, diabetes and cardiovascular diseases.

In this decade, there is some evidence to show that higher calcium in-

take reduces the risk of obesity. But does higher calcium intake reduce the risk of associated diseases? Sandeep Das and Dipayan Choudhuri at the Tripura University were curious. So they investigated the role of dietary calcium, in obesity-related diseases.

To induce obesity, the researchers fed 30 Wistar rats a high fat diet for 12 weeks. Then the obese rats were divided into three groups. Ten were fed a calcium-enriched high fat diet, ten received a high fat diet and ten were fed a calcium-deficient high fat diet. This part of the experiment which lasted 12 weeks included another group of 10 rats as controls which were fed a normal diet.

Throughout the experiment, weekly weight measurements and daily food consumption were recorded. The researchers found that even without any difference in daily food intake, the final body weight of obese rats with calcium-enriched diet was less than that of the other obese rat groups.

At the end of the experiment, the researchers tested samples of blood, and adipose and liver tissues from all the rats. The rats on a calcium-enriched diet had lower glucose and insulin levels, and better glucose tolerance. Their adipose tissue and liver masses were also less than those of the other two obese rat groups, suggesting less fat storage and better insulin production and metabolic breakdown of fat.

With the available data, the researchers now propose a complete pathway to explain how dietary calcium may help reduce the risk of insulin resistance, improve glucose tolerance and reduce cardio-vascular disease risk.

Besides confirming the role of dietary calcium in obesity, the researchers show that it reduces the risk of insulin resistance and diabetes – at least in obese rats.

Although the results provide hope for the obese with an easy alternative to keep a check on their weight, further testing and trials are required to understand and eliminate any risk or side effects associated with a calcium-enriched diet.

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### **Transmission Dynamics** *Modified Nipah model*

After the first reported cases in the Nipah village, Malaysia in 1999, the Nipah virus has caused many deaths in Asian countries. The transmission of the virus is not only from human to human, but also from animal reservoirs of the virus. Researchers do not yet have a suitable model to understand and predict the transmission dynamics of the virus.

Stochastic and deterministic approaches have been used to model this problem. The deterministic approach, using the classical differential operator to describe the dynamics of the virus, cannot capture the heterogeneity. The stochastic approach which assumes a Markovian process that is not dependent on the previous states also does not describe the phenomenon adequately.

Praveen Agarwal from the International Center for Basic and Applied Sciences, Jaipur and Ram Singh, BGSB University, Rajouri recently analysed the system, breaking it down into seven compartments: the virus, uninfected but susceptible bats, infected bats, bats capable of transmitting infectious virions, susceptible uninfected human population, exposed humans and infected humans. Thus they had seven distinct equations. Instead of using the classical differential equations, they used fractional differential equations that have proved successful in describing many natural phenomena.

The scientists replaced the local time differential operator with a differential operator using the Mittag-Leffler function, a special complex function that has proved to be a better filter than the exponential and power law functions for analysing such complex phenomena. And they could prove that it has non-negative solutions, that it shows possibilities of disease-free equilibrium, and that there are endemic equilibrium solutions which are stable.

They also tried the Atangana–Baleanu fractional derivatives, useful for modelling real world complex phenomena. Though more complex than the modelling done using the

Mittag-Leffler function, the researchers could solve the model numerically.

The models are now ready for testing in the original scenario, with real epidemiological data.

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### Detecting Parkinson's Disease Handwriting, age and sex

Parkinson's disease is a progressive disorder of the nervous system. It starts with tremors in the body but affects the movement, balance and coordination later on.

Early detection makes treatment easier. Available methods – imaging-based approach, speech or sensor-based gait analysis – are costly and call for specialized instruments and skills.

Deepak Joshi and team from IIT-Delhi reasoned that tremors would show up early enough in handwriting. They took handwriting samples from people with and without Parkinson's disease. The sample had both males and females of varying ages.

The researchers characterized the digitized handwriting samples using features such as x–y coordinates, timestamp, button status, pressure, tilt and elevation. And they extracted the kinematic, entropic, and energetic features from the handwriting signals.

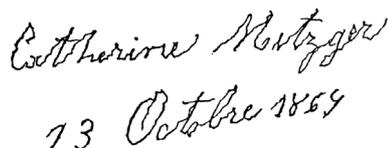


Image via Wikimedia Commons

Since the input feature data was large, they reduced it by removing redundant features using the Mann–Whitney U-test. Further, to investigate the sensitivity of the model for the number of features added and the order in which the features were added, they used the support vector machine ranking method. Though the results were encouraging, accuracy was low.

So, they considered the sex of the writers in classification and found that accuracy improved from 76% to 84%

with the female-specific classifier. When age-specific data was used, the accuracy improved to about 80% with the old-age dependent classifier. When age and sex information were both fed, 96% accuracy was achieved with the young female class.

But increasing the number of groups reduced the number of samples for training and testing in each group. Larger and more balanced datasets can further improve identification accuracy.

The trained model can identify Parkinson's patients at early stages with reasonable accuracy and does not require additional resources. Entrepreneurs can now create an app based on the approach to help clinical practice for the early detection of Parkinson's disease.

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### Automatic Cancer Detection From histopathology images

Histopathology imaging plays a significant role in cancer detection. The identification/detection of deformations in nuclei structure can help classify cancer. However, in histopathology images, nuclei often overlap, limiting the classification's dependability.

To improve upon the histopathology imaging method, recently, researchers from the Maulana Azad National Institute of Technology, the Jawaharlal Nehru Cancer Hospital and Research Center and the All India Institute of Medical Science, Bhopal used nuclei localization as a pre-processing step. The nuclei are stained darker, so that is simple. Then the images are converted to the grayscale format and enhanced. By applying the Gaussian of the difference between the two images and by applying Laplacian and Hessian transformations, the nuclei overlaps are identified. Thus each nucleus is initialised.

Now the problem is to estimate the boundary of each nucleus. The team used the normalised graph cut method to overcome the problem. To clarify the edges, they used the edge detection of small unit segments and took the weighted mean of all the edges.

Then they extracted a set of hundred and fifty shape features and created a bag of visual words to describe them.

In tumours, the size of the nucleus increases, the shape becomes irregular and the uniform staining of the nucleus gains heterochromatic regions. So the team separated the euchromatic and heterochromatic regions and applied nearest neighbourhood component analysis to finally extract 20 significant features from the localized images of nuclei. By applying Bayesian optimisation to small sets of training data, they determined the parameters for robustness.

Now the problem was to classify the images in terms of these features. The team decided to compare support vector machine which requires training and a multilayer perceptron for automatic recognition.

They also took easily available datasets of breast cancer histopathological images as well as a smaller dataset of microscopic images from other organs and analysed the performance. These datasets were used for performance analysis in the localization, classification, and evaluation parameters.

The nuclei localization method was found to be 92 per cent accurate. The multilayer perceptron model had the best accuracy of 95 per cent for cancer classification. The method is a significant improvement over earlier ones, say the researchers.

The method when converted into apps does not require human expertise and could be used in resource-poor clinical settings to accurately detect and classify cancer diagnosis.

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