Belousov-Zhabotinsky Reaction

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Background

We normally think of chemical reactions as reaching an equilibrium after some amount of time, but this is not always the case

There can also be chemical reactions that oscillate

- results of one chemical reaction become the reactants of another reaction
- the next reaction produces the initial reactants

This ends up producing a nonlinear chemical oscillator

Chemical Oscillators

In a general sense, occurs during reactions when the chemical concentrations exhibit periodic changes

Used as an example of non-equilibrium thermodynamics

BZ is one of the few known types of chemical oscillators

Theoretical models for simulating chemical oscillators:

-Lotka-Volterra (predator-prey equations)

-Brusselator

-Oregonator

Studies of BZ reactions

First discovered by Russian Chemist Boris Belousov in the 1950s

-initially could not publish his results because he could not explain the reaction to a satisfactory extent to the editors

-later studied by Anatol Zhabotinsky in the 60s

-BZ is thought to be extremely complex (at least 18 steps)

-in our model we show a simplified version with 3 substrates

Brusselator

-more complex model for chemical oscillators

-involves 4 reactions where two of the concentrations are taken to be constant

$$A \rightarrow X$$
$$2X + Y \rightarrow 3X$$
$$B + X \rightarrow Y + D$$
$$X \rightarrow E$$

$$\frac{d}{dt}\{X\} = \{A\} + \{X\}^2\{Y\} - \{B\}\{X\} - \{X\}$$
$$\frac{d}{dt}\{Y\} = \{B\}\{X\} - \{X\}^2\{Y\}$$

where instability can be seen when B > 1+A**2

Oregonator

Designed to simulate the BZ reaction

The simplest model of autocatalytic reactions

Dictated by the differential equations:

$$\epsilon\frac{\partial u}{\partial t} = u(1-u) - \frac{u-q}{u+q}fv + D_u\Delta^2 u$$

$$\frac{\partial v}{\partial t} = u - v + D_u\Delta^2 v$$

where u and v represent the concentrations of two chemicals

-activator and inhibitor (See notebook)

https://www.youtube.com/watch?v=PnOy1fSxBdI

Our BZ animation

-model using 3 chemical rate constants

$$
\begin{array}{ll}
\mathrm{A} + \mathrm{B} \to 2A & \alpha \\
\mathrm{B} + \mathrm{C} \to 2B & \beta \\
\mathrm{C} + \mathrm{A} \to 2C & \gamma
\end{array}
$$

using these, we create a simplified model defining the concentrations after each timestep:

$$
\begin{aligned}
[\mathrm{A}]_{t+1} &= [\mathrm{A}]_t + [\mathrm{A}]_t(\alpha[\mathrm{B}]_t - \gamma[\mathrm{C}]_t) \\
[\mathrm{B}]_{t+1} &= [\mathrm{B}]_t + [\mathrm{B}]_t(\beta[\mathrm{C}]_t - \alpha[\mathrm{A}]_t) \\
[\mathrm{A}]_{t+1} &= [\mathrm{C}]_t + [\mathrm{C}]_t(\gamma[\mathrm{A}]_t - \beta[\mathrm{B}]_t)
\end{aligned}
$$