

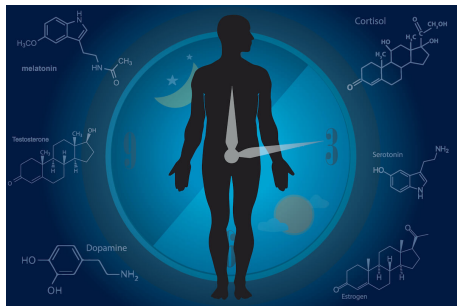
CAN WE BUILD RELIABLE CLOCKS ONLY USING CHEMICAL REACTIONS?

FINAL PRESENTATION - S4

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A QUESTION TO BEGIN



"Everybody has already heard talking about biological clocks. - Who has ever heard talking about chemical clocks?"

FIGURE: An illustration of the biological clock and the hormonal molecules involved - *risescience.com*.

WHAT IS AN OSCILLATION?

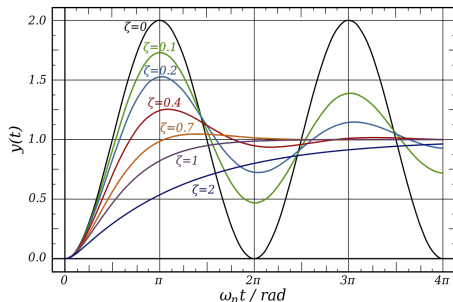


FIGURE: The effect of the damping ratio (ζ) on the oscillations - *Wikimedia Commons*.

A definition :

move or fluctuation around an equilibrium position.

- Harmonic oscillations : constant over time
- Damping : decreasing over time

WHAT IS AN OSCILLATION?

The equation that models the oscillations show their **periodicity/regularity**:

$$A(t) = A_0 \cos(\omega t + \phi)$$

Where A represents a physical quantity, depending on t the time.
 A_0 , ω and ϕ are constants.

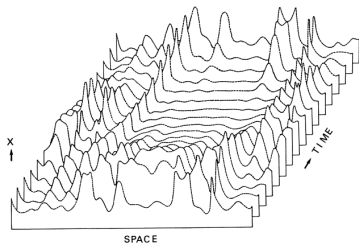


FIGURE: Illustration of the variations leading to chemical oscillations - *Chemical oscillations, waves, and Turbulence*. [2]

The most common oscillators: with iodine

- The *Briggs-Rauscher reaction* : iodine (I_2), malonic acid ($CH_2(CO_2H)_2$) and hydrogen peroxide (H_2O_2).
- The *Bray-Liebafsky reaction* : more simple reaction - iodine and hydrogen peroxide only.

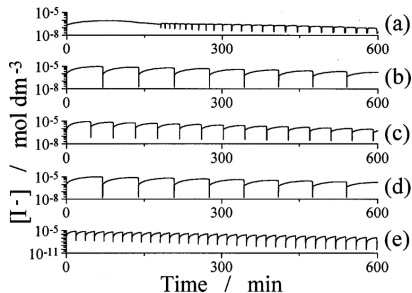


FIGURE: A numerical simulation of the Bray-Liebafsky reaction's behaviour - *Journal of Chemical Physics*. [4]

OTHER CHEMICAL CLOCKS

Candles flames can act as an oscillator

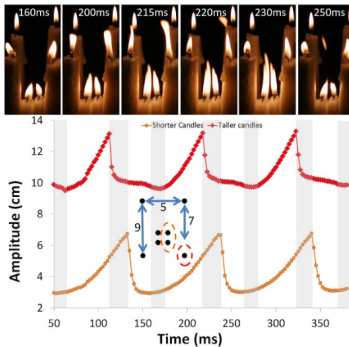


FIGURE: Illustration and study of candle's flames amplitude - *nature.com*. [1]

The Belousov-Zhabotinsky Reaction: uses bromine (KBrO_3) instead of iodine. Shows spatial oscillations.



FIGURE: Picture of the reactional media in Belousov-Zhabotinsky - *Saylor Academy*.

SPECIFICATIONS FOR ANSWERING OUR QUESTION

Let's have a concrete example: **A timer to help children with teeth washing, made with visual chemical oscillating reactions**

- Duration: 2 to 3 minutes after activation
- Periodicity: at most 1 full cycle within the expected duration
- Knowledge of the time: should be easy to understand (children)

ELEMENTS OF ANSWER

The **traffic light reaction**: A redOx reaction, involving color indicators

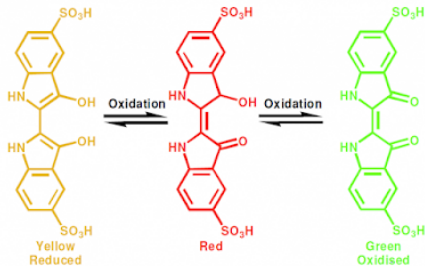


FIGURE: The color variations of the indigo carmine during the traffic light reaction - *According to the NCSUniversity.*

Spectroscopic study possible → determination of the right concentration of reactants → Thus the reaction can last 3 minutes

LIMITATIONS TO THE CHEMICAL REACTIONS

The safety ! In the traffic light experiment:

- Basis at high concentration (NaOH at 0,4 M)
- Harmful chemicals (indigo carmine: skin allergies, ...)

The reaction's requirements In the traffic light experiment:

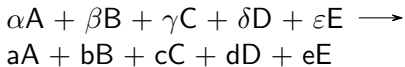
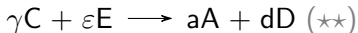
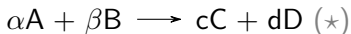
- Stirring during all the reaction
- Replacing chemicals between each experiment

TO GO FURTHER

Existing **links between mathematics and oscillating reactions** kinetics

"Chemistry is essentially a mathematical science" - Linus Pauling (1901-1994) - Nobel prize in chemistry (1954) and peace (1962)

Assuming the reactions :



The stoichiometric coefficients matrix[3] :

$$\begin{array}{ccccc} & \alpha A & \beta B & \gamma C & \delta D & \varepsilon E \\ \begin{array}{c} aA \\ bB \\ cC \\ dD \\ eE \end{array} & \left[\begin{array}{ccccc} X_{\alpha a} & X_{\beta a} & X_{\gamma a} & X_{\delta a} & X_{\varepsilon a} \\ X_{\alpha b} & X_{\beta b} & X_{\gamma b} & X_{\delta b} & X_{\varepsilon b} \\ X_{\alpha c} & X_{\beta c} & X_{\gamma c} & X_{\delta c} & X_{\varepsilon c} \\ X_{\alpha d} & X_{\beta d} & X_{\gamma d} & X_{\delta d} & X_{\varepsilon d} \\ X_{\alpha e} & X_{\beta e} & X_{\gamma e} & X_{\delta e} & X_{\varepsilon e} \end{array} \right] \end{array}$$

Linked to the reactions' speed, for example

$$v_{*} = k_1[A]^{\alpha}[B]^{\beta} = \frac{d[C]}{c \times dt}$$

$$\text{and } v_{**} = -k_2[A]^a[D]^d = -\frac{d[E]}{\varepsilon \times dt}$$

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- [1] Kolar-Anić L. (Bellegarde University) D Čupić Z. (Bellegarde University). "Contraction of the model for the Bray–Liebhafsky oscillatory reaction by eliminating intermediate I 2 O". In: *The journal of chemical physics* (1999).
- [2] Y. Kuramoto (Kyoto University). *Chemical Oscillations, Waves, and Turbulence*. Springer-Verlag, 1984.
- [3] Shanks N. *Modeling biological systems: the belousov–zhabotinsky reaction*. Kluwer Academic Publishers, 2001.
- [4] Forrester D. M. (Loughborough University). "Arrays of coupled chemical oscillators". In: *Openaccess nature.com scientific reports* (2015).