# SYSTEM DYNAMICS MODELING:
# FROM MECHANICS TO CHEMISTRY

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ABSTRACT
In this paper, we discuss a contribution toward the use of analogical reasoning by explicit system dynamics modeling of physical processes. The relational structures found in simple models are transferred to an example of chemical processes leading to chemical equilibrium. We present an experiment on the mutarotation of D-glucose. A dynamical model will be built that makes use of amount of substance and chemical potential differences in analogy to quantities of fluid and pressure differences in fluid phenomena, or electric charge and voltage in electricity. The model is simulated and results are compared to experimental data.

KEYWORDS
Dynamical Systems, Analogy, System-dynamics Modeling, Chemical Reactions, Chemical Potential, Mutarotation of D-glucose.

## 1 – INTRODUCTION

Analogical reasoning is considered a powerful tool for learning and thinking in the sciences (Fuchs, 2006). When dealing with macroscopic dynamical systems, analogical structures in physics emerge quite naturally. Explanations of processes commonly make use of a structure built upon the schema of (potential) differences of intensive quantities, and the schema of amount of fluid-like quantities (extensive quantities). The third element is the schema of force or power which is related to intensity and (fluid-like) quantity, and can be used to form the foundation of our energy principle. We call the overall structure a *force dynamic gestalt* (Fuchs, 2007).

Sadi Carnot’s description of the operation of heat engines serves as an example of this explanatory structure (Fuchs, 1996): *“D'après les notions établies jusqu'à présent, on peut comparer avec assez de justesse la puissance motrice de la chaleur à celle d'une chute d'eau […]. La puissance motrice d'une chute d'eau dépend de sa hauteur et de la quantité du liquide; la puissance motrice de la chaleur dépend aussi de la quantité de calorique employé, et de ce qu'on pourrait nommer, de ce que nous appellerons en effet la hauteur de sa chute, c'est-à-dire de la différence de température des corps entre lesquels se fait l'échange du calorique.”* (Carnot, 1824). Caloric is the fluid-like thermal quantity that falls through a potential difference (temperature difference) and as a result releases energy at a certain rate (power).

To be concrete, intensive and extensive quantities are pressure and volume in fluids, electric potential and charge in electricity, temperature and entropy in heat, and speed and momentum in translational motion.
For the simplest dynamical phenomena that commonly lead to equilibrium, explanations take the following form. A process consists of the flow of a fluid-like quantity (volume, charge, entropy, momentum) from one storage element to another. The flow is driven by a difference of the associated potential (pressure, electric potential, temperature, speed) and persists as long as the potential difference has not reached a value of zero (the relation between flow and potential difference is called flow

characteristic). The potentials themselves depend upon the *amount* of the fluid-like quantity stored in a system, and the storage element itself (capacitive characteristic). Analogies of this type become particularly evident when we use system-dynamics tools to convert the word model presented above into a formal mathematical model (see Fig. 1).

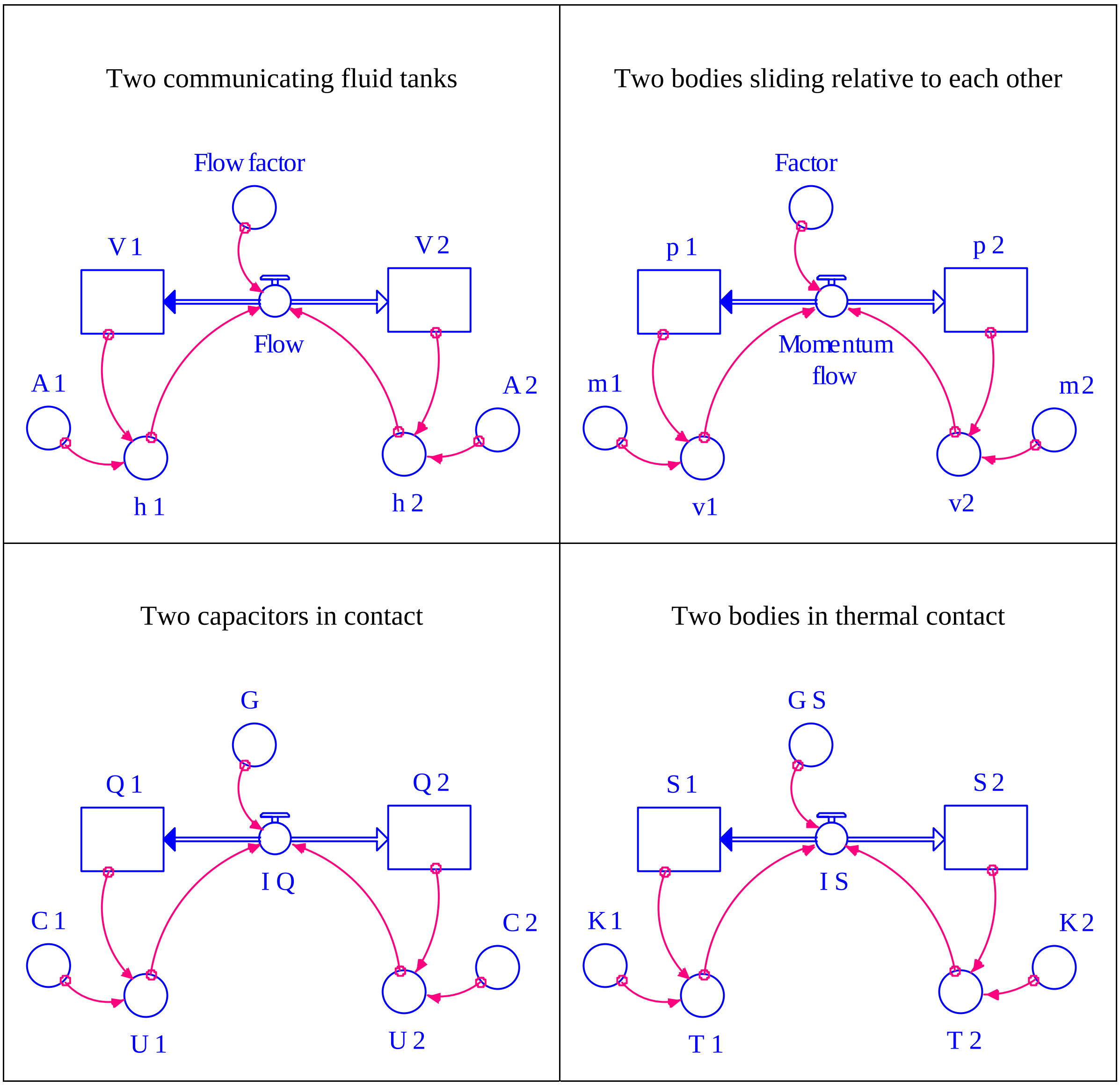

Figure 1. The phenomena of the equilibration of fluid levels, voltages, velocities, and temperatures can be explained with the help of analogous model structures. Rectangles symbolize fluid-like stored quantities; pipelines (fat arrows) stand for transports. (In the case of thermal equilibration, we have left out the production of entropy which, however, is commonly very small compared to the flow of entropy; Fuchs, 2006, p. 172).

These tools make use of a very few elements which allow us to translate our ideas into formal representations. We only need a symbol for stored quantities, another for flows (generally speaking, for rates of processes), and one for formulating special relations such as flow and capacitive laws.

Each of the system-dynamics models presented in Fig. 1 allow us to simulate the behavior of systems which tend toward equilibrium (Fig. 2).

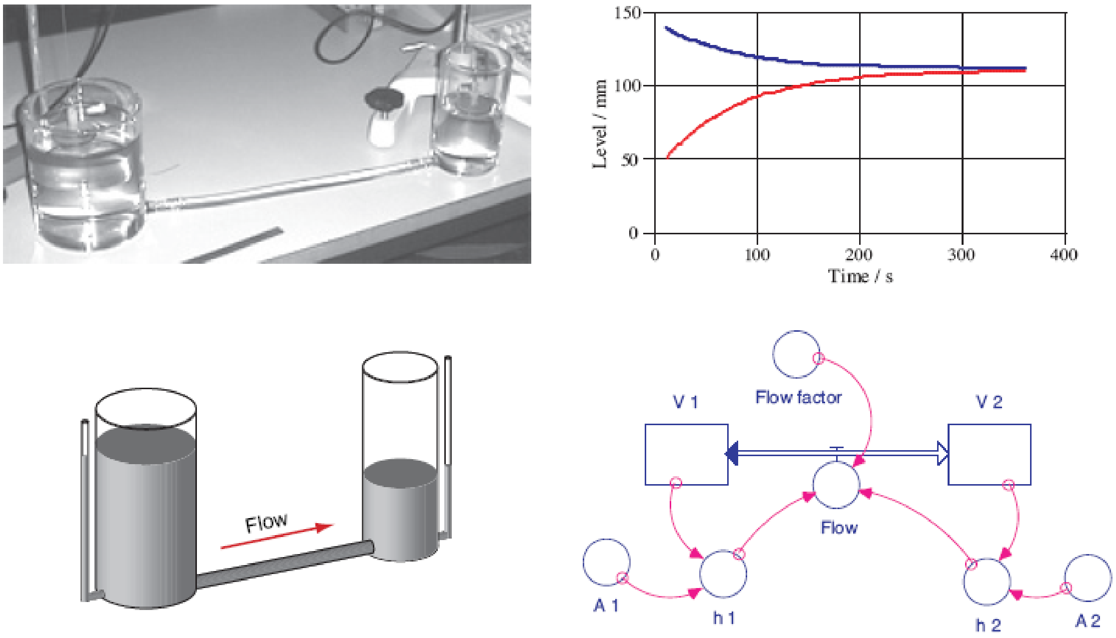

Figure 2. Two communicating oil tanks (top left), data of the equilibration of levels (top right), situation sketch (bottom left) and SD model diagram (bottom right).

Chemical phenomena are no strangers to this explanatory pattern. Chemical reactions running toward equilibrium are common, and the well known quantities of *amount of substance* ($n$) and the *chemical potential* ($\mu$) provide the conceptual background for explanations analogous to those used in fluids, electricity, heat, and motion. This we will demonstrate in the following sections where we consider the phenomenon of mutarotation of D-glucose.

## 2 - EXPERIMENT AND WORD MODEL

Here we present the background on and the results of an experiment measuring the mutarotation of D-glucose. The phenomenon will be explained with the help of a word model that makes use of the form of reasoning discussed in the Introduction.

Figure 3: Apparatus for measuring the rotation of the plane of polarization of light passing through a solution of D-glucose. The angle change in the course of time indicates that chemical reaction is taking place in the solution.

*Background and experimental procedure*

At the beginning of the 19th century, some dissolved substances were observed to rotate the plane of polarization of light (optically active substances, Fig. 3). Biot's law states that

$$\varphi = [\varphi] l c^* \tag{1}$$

Here, $\varphi$ is the angle of rotation, $[\varphi]$ denotes specific rotation of the particular solution (taken at 20°C and with the light of sodium), and $l$ and $c^*$ stand for the distance the light travels in the solution and mass concentration, respectively.

It has been observed that the specific rotation of some solutions can change over the course of time. It tends to assume a particular value which is independent of the initial composition of the solution.[1] It has been found that in such situations the substance under study can exist in two (or more) distinct forms, called anomers, each one characterized by its own specific rotation. In solution the mixture tends towards a well defined composition in equilibrium. The final condition depends upon the nature of the substance under study, the solvent considered, temperature, etc..

In an aqueous solution of D-glucose, these anomers (called $\alpha$-D-glucose and $\beta$-D-glucose) have different optical properties (different specific rotation $[\varphi]$, see The Merck Index, 2006):

$$\begin{aligned} \left[\varphi_\alpha\right] &= +112\,^\circ/\left(\mathrm{dm}\cdot\mathrm{g/mL}\right) = +1.12\,^\circ/\left(\mathrm{m}\cdot\mathrm{kg/m^3}\right) \\ \left[\varphi_\beta\right] &= +18.7\,^\circ/\left(\mathrm{dm}\cdot\mathrm{g/mL}\right) = +0.187\,^\circ/\left(\mathrm{m}\cdot\mathrm{kg/m^3}\right) \end{aligned} \tag{2}$$

For a solution which contains both forms of D-glucose the specific rotation can be expressed as follow:

$$\left[\varphi_{eff}\right] = (1-x)\left[\varphi_\alpha\right] + x\left[\varphi_\beta\right] \tag{3}$$

Where $x = n_\beta / n_{tot}$ is the $\beta$-D-glucose molar fraction. 1–$x$ stands for the molar fraction of $\alpha$-D-glucose. The time evolution of the angle measured in a typical experiment is reported in Fig. 4 (left). From the foregoing we easily obtain the molar fraction $x$:

$$x = \frac{\left[\varphi_\alpha\right] - \left[\varphi_{eff}\right]}{\left[\varphi_\alpha\right] - \left[\varphi_\beta\right]} \tag{4}$$

In order to obtain the time dependence of the chemical amounts we must remember that Biot's law involves mass concentrations $c^*$. Expressed as molar concentration $c$ we obtain

$$\begin{aligned} n_\beta(t) &= Vc_\beta(t) = Vc_{tot}x(t) = \frac{Vc^*_{tot}}{M}x(t) \\ n_\alpha(t) &= Vc_\alpha(t) = Vc_{tot}\left(1-x(t)\right) = \frac{Vc^*_{tot}}{M}\left(1-x(t)\right) \end{aligned} \tag{5}$$

for the amount of substance of the two forms of D-glucose as functions of time. The result of our experiment is shown in the graph on the right of Fig. 4.

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[1] See W. Pigman and H.S Isbell (1969) which refers to the pioneering works of A.P. Dubrunfaut (1846) and L. Pasteur (1848). H.T. Lowry (1899) first introduced the term mutarotation.

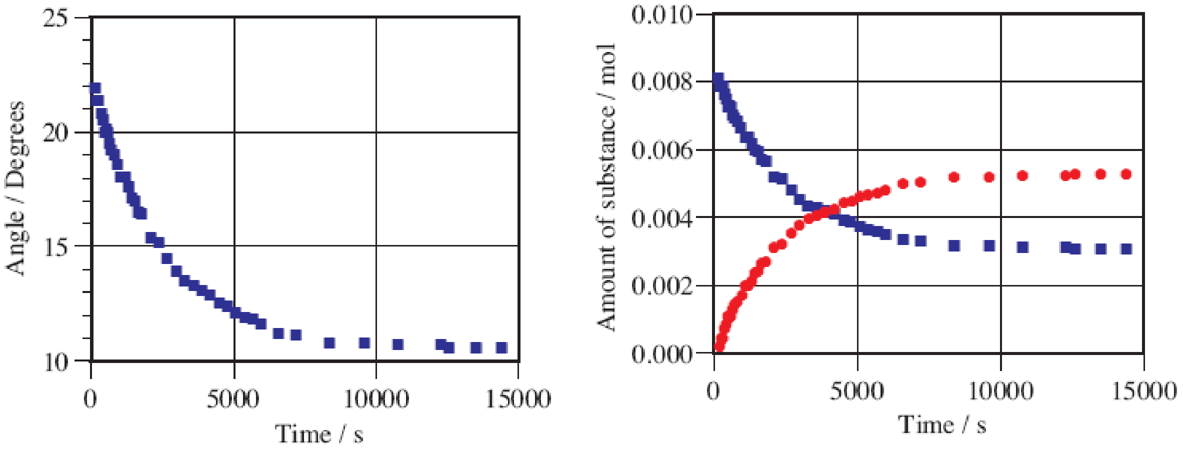

Figure 4: Angle of optical rotation measured in a typical experiment showing the mutarotation of D-glucose (left). The data has been transformed to obtain the amount of substance of $\alpha$- and $\beta$-D-glucose (right). We prepared 100.0 g of an aqueous solution containing 10.0 g of pure $\alpha$-D-glucose. The length of the optical path was 20.0 cm (see Fig. 3). Data was taken at room temperature.

*A word model*

Three things can be observed in the experiment. Firstly, the process runs fast at the beginning, slowing down as time goes on and, secondly, the reaction which leads to a change of the quantities of $\alpha$ and $\beta$–D–glucose reaches equilibrium. Finally, in equilibrium, neither the amount of substance nor the concentration of the two species have become equal. Since we have seen curves of the type presented in the diagram on the right of Fig. 4 in other phenomena in physics, it seems reasonable to use the same type of explanation for the present phenomenon.

The quantity of $\alpha$-D-glucose in solution decreases with time since some of it converts into $\beta$-D-glucose. As a result, the amount of $\beta$-D-glucose increases. The rates of change of amount of substance are equal to the rate of production or destruction of $\beta$- and $\alpha$-D-glucose, respectively. We now assume that the reaction rate depends upon the difference of an intensive chemical quantity. This difference will become zero in equilibrium. Obviously, the quantity in question *cannot* be the *amount of substance* (Fig. 4, right). We might be surprised, however, to find that the concentration of the substances is not the quantity we are looking for either. Rather, the intensive quantity is the *chemical potential*. The dependence of the chemical potential upon the concentration must be such as to make the potential difference vanish in equilibrium. If we assume that the chemical potential of a dissolved substance increases with increasing concentration, we now understand the slowing down and eventual halting of the reaction: The initial potential difference that drives the reaction becomes smaller as time goes on.

## 3 - CHEMICAL POTENTIAL OF DILUTE SOLUTIONS

The solutes of dilute solutions contribute to the pressure of the solution in a manner that is analogous to that of dilute (i.e., ideal) gases (see Fuchs, 1996, p. 496 for details):

$$p_s = RcT \tag{6}$$

Here, $R$ is the universal gas constant, and T is the (Kelvin) temperature of the solution. Since the chemical potential of ideal gases is

$$\mu(T,p)=\mu(T,p^0)+RT\ln\left(\frac{p}{p^0}\right) \tag{7}$$

(Fuchs, 1996, p. 478), an analogous relation holds for the chemical potential of the dissolved substance:

$$\mu(T,c)=\mu(T,c^0)+RT\ln\left(\frac{c}{c^0}\right) \tag{8}$$

$c^0$ is the standard value of concentration. This expression can be used to derive the relation of concentrations of two interacting (reacting) species in (chemical) equilibrium. We consider a reaction

$$\mathrm{A} \rightarrow \mathrm{B}$$

Since the difference of the chemical potential of the species must vanish in equilibrium, i.e.,

$$\mu_{\mathrm{A}}^0+RT\ln\left(\frac{c_{\mathrm{A}}^{eq}}{c^0}\right)=\mu_{\mathrm{B}}^0+RT\ln\left(\frac{c_{\mathrm{B}}^{eq}}{c^0}\right)$$

we have

$$\frac{c^0}{c_{\mathrm{A}}^{eq}}\frac{c_{\mathrm{B}}^{eq}}{c^0}=\mathcal{K} \tag{9}$$

where the equilibrium constant $\mathcal{K}$ is related to the chemical potential difference of the species for standard conditions:

$$\mu_{\mathrm{B}}^0-\mu_{\mathrm{A}}^0=-RT\ln\left(\mathcal{K}\right) \tag{10}$$

Note that since the standard concentrations of A and B are the same, the equilibrium constant equals the ratio of the equilibrium concentrations.

The case of mutarotation of D-glucose (Fig. 4) allows us to determine the numerical value of the chemical potential difference. Since, according to our data, $\mathcal{K}$ = 1.74, this difference turns out to be roughly – 1.36 kJ/mol at 295 K (temperature of the solution in the experiment). The value of the equilibrium constant calculated from the literature is 1.75 (The Merck Index, 2006).

## 4 - A SYSTEM-DYNAMICS MODEL OF MUTAROTATION

The word model presented above and our knowledge of the dependence of the chemical potential upon the concentration of a species of D-glucose lets us construct a simple system-dynamics model of the process of mutarotation (Fig. 5).[2]

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[2] We assume here that mutarotation of D-glucose can be treated as a direct reaction of $\alpha$-D-glucose into $\beta$-D glucose. This can be done since an intermediate form appearing in reality exists only in very low constant concentrations (Rasiel and Freeman, 1970).

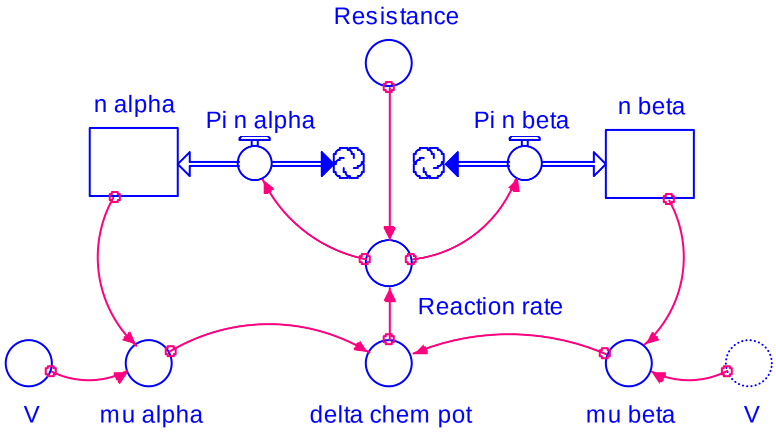

Figure 5: Diagram of a system-dynamics model representing the ideas expressed in the word model describing the phenomenon of mutarotation. Note the laws of balance of amount of substance for $\alpha$-D-glucose and $\beta$-D-glucose (rectangles and flows), the determination of the chemical potentials from the amounts, of the chemical potential difference from the chemical potentials, of the reaction rate in terms of the chemical potential difference, and of the production rates in terms of the reaction rate. The model diagram was constructed in Stella.

The model consists of the two laws of balance for $\alpha$-D-glucose and $\beta$-D-glucose

$$\frac{dn_\alpha}{dt} = \pi_{n\alpha} \quad , \quad \frac{dn_\beta}{dt} = \pi_{n\beta} \tag{11}$$

The production rates $\pi_{n\alpha}$ and $\pi_{n\beta}$ are directly related to the reaction rate $\pi_R$, where the concrete relation is a result of stoichiometry. In our case we have

$$\pi_{n\alpha} = -\pi_R \quad , \quad \pi_{n\beta} = \pi_R \tag{12}$$

Furthermore, the constitutive relations for the chemical potential difference is

$$\Delta\mu = RT\left[-\ln\left(\mathcal{K}\right) + \ln\left(\frac{c_\beta}{c_\alpha}\right)\right] \tag{13}$$

and the reaction rate is determine by

$$\pi_R = -\frac{1}{R_n}\Delta\mu \tag{14}$$

The last relation assumes the simplest form of a reaction driven by a chemical potential difference, namely, a rate proportional to the driving force. If we assume such a relation for the chemical reaction, we have to introduce a reaction constant. This can be done in the form of a *reaction resistance* $R_n$ (which is constant) as shown in Eq. (14). Whether or not the relation describes the actual progress of the reaction well enough can only be determined by comparing actual data to results of the simulation of our model. Quite obviously, for the present reaction, the assumption of a linear reaction law is satisfactory (Fig. 6).

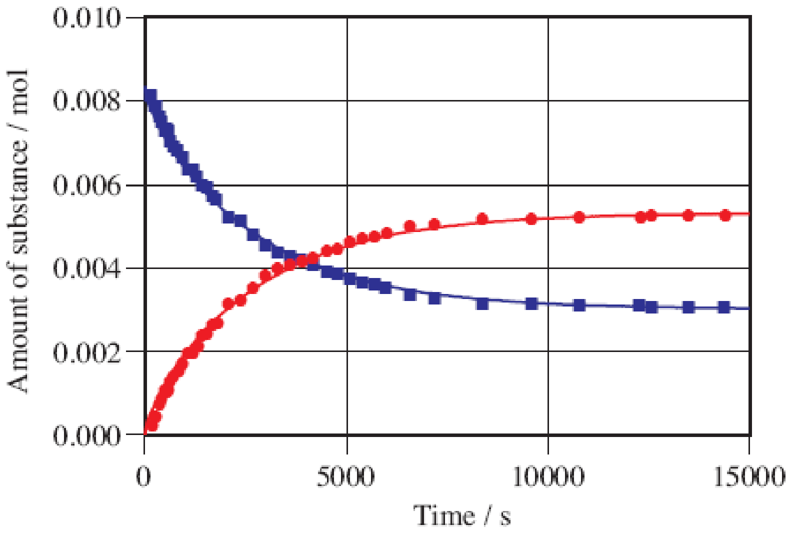

Figure 6: Data of the experiment and simulation results of the model presented in this section. Note that the linear form (linear in the difference of the chemical potential) of the reaction rate is satisfactory. The model was implemented and simulated in Berkeley Madonna.

## 5 - FORMAL CONSIDERATIONS

In chemical kinetics, a different expression for the reaction rates is commonly used. In the case of a reaction

$$\mathrm{A} \rightarrow \mathrm{B} \tag{15}$$

the simplest form of the production rate of species A is

$$\pi_{n\mathrm{A}} = -k\left(\mathcal{K} c_{\mathrm{A}} - c_{\mathrm{B}}\right) \tag{16}$$

$c$ stands for the concentration, and $k$ is a constant for this first order reaction. Note how this form follows from our intuitive model that uses the chemical potential difference as the driving force of the reaction. We simply linearize the expression for the chemical potential difference for conditions near equilibrium. If we use the equilibrium condition (*eq*) as the reference point for expressing the potentials, we have

$$\begin{aligned} \Delta\mu &= \mu_{\mathrm{B}}^{eq} - \mu_{\mathrm{A}}^{eq} + RT \ln\left(\frac{c_{\mathrm{B}}}{c_{\mathrm{B}}^{eq}}\right) - RT \ln\left(\frac{c_{\mathrm{A}}}{c_{\mathrm{A}}^{eq}}\right) \\ &= -RT \ln\left(\frac{c_{\mathrm{A}}}{c_{\mathrm{A}}^{eq}} \frac{c_{\mathrm{B}}^{eq}}{c_{\mathrm{B}}}\right) \approx RT\left(\frac{c_{\mathrm{A}}^{eq}}{c_{\mathrm{A}}} \frac{c_{\mathrm{B}}}{c_{\mathrm{B}}^{eq}} - 1\right) = RT\left(\mathcal{K}^{-1} \frac{c_{\mathrm{B}}}{c_{\mathrm{A}}} - 1\right) \end{aligned} \tag{17}$$

We can assume the production rate $\pi_{n\mathrm{A}}$ to be proportional to the concentration of the species A. This finally leads to an expression of the form

$$\pi_{n\mathrm{A}} = k^{'} c_{\mathrm{A}} \Delta\mu = k^{'} c_{\mathrm{A}} RT\left(\mathcal{K}^{-1} \frac{c_{\mathrm{B}}}{c_{\mathrm{A}}} - 1\right) = -k\left(\mathcal{K}\, c_{\mathrm{A}} - c_{\mathrm{B}}\right) \tag{18}$$

The result is the same as the typical form found in Eq.(16). This leads to an interesting question of the proper form of a reaction rate in a reaction such as the one discussed here. Since the standard form known from kinetics and our expression are the same near equilibrium, they cannot both hold far from equilibrium. A general decision as to the proper form cannot be made, however (Cukrowski and Kolbus, 2005). We know that Eq. (16) may not hold in general - sometimes nonlinear expressions must be used. So, a discussion whether or not a reaction is proportional to the difference of the chemical potential is pointless - it depends on the concrete case. All we can say is that, in general, constitutive laws for reaction rates and transports are nonlinear. Linear results are special cases. As we know, the same is true in electricity or fluids, i.e., characteristic relations for charge and fluid transports are nonlinear in general. The example of mutarotation of D-glucose can be satisfactorily dealt with by using the linear form with respect to the chemical potential difference.

## 6 - SUMMARY AND OUTLOOK

We have demonstrated here that a simple chemical reaction such as mutarotation of D-glucose can be successfully modeled using comparisons with electrical, hydraulic, mechanical, or thermal dynamical processes. Analogical reasoning suggests that the process (quantified in terms of a reaction rate) should depend upon a kind of driving force. In the case of fluids, electricity, heat, or motion, the driving force is a potential difference. The well known chemical potential serves a role analogous to pressure, electric potential, temperature, or speed, and the chemical potential difference of two species serves the role of the driving force of the reaction between the substances.

It seems to us that learning in chemistry and biology would greatly profit from an approach that makes use of direct system-dynamics modeling. As we have shown, analogical reasoning is at the core of SD modeling, i.e., different processes are represented by the same formal structures. In other words, our approach allows us to integrate not only different fields of physics, but also phenomena that go beyond physics proper, such as chemistry and biology. This can create a unity of subjects that are part of secondary education to an extent not normally seen in our schools. Since modeling commonly calls for experimental verification, this may well lead to more and stronger quantitative activities in the teaching of chemistry and biology (D’Anna, 2006). In fact, driven by modern computer technology and data acquisition, we have already seen a growth of experimental activities in the sciences ranging from physics through chemistry and biology all the way to applications such as physiology and environmental science. We believe that these activities would profit greatly from being supported by explicit system-dynamics modeling.

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