STUDENTS WORKING ON MODELS; AN ON-GOING EXPERIMENTATION IN MATHEMATICS AND CHEMISTRY

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This paper focuses on modelling at upper secondary level. The objective is to give students an understanding of mathematical concepts and methods in close relationship to a domain of reality, as well as to give them insight into the contribution of models of different kinds. This has led to the development of a framework for modeling activities based on the Mathematical Working Spaces theory. The questions at stake concern the operationality of this framework. To what teaching situations can it lead? How do students work in these situations? We examine these questions through an on-going experimentation on models of acid-base transformations.

APPROACHES TO MODELING IN MATHEMATICS EDUCATION AND SCIENCE DIDACTICS

Beginning in the 2000s, interest in involving real-world contexts has grown in mathematics education. The ICMI 14 study (Bloom 2002) kicked off a lively stream of research and focused on mathematics as an important activity in society. This stream seems to us marked by two lines of force, problem solving and the modeling cycle as a theorization of the modeling activity. Many authors indeed characterize modeling activities as solving authentic problems, but the activities they propose focus more on the solution to a contextualized problem than on models. For example, in Blum and Ferri (2009), the task involves a lighthouse of a given height and students have to find a value for the visibility distance that is valid specifically for that height. The authors identify steps in students' problem solving consistent with the modeling cycle, but these steps lead to the solution rather than to a model. Overall, the modeling cycle remains close to a classical resolution scheme where the problem and the solution are expressed at the extra-mathematical level and solving is done at the mathematical level. The cycle specifies steps and transitions and this allows, among other things, the interpretation of students' trajectories in their complexity. Nevertheless, the "real" and the "mathematical" remain two levels insufficiently intertwined to account for how working on a model articulates mathematics and real-world objects and phenomena (Czocher 2018).

In experimental science didactics, the main concern is the relationship between an "empirical referent" (Sanchez 2008) made up of objects and phenomena as they are perceived and spontaneously mobilized by the students, and a "scientific referent" consisting of theoretical elements. By appropriating a model, the students can relate these two referents and thus progress both in their perception of everyday objects and

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phenomena and in their understanding of scientific concepts. Nevertheless, the mathematical aspects of the model are generally not questioned as such, and science didactics privileges models where these aspects are minor for fear of complexity.

Thus, dominant approaches in mathematics education emphasize problem solving rather than working on models, and science didactics favors appropriation of a model while leaving aside mathematical aspects. Drawing on science didactics, we aim to engage students in explicit work on models, but we also want to include mathematics in this work. The experimentation we are carrying out starts from a laboratory technique taught in the chapter about acid-base reactions of the chemistry course in the non-vocational upper secondary stream in France. Students often describe this technique as “a cooking recipe”, since mathematical methods are used, but not explained with reference to acid-base reaction models. The purpose of the experimentation is then to look for ways to make students study models both in their chemical and mathematical aspects and get a better understanding of these aspects.

APPROACH AND FRAMEWORK

Lagrange et al. (forthcoming) distinguish between modelling and mathematization of a domain. While mathematization is global in scope, modeling aims to account for certain aspects of the domain in order to understand it, even partially, and to act on it. A corollary is that there is not a single model: several models are as many ways to approach a reality. Modeling thus has a subjective and social dimension: all models can be useful, but each one must be discussed and confronted with others. In each model, the contribution of mathematics results from a specific mathematical work, in collaboration with experts in the field, in order to make the model more intelligible and facilitate its use. Thus, there is not a real model on one side and a mathematical model on the other side, but a plurality of models, each with a specific implication of mathematics into the same domain of reality. We consider students’ activity in modelling as a work of appropriation of two or more models, and as a work of uncovering relationships between models, in order both to get better insight into the domain and to progress in the mathematical concepts used; for instance Lagrange (2018) proposed to consider four models of a suspension bridge for a high school teaching project, one based on a study of tensions, a second one on arithmetical relationships, a third one being a computer simulation, and finally a fourth model based on notions in real analysis (functions, integration, etc.).

Modelling implies collaboration between experts with different viewpoints (Lagrange et al. forthcoming) and that is why the above approach has led to organizing students’ work in a "jigsaw classroom". The work starts from a question. For the present study, the question will be about how a model of the reaction justifies the laboratory technique. There are four phases: (1) Presentation of the question and work on prerequisite concepts (2) Expert groups: each group works on a model from a specific viewpoint (3) Jigsaw groups: each group gathers experts from each expert group and progress in understanding the models (4) Whole class discussion and conclusion by the teacher.

Regarding the notion of work in educational settings, we refer to the theory of Mathematical Working Spaces (MWS). According to Kuzniak et al. (2016), a MWS is an abstract space that is organized to support mathematical work in an educational setting[1]. The theory of MWS distinguishes three levels:

- A reference working space (WS) is a space in which somebody educated in a specific domain is expected to do the work in this domain.
- A suitable WS helps manage the work for beginners in a teaching project.
- A personal WS is particular to individuals.

As Menares-Espinoza and Vivier (forthcoming) explain, beginners approach a new domain with their prior knowledge and cognitive processes. Teaching must design tasks to help students' personal WSs evolve towards the reference level and this requires designing suitable WSs. Here a reference WS is what allows for scientific thinking about the laboratory technique. Models on which this thinking can be based are described below. This paper focuses on suitable WSs, both a priori with reference to models of the reaction and a posteriori from student observation, leaving for further research a study of personal WSs.

The research question follows. RQ: What are the suitable WSs that provide a conceptual basis for a mathematical-chemical approach of acid-base reaction models? How do they predict students' behavior and cognitive processes?

MODELS, WORKING SPACES AND TASKS

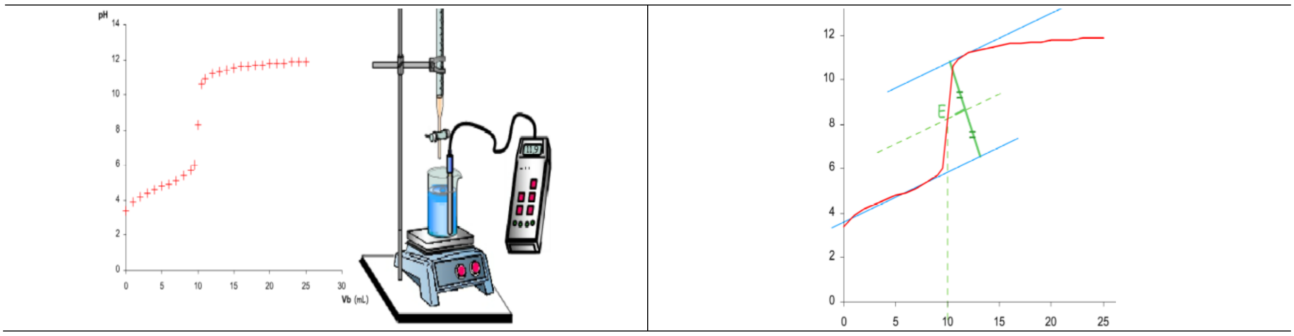

Table 1: The laboratory technique. Empirical procedure and tangent method.

The laboratory technique we start with is titration, i.e. the use of a solution of known concentration (titrant) to determine the unknown concentration of another solution (analyte). The titrant is added from a graduated buret to a known quantity of analyte. In case of an acid-base reaction, the analyte is an acidic solution, characterized by a preponderance of oxonium ions and the titrant is a basic solution characterized by a preponderance of hydroxides ions. During the titration, the oxoniums and the hydroxides react and then the pH (minus the decimal logarithm of the concentration

1 Because of limited space, we do not insist on the three dimensions that structure a MWS: semiotic, instrumental and discursive. However they are important in the domain of modelling, ensuring that mathematics are not simply considered as a "language".

in oxonium) of the mixture increases and a table of values (volume added, pH) is obtained (Table 1 on the left). The experimental curve is a sigmoid whose inflection point (called neutralization point) corresponds to a volume added for which the mixture is neutral, i.e. has equal concentration in oxoniums and hydroxides corresponding to pH 7. The position of the neutralization point allows to know the quantity of hydroxides added and consequently the concentration in oxoniums of the analyte. A geometrical technique (method of tangents) is used to determine this position. It is based on the quasi-symmetry of the experimental curve with respect to the inflection point (Table 1 on the right). As said before, no theoretical justification in chemistry and mathematics is given to students. The underlying model of the reaction is the evolution of the pH based on empirical observation, increasing and almost symmetrical with regard to the neutralization point. This is Model 1.

Titrant: 8 ml acid, oxinium concentration 0.0125 mole/liter.
Analyte: base, hydroxide concentration 0.01 mole/liter.

Oxinium concentration for *x* ml base< 10:

$$Ca(x) = \frac{10^{-4} - x \cdot 10^{-5}}{(8+x) \cdot 10^{-3}} = \frac{10 - x}{100 \cdot (x+8)}$$

pH for *x* ml base < 10:

$f(x) = -\log(10-x) + \log(8+x) + 2$

Hydroxide concentration for *x* ml base> 10:

$$Cb(x) = \frac{x \cdot 10^{-5} - 10^{-4}}{(8+x) \cdot 10^{-3}} = \frac{x - 10}{100 \cdot (x+8)}$$

pH for *x* ml base> 10:

$f(x) = \log(x-10) - \log(8+x) + 12$

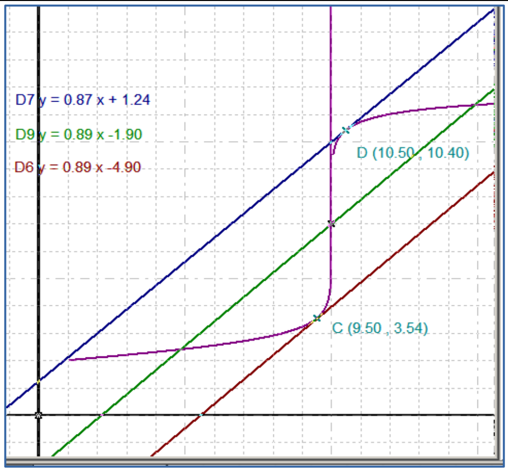

Table 2: Mathematical function based on assumption: mixture contains only one type of ions.

Model 2 is another model in which the titration curve is obtained by the calculation of a mathematical function (Table 2). It is based on a simplifying assumption: hydroxide and oxonium ions neutralize so that the mixture contains only one of the two types of ions. This assumption allows to obtain a function whose curve is coherent with the empirical curve, except in the vicinity of the neutralization point where the function tends towards infinity. This is a consequence of a phenomenon called partial dissociation of water, that contradicts the assumption: acidic solutions contain hydroxides and basic solutions contain oxoniums, but this is negligible except in the vicinity of the neutralization point. Because tangents are drawn at a distance from the neutralization point, the model is a basis for a mathematical work to justify the method. Mathematics also allows to question the simplifying assumption, and thus students working on the models should progress both in chemistry and mathematics.

In accordance with the RQ, the experimentation aimed to build and evaluate suitable

WSs thanks to which students could recognize Model 1 and 2 as the foundations of the titration technique, and compare the two models. These WSs are designed for the two group phases (expert groups and jigsaw groups). There are three expert groups. Students in group Ea should become experts in Model 1, students in Eb should become experts of the mathematical component of Model 2 and students Ec should develop an expertise in quantifying the evolution of concentrations throughout the titration. WSEa, WSEb and WSEc are suitable WS, each representing the respective expertise targeted in each group and WSJ is the suitable WS pour the Jigsaw groups. A presentation of the WSs and associated tasks follows, summarized in Table 3.

WSEa: Acid, base, neutralization (visual), pH (reading), measure, proportion, curve (experimental), tangents (visual).	**Task Ea:** Appropriate a simulation software. Simulate for given data. Operate the tangent method for varied positions and compare accuracy.
WSEb: Functions (symbolic), curve, tangents (software), decimal logarithms.	**Task Eb:** Study the function *f* (Table 1); growth, limits. Trace the curve and tangents at abscissas 10-x and 10+x for varied values of x ; observe the mid-lines.
WSEc: Ions, concentration, neutralization, pH. Volumes, ratios, formula.	**Task Ec:** Calculate hydroxides and oxynium concentration for varied added volume. Calculate pH for these values and draw curve.
WSJ: Idem Ec + symbolic calculations	**Task J:** Compare curves (Tasks Ea, Eb,Ec). Show how *f* (Task Eb) models the pH as a function of the added volume. Justify the tangent method.

Table 3: Suitable working spaces and tasks in the group works.

WSEa is suitable to work on Model 1 and thus includes elements of chemistry (ions, pH, concentration, etc.) but also of mathematics (measurements, curve, tangents, ratios, etc.) We choose to have Ea students work on computer software simulating titrations. The purpose of the software is to help systematize and reflect on the method: students must enter the data of a given titration; they obtain a curve simulating the empirical curve, they can choose points to perform the tangent method and observe the accuracy of the method (Task Ea).

WSEb is the space for a complete mathematical study of the Model 2 function. The signs, the theoretical frame of reference as well as the use of a software for functions belong to high school calculus, with the exception of decimal logarithms and the piece-wise function which are unfamiliar. Task Eb is a study of properties of the function. It is classical in the form, but the function is unusual.

WSEc is the space for students to numerically compute concentrations along the titration, using the assumption of complete neutralization. The elements of chemistry are the same as in Model 1, but they must be systematically quantified; pH formulas must be used. From a mathematical point of view it is an arithmetic space. Task Ec requires students to have a good mastering of chemistry notions, as well as ratios and unit conversion. The calculation of the concentration must take into account the quantity of ions, but also the increase of the volume along the titration.

WSJ correspond to the jigsaw groups in Phase 3. This is the space for students to understand Model 2, make the connection to the assumption that the mixture contains only one type of ions and make sense of the tangent method at a symbolic level. Task J should lead students to perform a computation similar to Task EC, but at a symbolic level as in Table 2, and to justify that two parallel tangents, one on each branch, are nearly symmetrical with regard to the neutralization point.

IMPLEMENTATION AND ANALYSIS

In the context of the pandemic in 2020, the experimentation was carried out in the form of a "lock-down online jigsaw classroom", i.e. the six participants were physically separated, communicating on a platform that allowed either all students to be gathered together (Phases 1 and 4) or split into groups (three groups of two in Phases 2, and two groups of three in Phase 3). The students were of average level, some more proficient in mathematics, other more in experimental sciences. They had previously performed titrations on real solutions. The platform allowed the recording of exchanges and productions. This data was completed by a e-mail survey. In the analysis of the data we leave aside the aspects related to the online work, underlining only that even online, the jigsaw classroom kept its potential for collaborative work.

This is the analysis of the group work phases (about one hour each). Table 4 presents extracts of the reports made by the three experts groups (Ea, Eb, Ec, Phase 2) and the two jigsaw groups (J1, J2, Phase 3). Ea appropriated the simulation software after having difficulty understanding menus and data needed. They were able to use the tangent method for several values and compare the accuracy. Eb's study of the function remained partial as the log decimal function was unfamiliar. As shown in their report they were also not comfortable with a piece-wise function. They noted an undefinitness, but did not mention infinite limits that would have shown inconsistency with the experimental curve. Pseudo-symmetry and use of parallel tangents for the position of the center were discussed. Ec was comfortable with the chemistry concepts and the various calculations, but had difficulty taking into account the variation in the volume of the solution. They made the connection with the titration curve. Overall, Ea and Ec's work can be seen as fitting in the suitable WSEa and WSEc after initial difficulties. This is not the case for Eb. The students were not comfortable with the function of Model 2, which is different from routine functions they had been trained with. They were able to draw curves and tangents thanks to the software. It was consistent with WSEc only for the use of software.

Group Ea	We used a software to enter the data, and we got curves for concentration and pH . We saw clearly the turning point that makes it go from acidic to basic. We used the tangent method to get the pH.

Group Eb	We had two functions, one for $x<10$ and the other for $x>10$, but it was the same function. The two functions are not defined in 10. We drew the curves with GeoGebra. The pH curve, was symmetrical with regard to the neutralization point. We placed the points A and B according to the given abscissas then we traced the tangents and the mid line on the computer to find the neutralization point.
Group Ec	We calculated the quantity of oxoniums for each added volume. Then we applied the formula m/V after converting the volume into liters to get the concentrations, and the formula -log(Ca) for the pH values. We did similar calculations for the hydroxides after neutralization. We saw that values increased and that it looked like the empirical curve.
Groups J	**J1** We observed that when we apply the formulas of group Eb, we obtain the data found by group C. We can therefore deduce that the curve representing pH are related to the function of group Eb. We calculated the derivatives to get the slopes of the tangents. When the difference between these is close to 0, we get more accurate results. **J2** We had to develop a formula that actually calculates everything at once. We made calculations like Ec did but with a variable *x* and we got the function of group Eb for the acidic part.

Table 4: Extracts of reports of students' group work.

Both J groups observed that the curves obtained by the three experts groups were similar. Group Eb's remark (the two functions are not defined in 10) did not lead students to observe a discrepancy between models near neutralization. Group J1 concluded that the similarity of curves is sufficient evidence that *f* is a model of pH evolution. They started a study of the slope of the tangents with regard to the accuracy of the method, using the derivative of *f* with difficulty. Group J2 looked for a an analytic proof that *f* is a model and succeeded only for the acid part. The behaviors in both groups show students' partial appropriation of WSJ, the suitable working space that should provide mastery of Model 2. One shortcoming is that students' symbolic calculation skills taught in math class were poorly enacted. Another shortcoming is that they were not able to recognize a discrepancy between the models. In Phase 4, after the J groups reported on their work, the teacher emphasized the use symbolic computation and the discrepancy between models near neutralization, which he explained by the dissociation of water. Answers to post-questions by email showed that these points were partially understood by students.

CONCLUSION AND PERSPECTIVES FOR RESEARCH

The suitable WSs prepared for this experimentation allowed the students some appropriation of the models both in their chemical and mathematical dimensions. A critical look highlights achievements and gaps. WSEa did not help students distinguish Model 1 from Model 2. WSEb was too demanding in symbolic calculation. WSEc seemed appropriate, with students Ec completing the task and contributing to the work in Phase 3. WSJ was affected by Ea and Eb's shortcomings.

Another implementation was then carried out in 2021 with a variation of the tasks. In Task Ea the simulation was a computer program that the students could read and interpret. In all tasks it was asked to get values of the pH (Tasks Ea and Ec) or of the function (Task Eb) very close to the neutralization point. The discrepancy between values obtained by Ea on one side and by Eb and Ec on the other side brought a discussion in groups J. The students did not reach a consensus. Some students emphasized the validity of the model underlying the computer program and its conformity with empirical observations, and others maintained that Model 2 was more reliable, stressing the inaccuracy of empirical observations compared to mathematics. These results may be somewhat surprising and unsatisfaying but they confirm the interest of this situation and provide insights for further experimentation.

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