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Mathematics in classroom chemistry. Towards STE ↔ M integration

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Mathematics in classroom chemistry. Towards STE ↔ M integration

This article begins by characterizing current conceptions that separate mathematics from STE by giving prominence to either mathematics (ste | M) or STE fields (STE | m), whereas education should help students develop joint understanding and reasoning in mathematics and STE (STE ↔ M.) In order to progress towards STE ↔ M, a theoretical framework is proposed, breaking with the way modelling is currently conceived in mathematics education research. The framework considers the intermediation role of models between an empirical referent composed of objects and phenomena as perceived by the learner and a theoretical referent. It is inspired by sciences education research but it differs by introducing mathematical reasoning as an important component of the theoretical referent.

In this framework, covariations between quantities are models that give meaning to processes perceived in the empirical referent. Modelling also makes it possible to treat covariations as dependencies between mathematical variables, thus establishing a link with the theoretical referent. Epistemological considerations point to two important dimensions: the plurality of models, and teamwork between people with different points of view.

Chemistry is chosen to illustrate and test this framework, as it is a field where mathematical reasoning and understanding is overlooked at school. Two models of the process involved in a laboratory technique are proposed, one based on a mathematical function and the other on a white-box simulation. Innovative tasks for grade 12 students are designed and evaluated in classroom implementations.

Keywords STEM integration, School chemistry, Mathematical reasoning in STEM, White-box simulation, Models, Empirical referent, Teamwork

Introduction

According to OCDE (2018) conceptualisations of STEM (Science, Technology, Engineering, and Mathematics) differ across countries: ‘while some focus on improving learning in stand-alone subjects, others emphasize STEM as an integrative approach to

learning.’ This integrative approach, or integrated STEM, has a potential for preparing students for the challenges of the modern world and in creating an holistic learning experience for students. For NAERC (2014), rather than teaching these subjects as separate and distinct areas integrated STEM education seeks to connect them in meaningful and relevant ways.

The goal of the research reported here is to investigate the role that mathematics can play in integrated STEM education. Mathematics is often described as an abstract domain. More precisely, Mitchelmore and White (2004) characterize mathematics as a self-contained system. In this view, although mathematical objects can derive from concepts in the physical and social world and are then useful for predicting and controlling real objects and events, they are separated from this world. Mitchelmore and White characterize the process of derivation as mathematical abstraction but also recognize being ‘far from a comprehensive theoretical answer to the challenge of mathematical abstraction in mathematics education.’ This conceptualization of mathematics and the physical and social world leaves open the question of how to conceive the M in STEM. Do Scientists, Technologists and Engineers just request from Mathematicians readymade constructs serendipitously available for application, separating the M from the other STEM (STE | M)? Or do they collaborate in building an understanding both in mathematics and in a domain of the physical and social world (STE ↔ M)?

At school, Kaiser and Maaß (2007) report on a dominant formalistic view of mathematics among teachers, giving the example of a teacher for which ‘Non-mathematical applications do not form a constitutive part of mathematics’ adding that

‘In mathematics lessons, students learn “the basic conditions of mathematics”, and everything else comes from the other subjects.’ On a larger scale, Kaiser and Maaß (2007) conclude that mathematics teachers’ view can be classified in two poles: one pole is a ‘Platonic view’ of the nature of mathematics which focuses on the internal logical structure, possibly gained and purified by abstraction from real life problems; the other pole is a ‘functional view’ where mathematics is treated as a language which describes and explains physical phenomena. Both these views allow teachers to teach mathematics independent of any application arguing that these applications certainly exist, and thus their students will eventually find the usefulness of the mathematics taught. Broadly, these mathematics teachers views separate mathematics from STE fields, and give mathematics a predominant role (ste | M.) Conversely, sciences or engineering teachers are able to consider notions of mathematics involved in their course as useful for formalizing and quantifying, but without paying much attention to conceptual aspects of these notions (STE | m.)

Teaching practices following these views leave students no opportunity to understand how mathematics and other STE fields work together to explain and act on the world. This has implications at the workplace. Czaplinski et al (2019) observed that many undergraduate mathematics students involved in a workplace experience regretted ‘a lack of understanding from the employers regarding the rich potential (...) offered by mathematicians.’

The motivation of this paper is then to explore ways to develop a STE ↔ M conception of STEM education. Because of the importance of models in STE as well as in the relationship between STE fields and Mathematics, the following sections study current didactic theorizations of models and modelling. Analysing their advantages and

limitations, a framework for STE ↔ M integration is proposed, helping to raise research questions and to design and evaluate a classroom situation. Before that, section 2 gives an example in a chemistry course in the French curriculum that suggests that opportunities for integrating mathematics are overlooked. It will be the starting point for proposing a framework and consequently tasks for students.

An example in a chemistry course

Chemistry was chosen because, at school, it is a scientific field generally taught without in-depth mathematics. Nevertheless, there is evidence of demands of undergraduate chemistry departments for a mathematical preparation of students. Craig (2000) mentions themes such as scaling, estimation and visualization. These themes are certainly important, and presumably sciences education does not ignore them. Craig also points to a theme that, by contrast, is rarely associated with learning chemistry: mathematical reasoning. Craig emphasizes a specific form of reasoning, involving the use of algebraic arguments¹, the treatment of mathematical expressions in relation to fundamental relationships, and a thoughtful use of notations. Mathematics education researchers such as Herscovics and Linchevski (1994) have suggested the existence of a cognitive gap between arithmetic and algebra. However, other researchers such as Carraher et al (2006) have shown that even elementary school children can reason algebraically. There are thus clear indications that the gap is a consequence of educators' representations and practices rather than learners' cognitive limitations: algebraic reasoning and notation have been considered difficult or too abstract for most students, unlike arithmetic, which is considered concrete. Introducing chemico-mathematical reasoning into school chemistry may well be possible, by breaking with

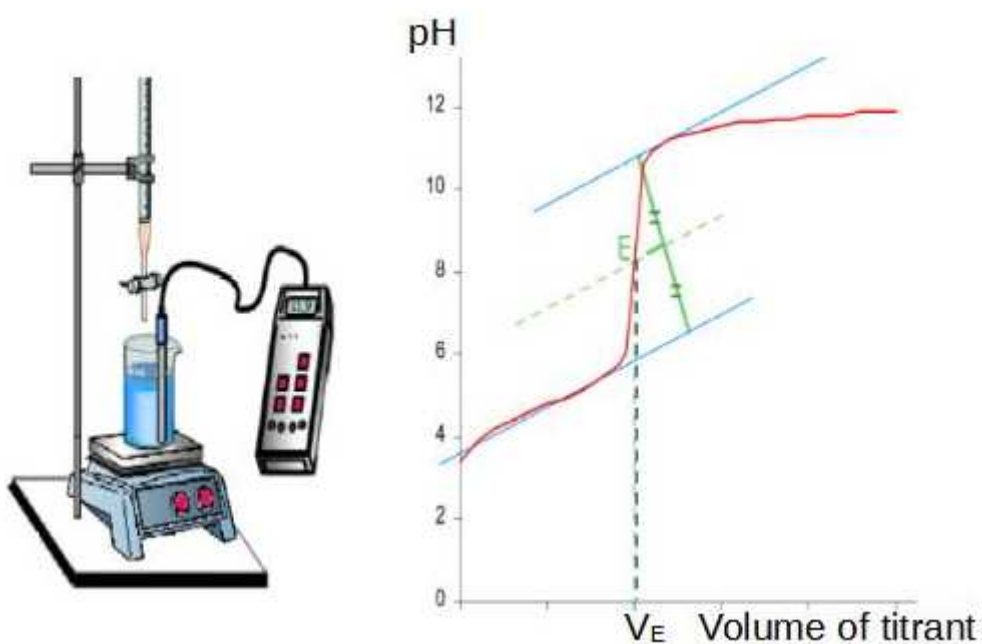
educators' current representations and practices.

In chemistry courses, laboratory techniques are part of the curriculum for non-professional students, the aim being to link theory with experimentation. However, this does not go as planned: Canac et al (2021) studied teacher discourse and teacher-student interactions during laboratory sessions on acid-base titration in the first year of undergraduate degree and concluded that in actual teaching, laboratory work is mainly focused on procedures and manipulative skills, without theoretical discussion. Titration is therefore a subject in which it is important to introduce theoretical reflection, including, where appropriate, chemical-mathematical reasoning.

Here is a brief introduction: titration is a laboratory technique using a solution of known concentration (titrant) to determine the unknown concentration of another solution, the analyte. In France, this technique is taught for acid-base titration in the 12th grade of non-professional secondary schools. The analyte is an acidic solution characterized by a preponderance of oxonium ions H_3O^+ . It is placed in a glass container which is continuously agitated. The titrant is a basic solution characterized by a preponderance of hydroxide ions OH^- . It is added to a known quantity of analyte from a graduated burette. During titration, the added hydroxides neutralize the oxoniums in equal amounts, so that the pH (minus the decimal logarithm of the oxonium concentration) of the mixture increases. A pH meter allows reading continuously the pH, and by recording values, a curve (volume of titrant, pH) is obtained (fig.1 left.) This experimental curve is a sigmoid whose inflection point (called the equivalence point) corresponds to an added volume for which the mixture is neutral, i.e. of equal oxonium and hydroxide concentration. This is the equivalent volume, V_E . It is used to calculate the quantity of hydroxides added and, consequently, the initial quantity and

concentration of oxoniums in the analyte. A geometric method (tangent method, appendix 2) is used to determine the equivalence point: two parallel tangents are drawn on the empirical curve; the equivalence point is at the intersection between the curve and the median line (fig. 1 right.)

Fig. 1: Titration



Profound notions and questions are at stake. What exactly happens in the process? Why does the tangent method work? What model(s) can be used? This is an opportunity to get students thinking about this technique, making the link between mathematics and chemistry. Two models of the titration process shed light on these questions.

Model 1 (annex 1) is a computer simulation, i.e. a program that iteratively calculates the pH throughout the titration process. It is a useful model for obtaining pH values for different volumes of base added, for automatically operating the tangent method at different points, and for thinking about the neutralization process in the acid-base reaction. The model takes into account the auto-ionization of water, a phenomenon in which water spontaneously dissociates into oxonium and hydroxide ions. It is assumed that in aqueous solutions, the product of the concentrations in acidic and basic

ions is a strictly positive constant K_w , whose value under normal temperature and pressure conditions is 10^{-14} . Taking this constant into account enables a simulation consistent with experimental curves, even for values close to the equivalence point.

For values of acid concentration below equivalence, the basic concentration is negligible: e.g. if $\text{pH}=6$ then $[\text{OH}^-] = 10^{-8}$ negligible compared to $[\text{H}_3\text{O}^+] = 10^{-6}$. Conversely, for values of acid concentration above equivalence, the basic concentration is predominant: for example, if $\text{pH}=8$, then $[\text{H}_3\text{O}^+] = 10^{-8}$ is negligible compared to $[\text{OH}^-] = 10^{-6}$. It is therefore possible to consider a model valid outside the vicinity by assuming $K_w=0$. This assumption allows the model to be expressed as a mathematical function. This is model 2 (annex 1.) The curve of the function is consistent with the empirical curve, except in the vicinity of the equivalence point where the function tends towards infinity. As the tangents are drawn at a distance from the equivalence point, the model provides a basis for mathematical work explaining the tangent method (annex 2.) Studying the model also enables students to question the simplifying hypothesis, so they can progress in both chemistry and mathematics.

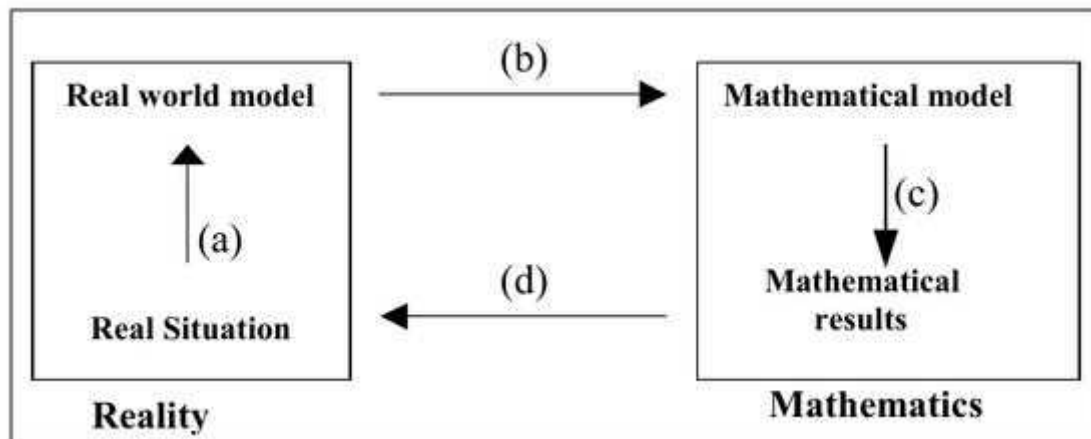
The following features stand out: a laboratory technique is taught without reflection on either chemistry or mathematics. Questions about the technique put forward two models that shed light on the neutralization process and the mathematical aspects of the technique. Model 1 is computational, consistent with empirical observation and useful for exploring the technique. Model 2 is a mathematical function, consistent with empirical observation except near the equivalence point, but useful for explaining the tangent method and challenging a simplifying assumption. This example suggests that modelling can bring mathematics and chemistry teaching closer together. The following section reviews current approaches to modelling.

Approaches to modelling in mathematics and sciences educational research

In mathematics education, interest in real-world contexts has been growing since the 2000s. The ICMI 14 study (Blum, 2002) kicked off a lively stream of research, focusing on mathematics as an important activity in society. This trend is marked by two main themes: problem solving and the modelling cycle. Many authors characterize modelling tasks as authentic problem solving, but the tasks they propose focus more on the solution to a contextualized problem than on the models. For example, in Blum and Ferri (2009), the task concerns a lighthouse of a given height, and students are asked to find a value for the visibility distance that is valid specifically for that height. The authors identify steps in the students' resolution of the problem. They interpret these steps as part of a cycle divided into two poles: a real model and a mathematical model.

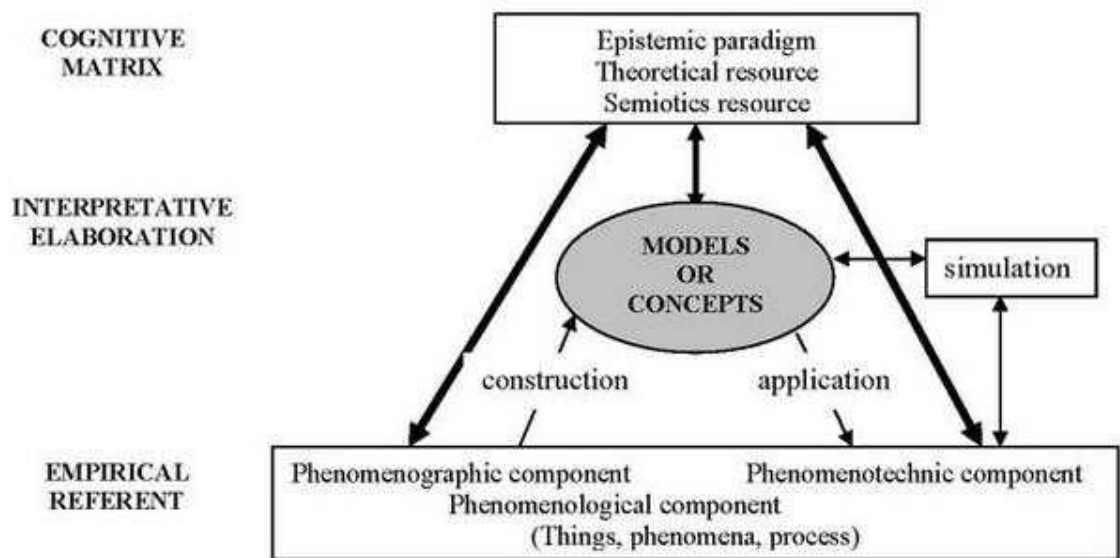
Overall, the organization of the modelling cycle remains close to a classic solving scheme where the problem and solution are expressed at the extra-mathematical level and solving takes place at the mathematical level (fig. 2.) Czocher (2018) objects that, in this cycle, the real and the mathematical remain insufficiently intertwined to account for how working on a model articulates mathematics and real-world objects and phenomena, particularly when students are engaged in a validation process. She proposes a framework that integrates real-world and mathematical reasoning. One of the limitations of Czocher's approach is that there is an imbalance between sciences and mathematics: although her study focuses on solving problems featuring scientific notions (movement of physical bodies, biological cells...), real-world reasoning is considered idiosyncratic to students and is therefore not investigated, unlike mathematical reasoning that she analyse with regard to mathematical notions such as differential equations (ste ↔ M.)

Fig. 2: A representation of the modelling process by Kaiser (1995.)



Sciences educational research takes a different view of modelling. Martinand (1995) proposed a representation of the role of models (fig. 3.) Drawing on this representation, Ganaras et al (2008) explain that models and concepts play the role of an ‘interpretative elaboration’ linking an ‘empirical referent’ made up of objects and phenomena as perceived and mobilized spontaneously by the learner, and a ‘cognitive matrix’ made up of scientific elements. Interpretative elaboration helps students to relate the two referents, and thus to progress both in their perception of sensible objects and phenomena, and in their understanding of a scientific theory. In sciences education, model has many meanings (Chamizo, 2013), and in analysing students' conceptions of the acid-base reaction, Ganaras et al (2008) do not distinguish model from concept, for example when they conclude ‘that the use and application of the concept of chemical equilibrium as an interpretive conceptual tool remains weak.’

Fig. 3 Martinand's framework of modelling in science education, from Ganaras and al (2008.)



Reflecting on tasks for students requires thinking of a model in an operational sense, explaining or predicting an aspect of a given phenomenon, as opposed to a concept that encompasses various interpretations and is intended to be integrated into a theory. The two models of the titration process presented above illustrate this idea. This conception of models for STE ↔ M will be developed in the next section. It is, however, compatible with Martinand's representation of modelling in sciences (fig. 3), which positions models at an intermediate level between an empirical referent and a cognitive matrix. This positioning also makes it possible to envisage work on models less systematically oriented towards problem-solving, in contrast to the dominant approaches in mathematics education described above: students can work on existing models, discussing their construction and application.

Blanquet and Picholle (2015) note that in physical sciences curricula, the notion of model is often coupled with mathematical symbolism reduced to a language.

Students are then faced with both epistemological difficulties concerning the idea of model and a poor understanding of symbolism. As a result, modelling, both in sciences teaching practice and in educational research, tends to be limited to elementary situations. Very simple mathematics is used, so students may overlook the role of mathematical reasoning (STE | m.)

Models and Modelling

Inspired by French epistemologists (Bouleau, 2014, Varennes, 2014) Lagrange et al (2022) distinguish between modelling and mathematizing. Mathematizing an experimental field consists in building a theory in which mathematical deduction is the source of truth: data from the field are interpreted in the theory, and conversely, facts produced within the theory without reference to the field are reinterpreted into the field. Modelling as it is conceptualized in mathematics education (fig. 2) is in fact mathematizing. In contrast, modelling has to be conceived as a process aimed at accounting for certain aspects of a field in order to understand it, even partially, and act upon it.

Modelling then enables local mathematical interventions that need to be continually controlled by knowledge of the field rather than treated as the only truth. From a pedagogical point of view, this implies that it is possible for students to develop a mathematical activity on models of an experimental phenomenon, while controlling this activity by an understanding based on experimental sciences notions. This is particularly the case in school chemistry: mathematizing chemistry would require notions linked to the structure of matter as well as highly advanced mathematics, both

well beyond secondary education, whereas the titration example suggests a potential for working on models of the process, combining mathematics and chemistry.

The corollary of the locality of modelling is that there is not a single model: several models are as many ways of approaching a reality. In each model, the contribution of mathematics is the result of specific work, in collaboration with experts in the field, to make the model more intelligible and easier to use. In this conception, there is not a real model on one side and a mathematical model on the other, but a plurality of models, each with a specific involvement of mathematics in the same field of reality. Because of plurality, modelling has a subjective and social dimension: all models can be useful, but each must be discussed and confronted with others. The locality of modelling and the dependence on simplifying assumptions mean that the students must learn to analyse the similarities and differences between models of the same reality. How do the models differ? For what purpose is one model more appropriate than another? How to assess the relevance of a model? This objective is closely linked to the epistemology of modelling, a major issue in the education of citizens. It also has implications for STEM, since it involves reasoning about objects in the field being modelled and their relationships. Finally, modelling is a social activity that involves the collaboration of specialists with different points of view (Wakes, 2015.)

Bagossi (2023) points out that modelling often requires reasoning on covariation. Covariation takes its meaning from the concrete experience of objects varying together in the sensible world. Quantifying the characteristics of covarying objects is an important step (Thompson and Carlson, 2017.) Graphs and tables of quantities can be used to progress towards a scientific conception of a phenomenon,

while maintaining a close link with objects in the sensible world. In the context of chemical kinetics, Rodriguez et al. (2018) emphasize the potential for learners of the physical meanings attached to inputs and outputs that make covariation take on ‘an interesting new meaning from the point of view of an expert reasoning with chemistry concepts.’ Beyond tabular and graphical representations of covariant quantities, mathematical functions express covariation as a dependency between variables, using the potential of algebraic representations as well as constructs not directly derived from empirical context. For example, the product of concentrations in the auto-ionization constant and the decimal logarithm in the definition of the pH are mathematical constructs that do not derive directly from the context of acid-base reactions. However, they enable calculations and reasoning that are not only useful for obtaining practical results, but also shed light on acid-base reactions.

Sciences, technology and engineering are fields in which data collection and exploitation play an important role. As mentioned above in the case of titration, laboratory techniques raise profound questions. Why does a technique work? Are there any conditions? What model can help? These questions can highlight the contribution of a mathematical function in a model. Students need to understand that mathematical functions are an effective way of making sense of a laboratory process, rather than a pure formalization. They also need to broaden their understanding of these functions to adapt to the characteristics of a non-mathematical field: decimal logarithms, for example, in chemistry and other fields.

Framework and research questions

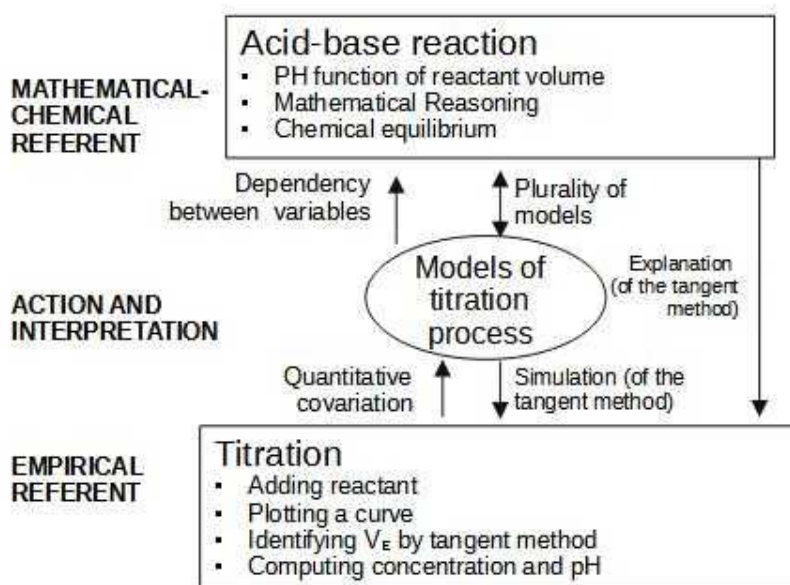
In this section, a framework is proposed to account for the role of models in STE ↔ M

integration. Consequences are then drawn for tasks to propose to students and their organization.

Models as intermediaries between empirical and theoretical referents

The framework outlined in fig. 4 is inspired by Martinand's representation (fig. 3.) It particularises to titration and acid-base reactions. The empirical referent is constituted by the titration process as perceived by a person operating in a laboratory. The mathematical-chemical referent includes mathematical reasoning and enables to think of titration as a continuous process of chemical equilibriums with particular properties (continuity, pseudo-symmetry, inflection, etc.)

Fig. 4: A framework for STE ↔ M integration instantiated to acid-base reaction.



Models play an intermediating role. In addition to interpreting empirical facts, they enable actions to be taken, first towards the empirical referent, by explaining, predicting and guiding, then within the models, by refining and comparing, and finally towards the mathematical-chemical referent, by highlighting potential theoretical elements. Upward arrows refer to covariation. The systematization of pH calculation enables to conceive of covariation between quantities involved in the process. Expressing covariation as a dependency between mathematical variables allows thinking of a continuous process. The similarities and differences between the models can then be studied in relation to the mathematical-chemical referent (two-way arrow), enabling equilibrium (ionic dissociation and neutralization) to be understood at a theoretical level.

The descending arrows deal with the tangent method. Using a model, the method can be simulated, enabling repeated application to find the optimum tangent positions for best accuracy. Explaining the method (why it works and how effective it is) requires elements of theoretical reference, considering pH as a mathematical function of the reactant volume.

The first research question is as follows

RQ1 Do models of the titration process help students make the link between empirical laboratory work and a mathematical and chemical conceptualization of acid-base reaction?

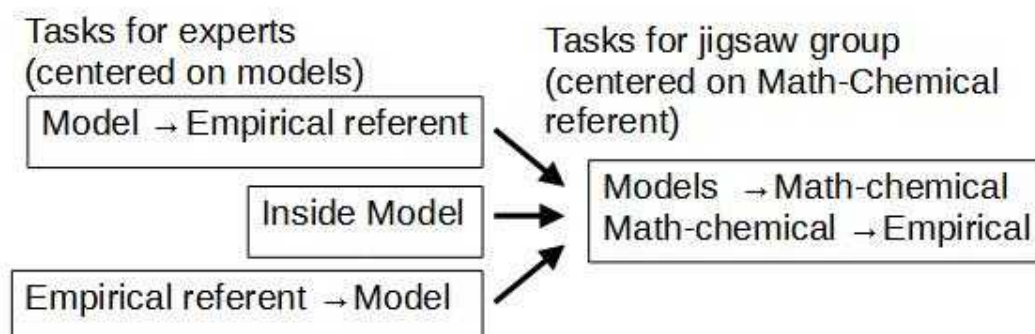
Tasks for students and collaboration

As explained in the introduction, the motivation of this paper is to explore ways of developing a STE ↔ M conception, i.e. ways that enable students to engage in a study of a field in science, technology or engineering , with the aim of developing an

understanding that links elements of the field with mathematics. The above framework then needs to be operationalized through tasks for students and an organization of these tasks. Fig. 5 proposes two stages. The first stage focuses on models, in relation to the empirical referent, or internally, examining their properties and coherence. The second stage focuses on the mathematical-chemical referent in relation to the models.

This organization makes it possible to divide the tasks of the first stage and assign different tasks to different students so that, in the second stage, students have to explain their task and how they solved it, and work together to complete tasks on the mathematical-chemical referent. This organization replicates the collaboration between experts with different points of view, which is important when working on models; it also enables students to go deeper into an aspect of the models and make it comprehensible to other students. This makes each student an expert in a given aspect, which is why the corresponding tasks are referred to as expert tasks. Second-stage tasks are handled through collaboration between experts, and are therefore labelled jigsaw tasks, in reference to the jigsaw class (Aronson, 2002)ⁱⁱ.

Fig. 5: An organization of tasks



A second research question follows:

RQ2 Does the experts-jigsaw organization of tasks engage students in collaborative work contributing to actualize the potential of models?

Method

The method consists in designing, implementing and evaluating a situation for a grade 12 class on the basis of two acid-base titration models. The task design reflects the assumptions about the role of the models and the organization outlined in the previous section. As explained, a first stage consists of model-centred tasks for experts. The tasks are defined in accordance with three aspects of a model.

(Ta) From model to empirical referent. The task uses a computer simulation of the titration process, according to model 1. There are two different versions. In version 1, the task consists in finding the result of the tangent method for different positions and comparing accuracy. The aim is for students to understand the idea of better accuracy as a function of position on the curve. In version 2, the task is to read, modify and interpret the code of the simulation. The aim is for students to understand the code, in particular by pointing out the hypothesis of incomplete neutralization (line23, in table 2, annex 2 while $N_{acid} * N_{base} > Eq$:)

(Tb) Within a model. The task is to study the function in model 2 and the tangents to its curve. The aim is for students to acquire an understanding of the mathematical properties of the function and the tangents, making a link with the tangent method seen in chemistry class.

(Tc) From empirical referent to model. The task is to obtain pH values for various volumes of added base by calculating the concentration of oxoniums or hydroxides under the simplifying assumption of model 2. The aim is for students to master the quantities, concentration and neutralization in order to quantitatively approach the covariation between pH and volume of added base.

A second stage begins with reports from the experts following tasks Ta, Tb and Tc. Then, tasks labelled T_{j1} , T_{j2} and T_{j3} aim to engage students in mathematical and chemical reasoning.

Table 1 shows the tasks as written for the students and summarizes the aims.

Table 1: Tasks and aims

<p>Ta: Appropriate a computer simulation (Model 1.) Simulate for given data.</p> <p>Version 1: Operate the tangent method for varied positions and compare accuracy.</p> <p>Version 2: Read the code and modify for values close to the equivalent volume. Interpret the code in the loop.</p>	<p>Aim:</p> <p>Version 1: make sense of the idea of a best accuracy, depending on a position on the curve.</p> <p>Version 2: understand the code, uncovering the hypothesis of incomplete neutralization.</p>
<p>Tb: Study the function f; growth, limits. With a graphing tool, obtain the curve and the tangents at abscissas $10-x$ and $10+x$ for varied values of x; observe the mid-lines.</p>	<p>Aim: a thorough understanding of the mathematical properties of the function in Model 2.</p>
<p>Tc: Calculate hydroxide and oxonium concentration for varied added volume with the hypothesis of Model 2. Calculate pH for these values and draw curve.</p>	<p>Aim: master quantities, concentration and neutralization in order to approach quantitatively the covariation between pH and added volume.</p>
<p>Tj₁: Link Tb and Tc. Demonstrate that the functions in Tb model the evolution of pH as a function of the volume of base added.</p>	<p>Aim: observe similarity between models in Tb and Tc. Prove algebraically. .</p>
<p>Tj₂: Investigate the tangent method algebraically.</p>	<p>Aim: Compute equations of parallel tangents and midline, and the intersection with the curve. Discuss accuracy.</p>
<p>Tj₃: Link Ta and Tc. Compare the two models of pH evolution as a function of the volume of base added in the two tasks.</p>	<p>Aim: Observe dissimilarity between models in Ta and Tc and identify underlying hypothesis.</p>

Implementation

Two implementations were carried out in the context of the 2020 pandemic, as an online classroom, i.e. participants were physically separated and communicated on a platform that allowed either to work as a whole class, or to be divided into groups. The students were in grade 12, of an average level, some more proficient in mathematics, others more in sciences. One implementation was carried out with Ta version 1 and six students, and another with Ta version 2 and thirteen students. All the students had already carried out titrations in previous laboratory work. The teacher was a doctor in didactics of sciences, specializing in chemistry and conducting research with the author in an interdisciplinary laboratory for didactics of mathematics and sciences. A mathematics teacher also participated in the implementation.

In both implementations, the organization was as follows: a 10-minute whole-class introduction, a first one-hour stage of group work, called GW1, a second one-hour stage of group work, called GW2, and a final 45-minute concluding discussion. In GW1, the students were divided into three groups Ga, Gb and Gc carrying out tasks Ta, Tb and Tc respectively. In GW2, the students were divided into Gj groups, each bringing together students from the three groups Ga, Gb and Gc. In order not to exceed one hour, each Gj group performed only one of the tasks Tj₁, Tj₂ or Tj₃. In the first implementation, one group performed task Tj₁, and another task Tj₂. In the second implementation, one group performed task Tj₁ and another task Tj₃.

All tasks were given according to the table 1, with the following data: Titrant: 8 ml acid, oxonium concentration $[H_3O^+]=0.0125$ mol/L; Analyte: base, hydroxide concentration $[OH^-]=0.01$ mol/L. With these data, $V_E=10$ ml.

Results

The link between laboratory work and mathematical-chemical conceptualization of the acid-base reaction

The results are organized into three dimensions. The first dimension *Quantitative covariation and dependency between variables* corresponds to the ascending arrows in the framework (fig. 3.) The second dimension *Simulation and explanation of the tangent method* corresponds to the descending arrows. The third dimension *Plurality of models*, corresponds to the two-way arrow. Extracts from discussions between students are analysed to assess their progress in linking mathematical-chemical and empirical referents along the arrows of the framework.

Quantitative covariation and dependency between variables

This part exploits the work carried out in the first implementation by the expert group Gc and a group Gj. It analyses how the students considered the covariation between analyte volume and pH. Although the task Tc involves calculating discrete values, the students in Gc recognized from the start a covariation. That is how they started.

S1. In fact, we want to see how the pH changes when sodium hydroxide is added.

S2. The evolution

S1. Whether it becomes more basic or more acidic when sodium hydroxide is added.

For each phase (acid, basic), students hesitated for the first calculation but iterated easily for the other values. Chemical concepts such as number of moles, concentrations and pH were used along with proportionality and decimal logarithms. After they

recognized a covariation, the students did not spontaneously think of a dependency between variables. This is a discussion with the teacher at the conclusion.

T. You took values for x and were able to find pH values... so we have a function that associates pH with x . Do you agree?

S1. Yes (not too convinced)

T. All the calculations you've made could have been done simply on x ...

S2. by associating a function in fact, our $f(x)$ would be ...

In their report to Gj, the students demonstrated an understanding of the covariation useful to check the values they obtained.

S1-S2. We did for all the acid values to get our pH (...) we can see that the values are increasing, so it is a good match. For the base, once again, the pH is increasing, so we are still on the right values and we have just transferred our values from the table to our graph and this gives us a curve, the same curve as the one we had obtained in the laboratory.

In their report, the students in group Gb pointed out that, although their task involved the mathematical study of a mathematical function, there was a similarity in the curves suggesting pH as a function of volume,

S3. We had two functions to study, in fact the same function: if x is less than 10, we had $f(x) = \dots$ and if x is greater than 10 ... We had to make the functions in GeoGebra, the brown curve and the red curve, and it looks like pH as a function of base.

The students had to be prompted by the teacher to provide a proof (task Tj1.)

T. Can you do the same calculation, number of moles then concentration, not with 5 but with x ?

S1. Do we have to find a formula that calculates everything at the same time?

S2. Do we have to start from $10^{-4} + x$ times 10^{-5} and arrive at the function (of Gb)?

After recognizing the possibility of constructing a formula, the students in group Gj engaged in the task, guided by the teacher and the calculation carried out by group Gc. The students did not easily transfer their calculus skills, and many mathematical difficulties were encountered. For example, it took the students a good part of the group work to simplify the expression $-\log\left[\frac{10^{-4} - x10^{-5}}{(x+8)10^{-3}}\right]$.

Simulation and explanation of the tangent method.

This part exploits the work done in the first implementation, the expert group Ga (Ta version 1) and a jigsaw group Gj doing Tj₂.

The students in Ga used simulation software. After a difficult appropriation, they recognized the empirical curve they dealt with in the laboratory. They simulated the tangent method at given points, using a dedicated software feature. In their report to Gj, they summarized their findings.

S10-11. We drew tangents at various points, and noticed that the closer they were to the pH jump, the more accurate the result. A pH value of 7 was expected.

Task Tj₂ was to examine this judgment, using the mathematical function studied by Gb. The students had to calculate the equations of three pairs of parallel tangents and the median line between them, then the coordinates of the intersection with the curve (annex 2.) But calculating the equations was a real problem. After much hesitation, they found that they had to calculate the derivative of the function to obtain the gradient of

the tangents. However, they were disconcerted because, in pairs of parallel tangents, the gradients they found were not strictly equal because of the approximation. Their conclusion was as follows.

Gj. Comparing the results of the three groups, we can see that calculating the derivative gives us the gradients of the tangents. When the difference between them is closest to 0, more accurate results are obtained by applying the method. This is because parallel lines have the same gradient.

This conclusion contradicts the results of S10-1, since it links the accuracy of the method to an insignificant difference in gradients due to numerical approximation, whereas S10-11 correctly made the link with the proximity of the pH jump. In the short time available, the students were unable to resolve this contradiction.

Plurality of models

This part is about the students' discussion of the similarities and differences between the mathematical function (Tb) and the simulated experimental model (Ta.) It first exploits an observation made in the first implementation. A student from group Gb reported on the mathematical function in Gj.

S4. Before 10 we have a function and after 10 we have another function (...) Both functions are not defined in 10, I mean $f(10)$ does not exist for both functions.

The idea of a piecewise-defined function is not clear to S4, but he has some notion of the discontinuous nature of the function, which is not consistent with experimental observation. However, this was overlooked by the other students in group Gj, who noticed no dissimilarity between the graphs obtained in expert groups Ga (simulated graph), Gb (mathematical function) and Gc (graph linking discrete values), and

concluded that they represented the same function.

This section also exploits an observation made in the second implementation. In this implementation, the Python language code was provided for the simulation of the Ta task (version 2.) The students in Ga, after being guided by the teacher, identified the dissociation of water in a line of code.

S5. (the line `while Nacid*Nbase > Eq:`) refers to the concentration of an aqueous solution, which is always 10^{-14} Are we talking about the acid concentration?

S6. It's the concentration of the product.

S5. Yes, I understand.

S6. The product of the concentration of acid and base.

S5. This is the product of the concentration of acid and the concentration of base, which in an aqueous solution is always 10^{-14} . This means that neutralization is never complete.

Students were also required to calculate pH values very close to the equivalence point. In Gj, the students compared the evolution in the two models (Python simulation and mathematical function, task Tj₃.) They noted something unexpected in the values obtained with model 2 (groups Gb and Gc.)

S7. We saw something a bit strange where it went up and down, under (the equivalence point) a slightly higher pH, and over (the equivalence point) a slightly lower pH.

Noticing a discrepancy with the continuously increasing values obtained with model 1 (task Ta), about half the students argued that the discrepancy was a consequence of the approximation in the Python program, which they assimilated to the inaccuracy of

experimental data, making a local phenomenon invisible.

S7. Python also gave fairly accurate results, but not as accurate as the mathematical formulas.

S8. Yes, to one tenth.

S7. We found the following explanation: we usually use experimental data, so we don't see that we have this odd variation of the pH.

T. Do you think that experimentally we can't see it?

S7. Yes, we're not accurate enough; before the equivalence point, the pH increases above 7.

S8. The margin of error..

These students interpreted the 'something odd' as a phenomenon not visible experimentally, because of a 'margin of error' in the data collection. Even after Ga identified water dissociation in the code of the simulation, S7 and S8 thought that a model given as a mathematical formula is necessarily more reliable, without questioning its relevance.

The other students recognized that water dissociation taken into account in model 1 and not in model 2 explains the difference. One of these students came to the following conclusion.

S9. For Gc and Gb, the same problem arises whenever values very close to 10 are reached, as pH tends towards plus infinity before 10 and minus infinity after 10. For values close to 10, the pH exceeds what is to be expected. Whereas for Ga, water dissociation cuts these problems short, and even if you get measurements that are perhaps a little less precise for certain values, I think it avoids this kind of problem.

When S9 says 'the values exceed what we're supposed to expect', it means he was

expecting a continuously growing function. He interprets the ‘something odd’ as infinite branches incompatible with the process of titration. He believes that the introduction of water dissociation ‘cuts these problems short’ and results in a model that better accounts for the process.

Collaborative work

This section analyses the responses of four students (labelled A1, A2, A3 and A4) to an e-mail post survey.

One of the questions was about the benefits of collaborative work in mathematics and chemistry. Students were also asked about any difficulties they had encountered. One student appreciated the collaboration between people with different backgrounds.

A1. It allows us to pool our knowledge to solve the problem.

Another student had the same appreciation and elaborated further, highlighting the benefits of collaboration between students with different skills in mathematics and chemistry. Beyond collaboration, she saw an advantage in considering a given problem from two points of view.

A2. I think there are only advantages. For example, I'm weak in maths but good in chemistry, so the fact that the main subject is the same but explained using different methods and by other groups who know their subject allows others (who may have gaps) to understand better in different ways. Thanks to this experience, I was able to understand in mathematical form the same problem I had studied in chemical form.

Although this assessment is positive, the student points out that the work was not easy, particularly because of the complexity.

A2. For me, the biggest difficulty was changing groups and having to put everything together and listen to the others. It's a lot of information to manage. I admit I was a bit lost on this part and tried to catch up as much as I could at the end, but then again that's also due to my lack of maths skills. Otherwise, for an average student who doesn't have too many gaps, this work doesn't present any great difficulties.

The other two answers stress the contribution to understanding and learning. A3 emphasizes independent group work, while A4 stresses the particular benefits of working together in a jigsaw group: learning to work as a team and, above all, formulating one's results for others.

A3. Overall, I had a good feeling about the lesson and the fact that we did the course ourselves helps us understand and assimilate more quickly.

A4. This type of work helps to improve your ability to work in a team, but also to improve the way you explain your work to partners who have never done it before.

This last student also explains, as A2 did, that the work requires bringing together different points of view, which was not easy.

A4. The difficulties I encountered were in making the connection between the different tasks with our partners' explanations only.

Observation of the students' work in the Gj groups is consistent with these answers. Each student reported carefully on his or her respective group in GW1 (Ga, Gb or Gc) while the others listened attentively. Afterwards, there were lively discussions with clear reference to the issues dealt with by these groups.

Discussion

By highlighting joint reasoning in mathematics and a field of STE, the theoretical

framework developed in this article breaks with the way modelling is conceived in mathematics education. It draws on science education research that considers the intermediary role of models between an empirical referent and a theoretical referent, but it also differs from this research by introducing mathematical reasoning as an important component of the theoretical referent.

In this new framework, covariations between quantities are models that account for processes perceived in the empirical referent. Covariations can be treated as dependencies between mathematical variables, thus establishing a link with the theoretical referent. The mathematical functions in this theoretical referent are then closely linked to the notions of a scientific field. Models can also serve as a basis for simulations of processes perceived in the empirical referent, thus providing a feedback link between theoretical and empirical referents. Epistemological considerations allow two important dimensions of modelling to be recognized: the plurality of models and teamwork between people with different points of view. These dimensions imply collaborative work on the models, refining and comparing them, as well as at the interface with the theoretical referent in order to account for the comparison.

School chemistry was chosen to illustrate and test this new framework, as it is a domain in which mathematics are generally not very present. This is particularly true of those mathematics, which enables algebraic-type reasoning rather than simple application of proportionality and arithmetic. To illustrate further, a laboratory technique has been chosen because there is evidence that students are generally trained in laboratory work without theoretical chemical or mathematical considerations. Two models of the process involved in this technique were proposed. The framework developed for this research was used to design tasks for grade 12 students, in which the

models are intended to play an intermediary role between the empirical referent of students trained in the technique, and a theoretical referent made up of mathematical and chemical elements enabling students to reason about a chemical reaction. The organization of tasks in a jigsaw classroom was chosen to allow students to work collaboratively from different points of view.

The students' achievements in the classroom implementations can be assessed in relation to the tasks and objectives for the jigsaw groups (three last lines of table 1.)

With regard to Tj₁, although the students clearly understood the quantitative covariation between the volume added and the pH after the report of G_c, the interpretation of this covariation as a dependency between variables was not spontaneous. The teacher's invitation to 'do the same calculation (...) not with 5 but with x' triggered the students' algebraic reasoning: 'a formula that actually calculates everything at once.' Despite the difficulties encountered in constructing a formula, the students seemed to recognize and appreciate the opportunity to 'understand in mathematical form the same problem studied in chemical form', as one student puts it in answer A2 above.

The students' work on Tj₂ (algebraic study of the tangent method) was disappointing. They had an adequate empirical estimate of the method's accuracy, thanks to the work done in G_a, but they failed to confirm with an algebraic calculation. It is surprising that grade 12 students were unable to calculate the tangent equations directly. The unusual form of the function may have been an obstacle. When students conclude 'we noticed that calculating the derivative allows us to obtain the gradients of tangents', it sounds like a discovery, which means that, although they have certainly been taught this, they had no previous opportunity to use this knowledge in context.

Context also implies dealing with approximation. Students have been confused by tangents that are supposed to be parallel, but do not have exactly the same gradient, and then drew a wrong conclusion contradicting an empirical observation. The observation points out the lack of time to solve this contradiction. Further implementations should take more into account the need for students to consolidate their understanding of the models especially between the first and the second stage. In addition to the need for time, dealing with approximation was a major difficulty: half the students misinterpreted the discrepancy between the software simulation and the mathematical function as the result of an approximate numerical calculation. Experienced scientists have no difficulty estimating whether a small difference due to approximation is or not significant. In contrast, the students need time and the help from the teacher.

The dissimilarity between the models (T_{j3}) was not investigated in the first implementation, although one student did notice a discontinuity in the function of model 2. The tasks were therefore revised for the second implementation: values of the base volume were suggested very close to the equivalence volume V_E ; the students had to examine the simulation code (model 1) and explain the loop in this code. As a result, the students became aware of the discrepancy. They should then have been able to conclude that Model 1 is closer to empirical observation, thanks to the water dissociation assumption introduced in the code. As observed above, half the students considered that model 2 was necessarily more accurate due to its algebraic nature. Beyond the difficulty in dealing with approximation analysed above, this suggests that teaching has constructed a representation of modelling that gives full confidence to algebraic models regardless of underlying simplifying assumptions. The fact that the other half of the class objected, pointing to the dissociation of water, indicates that tasks such as those

carried out in this implementation are able to challenge a misrepresentation of mathematical models.

Although sometimes disappointing or surprising, these findings help to understand students' difficulties with modelling, a consequence of the lack of adequate emphasis on models both in math and science courses.. Then this does not invalidate RQ1 and RQ2's assumptions about the potential of the tasks and their organization. While struggling with the tasks, and thanks to the mediation of the models, the students were confronted to mathematical reasoning in context, as well as to the notion of neutralization and chemical equilibrium in relation to the titration process. Collaboration in the second stage was productive thanks to the confrontation of the different areas of expertise acquired in the first stage.

Although two tasks mention models, the students didn't use this word. Instead, they referred to entities with which they were familiar: software for model 1 and function for model 2. This suggests, on the one hand, that the idea of models has not been emphasized in previous teaching, but also that the students' awareness that these entities play a role in relation to a concrete process is a good starting point for developing this idea.

Particular attention has to be paid to simulation. Wu et al (2021) reviewed 60 studies relating to technology-assisted learning in chemistry between 2010 and 2019 and found that most studies focused on student learning outcomes after the use of a computer simulation. The Ta task (version 1) follows this trend. The Ta task (version 2) is innovative. Whereas previous studies dealt with the use of a black-box computer simulation, this task introduces code analysis by the students (white-box simulation). The French mathematics curriculum includes algorithms and programming, so students

were able to carry out code analysis. However, this was a new subject in the classroom, which explains the difficulty of the task. It will become more familiar in the years to come, making tasks like version 2 even more relevant. This phenomenon is not unique to France: Fraillon et al. (2020a, p.34) reviewed school curricula in thirteen countries on three continents and found that ten countries included programming-related aspects, in particular the analysis of code, programs or macros.

There are other innovative aspects to the research presented in this paper. Firstly, covariation and mathematical function are deeply linked to chemistry in order to give meaning to a laboratory process and the associated method. Secondly, students are confronted with two different models, the comparison of which sheds light on the process. It is commonly accepted that for complex phenomena, it is advantageous to consider a plurality of models. For example, the geometric model of visibility at sea proposed in the study by Blum and Ferri (2009) could be usefully confronted with a model used by navigators, taking into account atmospheric refraction and a simplified formula. Curiously, this possibility is rarely offered to students at school. As Morgan and Morrison (1999) point out, "models teach us both about theories and about the world by providing concrete information about real physical and economic systems". The research presented in this paper suggests that this dual role is best achieved with complementary or alternative models. Finally, organizing the class as a jigsaw puzzle around specific model viewpoints encouraged productive collaboration between students.

The two implementations of tasks derived from the framework presented in this article are certainly not a conclusive validation of these innovations. They do, however, represent some progress towards STE ↔ M integration. Given current practices and

representations analysed in the introduction, there is a long way to go, and even small steps have their value.

This framework draws from a sciences education research and differs from frameworks in mathematics education in which mathematics and mathematical modelling competencies constitute the substantive part. The role of models as envisioned by sciences education research has proved consistent with an epistemological perspective. However, current approaches to sciences education research neglect the importance of mathematics in modelling. The classroom implementation suggests that the incorporation of mathematical reasoning is a sustainable step towards STE ↔ M integration, and opens up perspectives that exceed those offered by current STE and mathematics education frameworks. This should inspire researchers in both STE and mathematics education to consider how their theoretical frameworks might evolve in order to better support STE ↔ M integration.

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Annex 1: Models

The models 1 and 2 are instantiated below for the titration of a strong acid (for instance HCl) by a strong base (for instance NaOH). In this case the concentrations of oxoniums and hydroniums are equals at the equivalent point and then the pH at this point is 7.

The volume of acid is 8 ml and the concentration $[H_3O^+] = 0.0125$ mol/L. The concentration of base is $[OH^-] = 0.01$ mol/L.

Model 1

It is a computer simulation that calculates iteratively the concentrations and the pH along the titration. It takes into account the water self-ionization quantified by

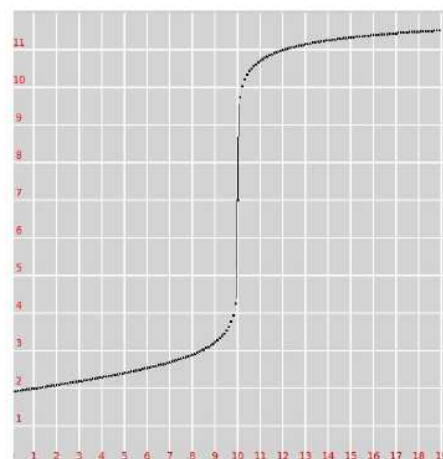
Table 2. The code of the simulation

1. *# Constant of water dissociation*
2. $K_w = \text{float}('1e-14')$
3. *# 1/100 ml added at each step*
4. $\text{AddedBase} = \text{float}('1e-5')$
5. *# Concentration of the reactant (mole/liter)*
6. $\text{Creactant} = 0.01$
7. *# Number of moles of reactant added at each step*
8. $\text{NbAdded} = \text{AddedBase} * \text{Creactant}$
9. *# Initial values of variables*
10. $\text{Vsol} = 0.008$ *# Initial volume in the becher (liters)*
11. $\text{H3Oplus} = 0.0125$ *# Initial concentration of acid (mole/liter)*
12. $\text{Nacid} = \text{Vsol} * \text{H3Oplus}$ *# Initial number of acid moles*
13. $\text{OHmoins} = K_w / \text{H3Oplus}$ *# Initial concentration of base (mole/liter)*
14. $\text{Nbase} = \text{OHmoins} * \text{Vsol}$ *# Initial number of basic moles*

```

15. def add():
16.     #Addition of base
17.     Nbase=Nbase+NbAdded
18.     Vsol =Vsol + AddedBase
19.     # product of number of base and acid at
        equilibrium
20.     Eq=K_w*Vsol*Vsol
21.     # number of moles neutralized at each step
22.     epsilon =Eq/(Nbase+Nacid)/10
23.     while Nacid*Nbase > Eq:
24.         # Neutralization
25.         Nacid = Nacid - epsilon
26.         Nbase = Nbase - epsilon
27.         # New acid concentration and pH
28.         H3Oplus=Nacid /Vsol
29.         pH=-log(H3Oplus,10)

```



The table 2 displays a part of the code the python language submitted to the students.

The lines 1 to 8 define the constants K_w and the characteristics of the reactant. The lines 10 to 14 initialize the variables, particularly the initial number of acid moles (Nacid) and of basic moles (Nbase), and the initial volume of the solution Vsol that will evolve along the process.

The lines 15 to 29 define the elementary procedure modelling the equilibrium after the addition of 1/100 ml of reactant. After the addition, the number of basic moles and the volume of the solution are updated and the expected product of number of base and acid at equilibrium Eq is calculated. The goal of the loop (lines 23 to 26) is to calculate the numbers of acid mole and base mole such that the hypothesis $Nacid \times Nbase = Eq$ (equivalent to $[H_3O^+] \times [OH^-] = K_w$) holds by operating neutralization by small volumes epsilon.ⁱⁱⁱ Finally after the loop, the lines 28 and 29 compute the concentration in oxoniums and the pH. Plotting the pH against the volume of solution and repeating 2000 times, a graph is obtained (right).

Model 2

It is a mathematical function based on a simplifying assumption: oxoniums and hydroxides do not coexist in the solution.

With a volume 8 ml and a concentration $[\text{H}_3\text{O}^+] = 0.0125 \text{ mol/L}$, the number of acid moles is initially 10^{-4}

x volume of base added in ml. With a concentration $[\text{OH}^-] = 0.01 \text{ mol/L}$, $x \cdot 10^{-5}$ basic moles are added.

Below the equivalent point ($x < V_E$) the added basic moles neutralize with the same quantity of acid.

The number of acid moles, initially 10^{-4} , is $10^{-4} - x \cdot 10^{-5}$.

The volume of the solution, initially $8 \cdot 10^{-3}$, is $(8+x) \cdot 10^{-3}$

Hence the concentration in oxonium is

Above the equivalent point ($x > V_E$) the acid moles initially 10^{-4} have been entirely neutralized with the same quantity of base. The remaining quantity of base is $x \cdot 10^{-5} - 10^{-4}$. Hence the concentration in hydroxide is:

The pH is calculated from the above concentrations:

for $x < 10$: $f(x) = -\log$

for $x > 10$: $f(x) = 14 + \log$

Annex 2. The tangent method

Mathematically, the tangent method is based on the symmetry of a curve with regard to a point. In this case, two parallel tangents to symmetrical branches are also symmetrical.

The centre of symmetry lies on the midline between the tangents.

Consider the function f of model 2 above.

$$\frac{1}{2}(f(x) + f(20-x)) = 7 + R(x) \text{ with } R(x) = \frac{1}{2} \log\left(\frac{8+x}{28-x}\right)$$

$R(10) = 0$, $R(11) = -R(9) \approx 2.5 \cdot 10^{-2}$. R is mostly negligible in the vicinity of 10.

It means that the curve of f is nearly symmetrical with regard to the point (10 ; 7). Thus the construction by the tangent method yields to a point very near to this point if the points of tangency are close to the jump. So the method has to be applied with positions of the tangents not too far from the jump. Tangents should also not be drawn too close to the jump in order that the midline intersects the curve at an angle.

Symmetry of curves and tangents are not in the French secondary curriculum, thus a reasoning like above cannot be expected from students. Yet, they can use the function f to compute equations of the tangents using a formula like

$Y = f'(x)(X - x) + f(x)$ for a tangent at $(x; f(x))$, and then of the midline. V_E is computed as the x-coordinate of the point on the mid-line of y-coordinate 7, the pH of a neutral solution. Applying around the jump one can get an evaluation of the accuracy of the method in given points as in the table 3. The table displays three choices of points C and D of the curve for which tangents are nearly parallel. For each choice, the equations are computed using the above formula. The equation of the midline has the same directional coefficient and the ordinate at the origin is the mean of those of the two tangents. The equivalent volume V_E is the x-coordinate of the point on this line whose y-coordinate is 7. Calculation shows that the choice of C and D close to the jump gives the better approximation of the equivalent volume.

Table 3. The tangent method applied to three pairs of tangents.

<p>C and D are the points on the curve with x-coordinate respectively 5.01 and 13.</p> <p>The equation of the midline is $y=0.12x + 5.7$ and then the equivalent point given by the method is for</p> $= \frac{7-5.7}{0.12} \cong 10.83$ <p>V_E</p>	<p>C and D are the points on the curve with x-coordinate respectively 9.04 and 10.9.</p> <p>The equation of the midline is $y=0.48x + 2.18$ and then the equivalent point given by the method is for</p> $= \frac{7-2.18}{0.48} \cong 10.04$ <p>V_E</p>	<p>C and D are the points on the curve with x-coordinate respectively 9.5 and 10.5.</p> <p>The equation of the midline is $y=0.89x - 1.90$ and then the equivalent point given by the method is for</p> $= \frac{7+1.9}{8.9} = 10$ <p>$V_E = 7+1.9-V_E$</p>

- i In this paper, algebra is extended to expressions made up of constants, variables and basic functions (such as the logarithms) linked by arithmetic operations.
- ii The idea of jigsaw class was introduced to enable pupils in recently desegregated schools to interact in ways that reduce suspicion and mistrust. The benefits in achievement, peer attitudes and prejudice have been discussed in psychology research. What is expected here is different: the organization of the puzzle is aimed at student collaboration, but the collaboration is between experts in specific aspects of a question, rather than between learners with specific profiles.
- iii In textbooks, the equilibrium is calculated by solving a quadratic equation. A loop calculation has been chosen in order to make the process closer to the intuitive idea of neutralization. In the code, epsilon is calculated in order that the relative error on the product of concentrations at equilibrium is below 1/10. Implementing the solution of the quadratic equation instead of the loop would be faster but not congruent to the process of neutralization.