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what does that take?

Blomhøj, Morten; Niss, Mogens Allan

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Decoding, understanding, and evaluating extant mathematical models: what does that take?

Descodificar, compreender e avaliar modelos matemáticos existentes: o que é que isso requer?

Morten Blomhøj
Danish School of Education, Aarhus University
Denmark
blomhoej@edu.au.dk

Mogens Niss
IMFUFA, Roskilde University
Denmark
mn@ruc.dk

Abstract. The far majority of theoretical and empirical studies in the didactics of mathematical modelling focus on actively putting mathematics to use in dealing with extra-mathematical contexts and situations. However, modelling competency as conceptualised in, e.g., the Danish KOM Project, also involves the ability to analyse and relate to extant mathematical models. This ability has only been sparsely considered in research. The present paper proposes a systematic approach to such investigations. It takes its departure in in-depth accounts and analyses of two extant models, the so-called Reilly model of the attraction of shopping centres, and the well-established Michaelis-Menten model of enzyme kinetics. The paper aims at identifying what it takes to grasp and critically analyse such and other extant models and finishes by outlining didactical consequences for fostering students' ability to undertaking model analysis, a highly important component of the modelling competency.
Keywords: modelling competency; authentic models; critical model analysis; didactical consequences.

Resumo. A grande maioria dos estudos teóricos e empíricos na didática da modelação matemática foca-se em colocar ativamente a matemática em utilização para lidar com contextos e situações extramatemáticos. Contudo, a competência de modelação matemática, tal como é entendida, por exemplo no Projeto KOM Dinamarquês, também envolve a capacidade de analisar e de compreender modelos matemáticos existentes. Essa capacidade tem sido apenas residualmente considerada na investigação. O presente artigo propõe uma abordagem sistemática para produzir tais estudos. O artigo tem como ponto de partida a análise e a descrição detalhada de dois modelos existentes, o

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chamado modelo Reilly da atração de centros comerciais e o modelo bem estabelecido da cinética enzimática de Michaelis-Menten. O artigo visa identificar o que é necessário para captar e analisar criticamente esses e outros modelos existentes e termina com a apresentação de consequências didáticas para promover a capacidade dos alunos de fazer a análise de modelos, uma componente altamente importante da competência de modelação.
Palavras-chave: competência de modelação; modelos autênticos; análise crítica de modelos; consequências didáticas.

Introduction: modelling competency

Internationally, development of and research on mathematical models and modelling in the context of mathematics education has primarily focused on fostering and furthering students' ability to undertake active modelling of extra-mathematical situations. This is not at all surprising, given how important this ability is for students' current and future lives as well as for society at large. The emphasis on active modelling has given rise to the introduction of the notion of modelling competency and its cognates and to lots of theoretical and empirical papers about this notion (Blomhøj & Jensen, 2003; Kaiser & Brand, 2015). Blum (2015) gives an overview of what has been achieved in this endeavour.

While most definitions of mathematical modelling competency (and (sub)competencies) (see, e.g., Niss & Blum, 2020) focus on individuals' ability to engage in active modelling work, there is, in fact, another important aspect of modelling competency worthy of consideration, even if this aspect has received less attention in the literature. In this paper, we shall adhere to the characterisation of the modelling competency offered in the Danish KOM project (Niss & Jensen, 2002), also adopted in much of the modelling literature (e.g., Niss, Blum & Galbraith, 2007). The following definition is quoted from (Niss & Højgaard, 2019, p. 16):

> This competency focuses on mathematical models and modelling, i.e., on mathematics being put to use to deal with extra-mathematical questions, contexts and situations. Being able to construct such mathematical models, as well *as to critically analyse and evaluate existing or proposed models, whilst taking purposes, data, facts, features and properties of the extra-mathematical domain being modelled into account*, are the core of this competency. (Our italics)

The italicised part of this characterisation is our focus in this paper. The ability to critically analyse and evaluate existing or proposed models is sometimes named the analytic aspect of the modelling competency, to distinguish it from the active or constructive aspect of the competency. Although the analytic aspects have been present in the discussion for quite some time, very little research has been done on what it takes to be able to handle the analytic aspect of the modelling competency, both in conceptual/theoretical and in empirical terms. This gives rise to the following

Research question (RQ): What are the key epistemological and cognitive components involved in the ability to handle the analytic aspects of the modelling competency?

The reason why in the RQ we emphasise the epistemological and cognitive components of the analytic aspect of the modelling competency is not that we find affective, dispositional and volitional components unimportant. Rather, we see them as conceptually and analytically distinct from the epistemological and cognitive ones, so the two sets of components ought not to be mixed up. The approach taken in this paper to answer the research question is of a conceptual and theoretical nature. So, we are not, in this paper, offering any empirical investigations into individuals' actual dealing with the analytic aspect of the modelling competency. As to methodology, we analyse, in considerable detail, two examples of extant models presented in written form in the English version of WikipediA. This presentation of the model then constitutes the primary data on that model. In each case, multiple other descriptions of the same or a very similar model can be found in other publications, or in oral presentations such as lectures, but such descriptions will not be taken into consideration in our analysis. This implies that we are not dealing with each model as an equivalence class of all the existing presentations of what may be perceived or known as "that model", but with the specific version retrieved from WikipediA and presented verbatim below. The reason for this is that the analytic aspect of the modelling competency will only be exercised when an individual is confronted with a specific prima facie presentation of a model and tries to come to grips with it as it stands. Of course, in "real life", a person analysing a model will have access to various sources. However, in order to establish a well-defined methodological basis for answering the research question, we delimit our analyses to an imagined situation where the WikipediA presentation is the only source of information for analysing the model in each of the two examples. Thus, our analyses of the models are delineated by the selected presentations. At certain points in the analyses, however, it is relevant to include information from background disciplines or areas of application related to the models. We will be explicit about such aspects when considered.

As part of our method in this paper, we have chosen WikipediA as our data source rather than more or less randomly selected article or textbook versions of the models at issue, because the WikipediA versions are accessible to a wide public and is oftentimes, by many people, used as a first source of information on a topic. So, WikipediA was not chosen as a result of an assessment of the quality of the exposition of the models. Actually, one of the points in this paper is that we do have serious issues with the model expositions. The fact that the WikipediA versions of the models constitute our date source also implies that we are not free to change the presentations at will. That would distort our object of study. After the presentation of the model, one is, of course, free to interpret what is being stated in the presentation as long as the interpretation pays due respect to formulations given in the presentation.

Based on our detailed analyses of the two examples of model presentations, we will attempt to extract some general features of model analysis and of the analytic part of the modelling competency. In that respect the two examples do, at least to some extent, serve as generic examples.

Two examples of extant models

Obviously, selecting just two model examples for analysis among a plethora of extant examples involves a lot of considerations, but cannot avoid, however, being somewhat haphazard. The most important selection criteria adopted were the following: The models should not be too well-known standard examples from publications on models and modelling. However, they should be authentic in the sense that they are accepted as serious models in their respective fields. We wanted one of them to be a qualitative model in the social sciences built on an essential idea borrowed from a natural science domain, without it pretending to offer an accurate quantitative description of the situation it purports to model. We wanted the other example to be a crucial model – generally recognised and utilized, both in qualitative and in quantitative terms – within an established discipline of natural science. Finally, it was important that the models were not so specialised or technically complicated that they could not be introduced, within a relatively limited space, to well-educated readers in the didactics of models and modelling who are not, however, experts in the specific domains of the models, while also making sufficient room for thorough analysis. Needless to say, a multitude of alternative choices satisfying these criteria could have been made instead. Nevertheless, we want to maintain that our examples are sufficiently rich, both with regard to their extra-mathematical features and with regard to the mathematics involved, to allow for bringing forward significant analytic characteristics.

In what follows we focus on the presentations of the models only, not on their actual or potential use.

Example 1: Reilly's law of retail gravitation (quoted from WikipediA)

> In economics, Reilly's law of retail gravitation is a heuristic developed by William J. Reilly in 1931 [Reilly, 1931]. According to Reilly's "law", customers are willing to travel longer distances to larger retail centers given the higher attraction they present to customers. In Reilly's formulation, the attractiveness of the retail center becomes the analogy for size (mass) in the physical law of gravity.
>
> The law presumes the geography of the area is flat without any rivers, roads or mountains to alter a customer's decision of where to travel to buy goods. It also assumes consumers are otherwise indifferent between the actual cities. In analogy with Newton's law of gravitation, the point of indifference is the point at which the "attractiveness" of the two retail centres (postulated to be proportional to their size and inversely proportional to the square of the distance to them) is equal:

$$\frac{d_A}{d_B} = \sqrt{\frac{P_A}{P_B}},$$

where d_A is the distance of the point of indifference from A, d_B its distance from B, and P_A/P_B is the relative size of the two centres. If the customer is on the line connecting A and B, then if D is the distance between the centres, the point of indifference as measured from A on the line is

$$d = \frac{D}{\left(1 + \sqrt{\frac{P_A}{P_B}}\right)}$$

As expected, for centres of the same size, $d = \frac{D}{2}$, and if A is larger than B, the point of indifference is closer to B. As the size of A becomes very large with respect to B, d tends to D, meaning the customer will always prefer the larger centre unless they're very close to the smaller one.

We begin the analysis of this model by identifying its basic elements, which appear with varying degrees of explicitness in the text. All elements are introduced in the 2nd paragraph. Firstly, the model involves two retail centres, A and B, which are located as points in a homogeneous plane. The distance between them is the magnitude D (dimension "length"). The centres are referred to as "actual cities", whose "attractiveness" is measured by their sizes, P_A and P_B, respectively. It is not specified what "size" means, but the choice of the symbols P_A and P_B seems to suggest that "size" is equal to "population size". This also corresponds to the gravitational analogy according to which a fixed point mass attracts another point mass according to Newton's law of gravitation. Secondly, the model refers to a so-called "point of indifference" such that a customer positioned at that point is indifferent to shopping in A or in B. By speaking of "the point of indifference" it is tacitly taken for granted that there is only one such point, which by the way is not denoted by a symbol in the text. The final basic elements of the model are the distances d_A and d_B of the point of indifference to A, respectively B. Without stating it explicitly, the goal of the model is to obtain a formula to determine d_A for the point of indifference for a customer positioned on the line connecting A and B. This value is denoted by the symbol d.

Now let us look at the explicit and implicit *assumptions* that are in play in the formulation of the model. The first two assumptions are that a customer's choice of which of the two centres to shop in is solely determined by the sizes of the centres A and B and the customer's distance to them. Then comes the key assumption, formulated in qualitative and partly implicit - in some cases even vague - terms, that for each point in the plane the "attractive-ness" of each retail centre for a person positioned in that point is directly proportional to the size of the centre and inversely proportional to the square of the person's distance to it. This assumption is stated as being in analogy with Newton's law of gravitation in physics, where "mass" (of a physical object) is replaced by "size" (of a city). The final, although rather implicit, assumption is that only points on the line connecting A and B are of interest as points of indifference, and as mentioned above it is tacitly assumed that there is only one such point.

The choosing of elements and the making of the assumptions listed above constitute a process oftentimes called *pre-mathematisation* as it is crucial in preparing the situation for subsequent mathematisation.

The core of the construction of the model is the *mathematisation*. Taking its point of departure in the qualitative statement of the "gravity" attractiveness postulate, mathematisation consists in stating the equation

$$(*)\ \frac{d_A}{d_B} = \sqrt{\frac{P_A}{P_B}}.$$

No comments are offered in the text to explain how this equation follows from the attractiveness postulate, which in the formulation given is not identical to the equation.

Once the model has been established it is used to obtain the conclusion that, for a customer on the line between A and B, d is determined by the formula

$$(**)\ d = \frac{D}{\left(1+\sqrt{\frac{P_A}{P_B}}\right)}.$$

The pathway leading to this conclusion is invisible in the text.

The final part of the modelling undertaken is to draw consequences for the location of the "real world" point of indifference of different initial sizes of the centres A and B: if the centres have the same size, if A is larger than B, and finally if A is much larger than B. In the latter case it is concluded that customers will always prefer to shop in the larger centre, unless "they're very close to the smaller one". This last statement is not explicitly corroborated by the model as described. Rather, its status is that of an additional assumption.

It is interesting to observe that the text makes no attempt to evaluate the model, except by noting that the consequences of equal sizes for A and B, and of A being larger than B are "as expected". It is also interesting to note that no units are mentioned in the presentation text.

Up till this point, we have familiarised ourselves with Reilly's model by identifying its different underlying ideas and components. Along the road we encountered some obscure, vague or missing points, especially as far as explanations are concerned. The next step in our analysis is to try to *understand* and *make sense of the model* and its description. In so doing, we focus on understanding how the analogue of Newton's gravitation model in the context of retail is actually constituted, since the presentation text explicitly refers to that model. For this to be possible it is necessary to activate knowledge of Newtonian gravitation that is not spelled out in the text. According to the law of gravitation, two physical objects with centres at the distance d between them and masses m_1 and m_2, respectively, exert a gravitational attraction of each another given by the magnitude Gm_1m_2/d^2, where G is the gravitational constant (measured in kg·m/sec^2). If one of the objects has mass 1, say $m_1 =$

1, the gravitational attraction from the other object is $G \cdot m_2/d^2$. For physical masses being replaced by (population) sizes P_A and P_B it is assumed that centres A and B attract an individual positioned at distance d_A from A and d_B from B, by the "forces" P_A/d_A^2 and P_B/d_B^2, respectively. It is important to observe that this does not require the individual to be positioned on the line connecting A and B. With this in hand we can then ask: What can we say about the relationship between the variables P_A, P_B, d_A and d_B for an individual positioned at a point in which the attraction from the two centres A and B are identical? Well, for such a point $P_A/d_A^2 = P_B/d_B^2$, which implies that, which is exactly equation (*). So, the mathematisation presented in equation (*) actually is derived from a preliminary mathematisation consisting of translating the verbally formulated centre attractions into mathematical expressions P_A/d_A^2 and P_B/d_B^2, and subsequently equating them.

It is interesting to observe that the presentation text makes no attempt to justify the use of Newton's law of gravitation in the context of economic geography. This suggests that the mere invocation of an analogy borrowed from a well-established scientific field is supposed to be convincing in and of itself.

If the point of indifference is located on the line between A and B, being at the distance D from each other, equation (*) yields $d_A/(D - d_A) = d_A/d_B = \sqrt{P_A/P_B}$, which implies that $d_A = (D - d_A)\sqrt{P_A/P_B}$, from which we obtain $d_A + d_A\sqrt{P_A/P_B} = D\sqrt{P_A/P_B}$, and further

$$d_A = \frac{D\sqrt{P_A/P_B}}{\left(1+\sqrt{P_A/P_B}\right)} = \frac{D}{\left(1/\sqrt{P_A/P_B}+1\right)} = \frac{D}{\left(\sqrt{P_B/P_A}+1\right)}$$

which is exactly equation (**) with d_A replaced by d. This step consists of drawing mathematical consequences of (*), while implicitly making use of the relationship $D = d_A + d_B$, which in turn presupposes that the point of indifference is located between the centres A and B. As already mentioned, the presentation text takes it for granted that there are no other indifference points on the line connecting A and B. We return to this issue below.

In order to come to grips with the model as presented it was necessary to perform some "model archaeology", i.e. to uncover quite a bit of tacit or hidden components of the model. So, by adding assumptions that aren't explicit in the quoted presentation of Reilly's model, we were able to uncover the way in which the model was most probably generated as well as the conclusions arrived at by means of the model.

As the presentation text offers no *evaluation* of the model, a reader who would like to see such an evaluation would have to undertake it him- or herself. In what follows, we'll be outlining a brief evaluation of the Reilly model, without going into excessive detail. There are several ways to evaluate a mathematical model, including: (1) Evaluating the grounds on which it has been built, including the assumptions, simplifications and choices made; (2) evaluating outcomes of the model vis-à-vis its original purpose, including confronting these outcomes with known facts and data; (3) evaluating qualitative properties of the model, especially with regard to its scope and range; and (4) evaluating the actual or potential use of the model.

As to evaluation mode (1), the model rests on two ideas, one being an analogy between commercial attraction and gravitational attraction in which “size” of a city and mass of a physical object are the sources of attraction, and the other one being an analogy between the strength of the attraction in the two cases as being inversely proportional to the squared distance between the attracting and the attracted entity. While in mechanical gravitation attraction works both ways between the two objects – they are both attracting and attracted objects - this makes no sense when it comes to retail attraction, since an individual customer does not attract a centre. The analogy between the commercial and the physical situation is not supported by intrinsic features and properties of the two situations beyond the very idea inherent in the notion of “attraction”. Moreover, the fact that the distance in the physical situation occurs in the model exactly as its squared inverse, and not in any other of infinitely many possible forms, is deeply rooted in the nature of physical space itself and in the nature of gravitational force, whereas nothing similar can be said about the way distance occurs in the retail situation. So, in this situation the inverse power of 2 is just a result of sheer emulation. Furthermore, in the Reilly model there is no explicit analogy to the gravitational constant G. Therefore, the unit of the attraction to a centre experienced by a customer seems to be calculated in the model in the unit m^{-2}, which does not make any sense at all. Altogether, the conceptual foundation of the Reilly’s model is nothing but “associational inspiration” from Newtonian gravitation, which means that a serious evaluation of the model has to rest on the other three evaluation modes listed.

When it comes to evaluating the outcomes of the model vis-à-vis its purpose – mode (2) – this would require some form of empirical set-up in which the behaviour of actual customers living in some area with at least two retail centres of different sizes could be investigated. The purpose would be to find out whether the centres do in fact attract customers according to Reilly’s “law “. Setting-up a reasonable empirical study that could yield trustworthy data to admit such an investigation would be a very demanding and sophisticated task, which would go far beyond the possibilities of the average reader of the model exposition. Apart from that, the common-sensical comments in the text that the location of the point of indifference in various situations is “as expected” can be perceived as a (very limited) qualitative evaluation of the outcomes of the model in one particular respect.

Evaluation of the qualitative properties of the model – mode (3) – can take several different forms. Here, we shall focus on one aspect only. According to the model, what are the possible points of indifference in the plane? Is there only one, as suggested in the presentation text, which is located on the line connecting A and B? If not, what other indifference points are there?

To answer this question, let us introduce a coordinate system, whose first axis is the line connecting A and B, and whose second axis is the line perpendicular to the first axis through the point A, placing A in the origin. So, the coordinates of A are $(0,0)$, and of B $(D,0)$. For an arbitrary point $P(x,y)$ in the plane, the "Reilly attraction" of P from A is $P_A/(x^2+y^2)$, whereas the attraction of P from B is $P_B/((x-D)^2+y^2)$. P is a point of indifference if and only if

$$(\Delta)\ \frac{P_A}{x^2+y^2} = \frac{P_B}{(x-D)^2+y^2}$$

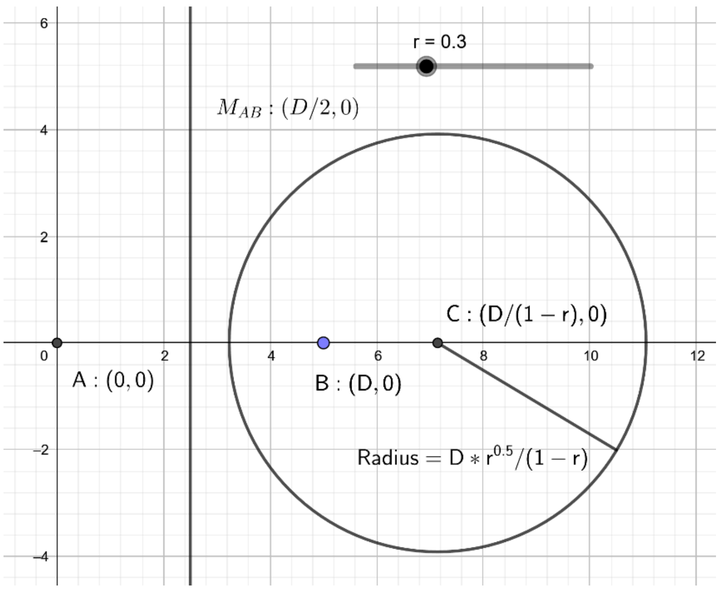

Figure 1. The points of indifference in the cases $P_B/P_A = 1$ and $r = P_B/P_A = 0.3$

In case $P_A = P_B$, points of indifference are those that satisfy the equation $x^2+y^2 = (x-D)^2+y^2$, i.e., the equation $x^2 = (x-D)^2$, the solution of which is $x = D/2$, while y can take any value. In other words, in this special case, the points of indifference are all points of the form $(D/2y)$, y arbitrary, corresponding to the midpoint normal of the line segment between A and B.

If $P_A \neq P_B$, equation (Δ) is equivalent to $P_A((x-D)^2+y^2) = P_A(x^2+y^2)$, which after a few calculations and some rearranging is equivalent to the equation (noting that $P_A \neq P_B$)

$$x^2 - x^2 P_A D/(P_A - P_B) + y^2 = -P_A D^2/(P_A - P_B).$$

Letting $r = P_B/P_A\ (\neq 1)$ and factoring P_A out in the two fractions, this equation takes the form

$$x^2 - 2xD/(1-r) + y^2 = -D^2/(1-r).$$

Completing the square of the quadratic polynomial in x on the left-hand side and rearranging yields

$$(x-D)/(1-r)^2 + y^2 = D^2 r/(1-r)^2.$$

This shows that the points of indifference in the plane are exactly the points on the circle with the centre $(D/(1–r), 0)$ and radius $D\sqrt{r}/|1 - r|$. Since this circle of indifference intersects the line through A and B, the first axis, in the two points $(D/(1 - r) - D\sqrt{r}/|1 - r|, 0)$ and $(D/(1 - r) + D\sqrt{r}/|1 - r|, 0)$ that line actually contains two indifference points and not only one as suggested in the presentation text.

This analysis shows that, and how, the construction principles on which the Reilly model is based lead to a much wider range of consequences than those pointed out in the presentation text. To assess whether this is reasonable, one has to look at the different possible instances of these consequences. For example, if $r = P_B/P_A = 2$, i.e., if B is twice as attractive as A, the centre of the indifference circle is located to the left of A, at $(-D, 0)$, and so is the leftmost indifference point on the line connecting A and B, namely $(-D– D\sqrt{2}, 0)$. This implies that a person positioned in that point is indifferent to shopping in A, at the distance $D + D\sqrt{2}$ away from the shopper, or in B at the distance $2D + D\sqrt{2}$ away from the shopper. It appears to be less than reasonable to drive markedly farther through A to B, than just to A, in a situation where A and B are equally attractive. This is a consequence of the very assumption behind the Reilly model: That "shopping centre attraction" is analogous to Newtonian gravitation.

As finally regards mode (4), it is not clear what actual or potential use may be made of the Reilly model as presented in the WikipediA text, except perhaps to understand how people positioned in an area containing A and B would behave when it comes to making shopping decisions. In view of the oddities and weaknesses uncovered by the evaluation outlined above, this goal would require a very convincing result of an empirical evaluation as indicated in mode (2).

Example 2: The Michaelis-Menten model of enzyme kinetics (quoted – in excerpts – from WikipediA)

> In biochemistry, Michaelis-Menten kinetics is one of the best-known models of enzyme kinetics. It is named after German biochemist Leonor Michaelis and Canadian physician Maud Menten. The model takes the form of an equation describing the rate of enzymatic reactions, by relating reaction rate v (rate of formation of product, [P]) to [S], the concentration of a substrate S. Its formula is given by
>
> (#) $V = d[P]/dt = V_{max} [S] / (K_M + [S])$.
>
> This equation is called the Michaelis-Menten equation. Here, V_{max} represents the maximum rate achieved by the system, happening at saturating substrate concentration. The value of the Michaelis constant K_M is numerically equal to the substrate concentration at which the rate is half of V_{max}. Biochemical reactions involving a single substrate are often assumed to follow Michaelis-Menten kinetics, without regard to the model's underlying assumptions.

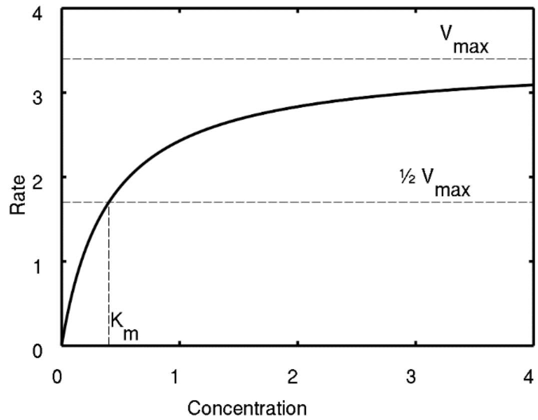

Figure 2: Reaction velocity as function of the substrate concentration (WikipediA)

Model:

In 1901, French physical chemist Victor Henri found that enzyme reactions were initiated by a bond (more generally, a binding interaction) between the enzyme and the substrate. His work was taken up by [...] Michaelis and [...] Menten, who investigated the kinetics of an enzymatic reaction mechanism, invertase, that catalyzes the hydrolysis of sucrose into glucose and fructose. In 1913, they proposed a mathematical model of the reaction. It involves an enzyme, E, binding to the substrate, S, to form a complex, ES, which in turn releases a product P, regenerating he original enzyme. This may be represented schematically as

$$\mathrm{E} + \mathrm{S} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{ES} \xrightarrow{k_{\mathrm{cat}}} \mathrm{E} + \mathrm{P}$$

where k_f (forward rate constant), k_r (reverse rate constant), and k_{cat} (catalytic rate constant) denote the rate constants, the double arrows between S (substrate) and ES (enzyme-substrate complex) represent the fact that enzyme-substrate binding is a reversible process, and the single forward arrow represents the formation of P (product).

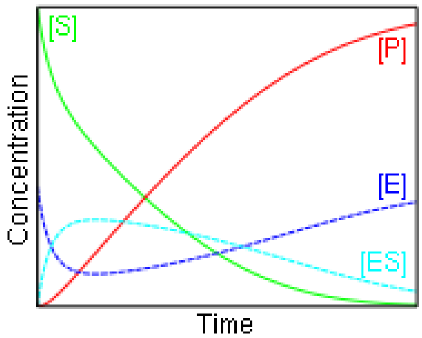

Figure 3. Model results: Reactant concentrations as functions of time (WikipediA)

Under certain assumptions – such as the enzyme concentration being much less than the substrate concentration – the product formation rate is given by

$$v = d[P]/dt = V_{max}\,[S] \;/\; (K_M + [S]) = k_{cat}\,[E]_0\,[S] \;/\; (K_M + [S]).$$

The reaction order depends on the relative size of the two terms in the denominator. At low substrate concentrations $[S] << K_M$, so that the reaction rate k_{cat} $[E]_0$ $[S]$ / K_M varies linearly with substrate concentration [S] (first-order kinetics). However at higher [S] with

[S] >> K_M, the reaction becomes independent of [S] (zero-order kinetics) and asymptotically approaches its maximum rate $V_{max} = k_{cat} [E]_0$, where $[E]_0$ is the initial enzyme concentration. This rate is attained when all enzyme is bound to substrate. K_{cat}, the turnover number, is the maximum number of substrate molecules converted to product per enzyme molecule per second. Further addition of substrate does not increase the rate which is said to be saturated.
[...]

Derivation:

Applying the law of mass action, which states that the rate of reaction is proportional to the product of the concentrations of the reactants (i.e. [E][S]), gives s system of four non-linear ordinary differential equations that define the rate of change of reactants with time t [ODE labelling is ours]

[ODE1] $d[E]/dt = -k_f [E][S] + k_r [ES] + k_{cat} [ES]$

[ODE2] $d[S]/dt = -k_f [E][S] + k_r [ES]$

[ODE3] $d[ES]/dt = k_f [E][S] - k_r [ES] - k_{cat} [ES]$

[ODE4] $d[P]/dt = k_{cat} [ES]$.

In this mechanism, the enzyme is a catalyst, which only facilitates the reaction, so that its total concentration, free plus combined, $[E] + [ES] = [E]_0$ is a constant (i.e. $[E]_0 = [E]_{total}$). This conservation law can also be observed by adding the first and third equations above.

Equilibrium approximation:

In their original analysis, Michaelis and Menten assumed that the substrate is in instantaneous chemical equilibrium with the complex, which implies
kf [E][S] = kr [ES].

This is in fact the law of mass action for the first reaction. From the enzyme conservation law, we obtain $[E] = [E]_0 – [ES]$. Combining the two expressions above, gives us

$k_f ([E]_0 – [ES]) [S] = k_r [ES]$, $k_f [E]_0 [S] – k_f [ES] [S] = k_r [ES]$,

$k_r [ES] + k_f [ES] [S] = k_f [E]_0 [S]$

$[ES](k_r + k_f [S]) = k_f [E]_0 [S]$, $[ES] = k_f [E]_0 [S] / (k_r + k_f [S])$,

$[ES] = k_f [E]_0 [S] / k_f (k_r /k_f + [S])$.

Upon simplification, we get

$[ES] = [E]_0 [S] / (K_d + [S])$,

Where $K_d = k_r / k_f$ is the dissociation constant for the enzyme-substrate complex. Hence the velocity v of the reaction – the rate at which P is formed – is

$$V = d[P]/dt = V_{max} [S]/(K_d + [S]),$$

where $V_{max} = k_{cat} [E]_0$ is the maximum reaction velocity.

Quasi-steady-state approximation:

An alternative analysis of the system was undertaken by British botanist G.E. Briggs and British geneticist J.B.S. Haldane in1925. They assumed that the concentration of the intermediate complex does not change on the time-scale of product formation - known as the quasi-steady-state assumption or pseudo-steady-state hypothesis. Mathematically, this assumption means that:
k_f [E][S] = k_r [ES] + k_{cat} [ES] = (k_r + k_{cat}) [ES].

This is mathematically the same as the previous equation, with k*r* replaced by k*r* + k*cat*. Hence, following the steps as above, the velocity v of the reaction is
v = V*max* [S] / (K_M + [S]),
where K_M = (k_r + k_{cat})/k_f is known as the Michaelis constant.

In order to come to grips with the Michaelis-Menten model as just presented, we begin by identifying its *basic elements* from the presentation above. The most important elements are four chemical substances, a substrate S, an enzyme E, an enzyme-substrate complex ES, and a product P, all involved in a chemical reaction, which in fact consist of three different reactions. The respective concentrations [S], [E], [ES], [P], are all perceived as functions of time t. The original concentration of the enzyme added to the chemical reactor is $[E]_0$. Next comes the reaction velocity, v, the rate of change for the product P:

v = d[P]/dt,

the catalytic rate constant k_{cat} characteristic of the production of P:

$$ES \xrightarrow{k_{cat}} E + P,$$

the forward rate constant k_f concerning the formation of ES:

$$E + S \xrightarrow{k_f} ES,$$

and k_r, the reversed rate constant concerning the dissociation of ES into E and S:

$$E + S \xleftarrow{k_r} ES.$$

These rate constants are proportionality constants characterizing the three reaction rates for the processes expressed in ODEs 1-4. In addition, the final model involves two constants, V_{max}, the maximum reaction velocity for the production of P, and K_M, the Michaelis constant.

The Michaelis-Menten model rests on quite a number of assumptions, some of which are made explicit in the presentation text, whereas others are implicit. The most fundamental assumptions are of a rather general chemical nature. Firstly, it is (tacitly) assumed that all chemical reactions take place in a closed system with free motion of the molecules and are determined by the concentrations of the substances at any time. In vitro, in a chemostatic environment for experiments or enzymatic production, the concentrations can be measured and controlled within a constant volume. In vivo, in living cells, the situation is of course more complicated. The basic assumption is that the concentrations of the substance are well-defined in a closed system, and that the reactions in a state of quasi-equilibrium are governed by the law of mass action. Moreover, there is a reversible process by which an enzyme added to the substrate gives rise to a complex composed of the two substances and that this complex can be decomposed into the original constituents. The third process by which the enzyme-substrate complex releases a product (P), implicitly stemming from the substrate, and regenerates the original enzyme is - in the model as presented - assumed to be irreversible. In other words, the production process is catalysed by the enzyme without actually consuming it.

In the derivation of the model additional assumptions are made. First of all, it is tacitly assumed that the enzyme has one active site only, and that the formation of one product molecule releases one intact enzyme molecule. Secondly, it is further assumed that the total concentration of the enzyme in free or in bounded form is constant, i.e., $[E] + [ES] = [E]_0$. And it is assumed that the reaction rate for the product P at all times is proportional (proportionality constant k_{cat}) to the concentration of the complex, [ES], and that the entire set of reaction rates are engaged in balancing the rate of change of the [E], [S], and [ES] according to the four ODEs governing the system.

When it comes to the approximations made, the equilibrium approximation rests on the assumption that the substrate and complex are in instantaneous chemical equilibrium, meaning that the rate of change of [S] is 0, i.e. $d[S]/dt = 0$, which implies (ODE2) that $k_f[E][S] = k_r[ES]$. In contrast, the quasi-steady-state approximation rests on the assumption that the rate of change of [ES] during the product formation is 0, i.e.,

$d[ES]/dt = 0$, which implies (ODE3) that $k_f[E][S] = k_r[ES]+k_{cat}[ES]$.

As with any mathematical model, the core of the Michaelis-Menten model is the *mathematisation* undertaken. In the presentation text, in addition to choosing the elements seen as relevant for the enzymatic reaction and making the assumptions listed above, taken at face value the key component of the mathematisation consists in stating the Michaelis-Menten equation (#):

$v = d[P]/dt = V_{max}\, [S] / (K_M + [S])$

However, in the text this equation is in fact a result derived from the underlying system of four linked ODEs, ODE1-4, representing the dynamics of the chemical system at issue. In other words, these ODEs actually constitute the fundamental mathematisation of the system. Based on mathematical deductions and the activation of the assumption of enzyme conservation and the quasi-steady-state assumption that the concentration of the complex remains constant, the Michaelis-Menten equation is obtained by also observing that the theoretical maximum production velocity for P, i.e. the maximum value of

$$d[P]/dt = k_{cat}[ES] = k_{cat}([E]_0 - [E]) \le k_{cat}[E]_0, \text{ has to be } k_{cat}[E]_0, \text{ so } V_{max} = k_{cat}[E]_0.$$

It is claimed in the presentation that the numerical value of K_M is equal to the substrate concentration at which the reaction rate is $\frac{1}{2}V_{max}$. This is not argued for in the text, but can be deduced as follows:

$\frac{1}{2}V_{max} = V_{max}[S] / (K_M + [S])$, is equivalent to $K_M + [S] = 2[S]$, corresponding to $[S] = K_M$.

The model arrived at is of a general, principal nature, based on a number of critical assumptions, not a model dealing with a specific enzymatic reaction involving specific chemical substances or concrete data. As regards an evaluation of the model, the article from which the presentation is quoted, contains a qualitative discussion, which we haven't quoted due to space limitations, of the conditions under which the various assumptions made are likely to hold. It also contains a section on the determination of the model constants and a table of K_M (measured in M (molar concentration), and k_{cat} (measured in sec^{-1}) for different enzymatic reactions.

The next step in our analysis is to try to *understand* and *make sense of the model*. The presentation of the model and the foregoing considerations are helpful in this endeavour. As mentioned, the Michaelis-Menten model is actually derived as a secondary model from a primary model consisting of four linked ODEs. These ODEs represent a dynamical system, involving four state variables, at which we now take a closer look.

The general enzymatic reaction represents a transformation of chemical substances, which leads to a change of concentrations of the substances involved. In situations with constant physical and chemical conditions, such as temperature, pressure, and pH, as assumed in the Michaelis-Menten model, the kinetics of the involved reactions will be determined by the concentration of reactants according to the equations given above. The general enzymatic reaction can be represented as a dynamical system by means of a compartment diagram, see Figure 4.

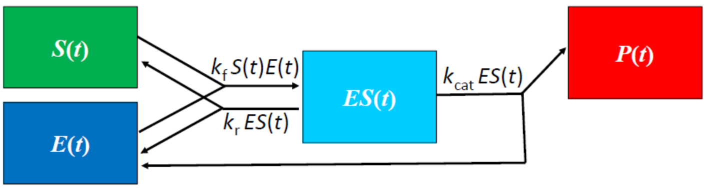

Figure 4. A compartment diagram of the generalised enzymatic reaction

In Figure 4, the four compartments represent the changing levels of concentration of each of the four substances as a function of time. The connections (the arrows) between the compartments represent the flows of substances caused by the chemical transformations in the three reactions, which are leading to changes in the *concentrations* of the substances. We denote the four concentrations as functions of time by S(t), E(t), ES(t), and P(t) respectively. Obviously, they are mathematised versions of [S], [E], [ES] and [P], where the time dependence is made explicit.

Although the compartment diagram is analogous to the chemical reaction scheme, the construction of the diagram exposes some important aspects of the situation. First of all, it makes the abstraction of perceiving an enzymatic reaction as a dynamical system of flows of substance causing a change in concentrations explicit. Also, the diagram offers a clear representation of the assumption that the enzyme has one active site only, means that the flows from E and S into ES are equal, as is also the case with the reverse flows. Moreover, the other basic assumption that the formation of one product molecule release one intact enzyme molecule becomes explicit in the construction of the diagram. The formation of the product from the ES compartment causes equal flows of concentration into the P and the E compartments. In the diagram, these characteristics are represented with the fork arrows, where the branching points represent the formation, dissociation or transformation of the enzyme-substrate complex.

From the diagram, it is seen that the sum of the concentrations of E and ES is constant. The sum of the flows in and out of E and ES is, for both compartments, equal to zero. In the derivation of the model in the presentation text it is stated as a basic assumption, that the concentration of total enzyme is constant, and equal to an initial concentration of free enzyme $[E]_0$, that is $[E]_0 = [E] + [ES]$. However, if no enzyme is added or removed externally, this assumption follows form the assumption that an intact enzyme molecule is released every time a substrate molecule has been transformed into a product molecule. By reading the compartment diagram it also becomes clear that the rate constants (must) have different units. The units of k_{r} and k_{cat} are s^{-1}, so that the respective flows get the unit Ms^{-1}, whereas the unit of k_{f} is $M^{-1}s^{-1}$ so that the flow into ES is in M/sec. As in the WikipediA article, the units of the rate constants are typically not discussed explicitly in standard derivations of the model.

From the diagram it is possible to set up differential equations based on the general principle that the net-rate of change for each compartment is the sum of inflows minus the sum of outflows for that compartment. This yields the following non-linear system of four ordinary differential equations (ODE), which are simply ODEs1-4 written in mathematical form:

$$S'(t) = -k_{\mathrm{f}}\, S(t)E(t) + k_{\mathrm{r}}\, ES(t)$$

$$E'(t) = -k_{\mathrm{f}}\, S(t)E(t) + k_{\mathrm{r}}\, ES(t) + k_{\mathrm{cat}}\, ES(t)$$

$$ES'(t) = k_{\mathrm{f}}\, S(t)E(t) - k_{\mathrm{r}}\, ES(t) - k_{\mathrm{cat}}\, ES(t)$$

$$P'(t) = k_{\mathrm{cat}}\, ES(t)$$

This system cannot be solved analytically. If the rate constants and the initial conditions are known, the system can of course be solved numerically. Figure 3 shows principal solution curves for the four concentrations during an enzymatic reaction.

The purpose of the Michaelis–Menten model is not only to predict the evolution of specific enzymatic reactions, but also to contribute to a theoretical understanding and characterisation of such reactions. Moreover, when the model was developed in 1913, it was not possible to solve the ODE system, neither analytically nor numerically. Accordingly, the

ODE system is not given as the final model. Instead, it is the starting point for deriving the Michaelis-Menten equation by way of an approximation.

As mentioned in the model presentation, one way of analysing the behaviour of system is to assume that the concentration of ES is kept in a quasi-steady-state during the reaction. This means, that ES’(t) is close to zero, i.e., the concentration of the ES complex does not change on the time-scale of the product formation. Assuming that ES’(t) = 0, which in terms of the compartment diagram means that the inflows balance the outflows for the ES compartment, allows for developing the Michaelis-Menten model through the following steps:

$$k_{\mathrm{f}}\, S(t)E(t) = k_{\mathrm{r}}\, ES(t) + k_{\mathrm{cat}}\, ES(t)$$

By using the conservation of the enzyme to substitute $E(t) = E_0 - ES(t)$ we get:

$$k_{\mathrm{f}}\, S(t)E_0 - k_{\mathrm{f}}S(t)ES(t) = (k_{\mathrm{r}} + k_{\mathrm{cat}})\, ES(t)$$

$$k_{\mathrm{f}}\, S(t)E_0 = (k_{\mathrm{r}} + k_{\mathrm{cat}} + k_{\mathrm{f}}S(t))\, ES(t)$$

$$S(t)E_0 = \left(\frac{k_{\mathrm{r}} + k_{\mathrm{cat}}}{k_{\mathrm{f}}} + S(t)\right) ES(t)$$

By introducing the Michaelis-Menten constant $K_{\mathrm{M}} = \frac{k_{\mathrm{r}} + k_{\mathrm{cat}}}{k_{\mathrm{f}}}$, with the unit M, we get:

$$ES(t) = E_0 \frac{S(t)}{K_{\mathrm{M}} + S(t)}$$

Multiplying this equation with k_{cat} yields the Michaelis-Menten model for the reaction rate for the formation of the product P:

$$v = P'(t) = V_{\mathrm{max}} \frac{S(t)}{K_{\mathrm{M}} + S(t)}\ ,$$

where $k_{\mathrm{cat}}\, E_0$ is called V_{max}, since it expresses the theoretical maximum for the production rate $P'(t)$, corresponding to the situation where all enzyme molecules are in a complex with a substrate molecule.

In their original analysis, Michaelis and Menten assumed that the substrate is in instantaneous dynamical equilibrium with the complex. This assumption is a stronger but conceptually simpler assumption compared to the quasi-steady-state one. In terms of the compartment diagram this assumption means that the in- and outflows of the S compartment are in balance. Making an analogous mathematical derivation to the previous one, we obtain

$$v = P'(t) = k_{\mathrm{cat}} \frac{E_0 S(t)}{K_{\mathrm{d}} + S(t)} = V_{\mathrm{max}} \frac{S(t)}{K_{\mathrm{d}} + S(t)},$$

again $k_{\mathrm{cat}}\, E_0$ is replaced by V_{max} . $K_{\mathrm{d}} = k_{\mathrm{r}}/k_{\mathrm{f}}$ is called the dissociation constant.

This expression for the production rate is almost identical with the expression of the Michaelis–Menten model. Both models describe the reaction rate of the product formation as a concave function of the substrate concentration having the same horizontal asymptote, $v(S) = V_{\mathrm{max}}$. The only difference between the two models are the constants K_{M} and K_{d}. Both models produce graphs of the form shown in Figure 2 and in both models the interpretation of the constant is that it is equal to the substrate concentration corresponding to the reaction rate $V_{max}/2$. However, the similarity in the mathematical structure of the derivations of the two models should not conceal the fact that they are based on two different assumptions.

The Michaelis-Menten model is a *theory-generating* model. It encapsulates the theoretical understanding of enzymatic kinetics in its simplest form. Although historically the model was developed to describe specific enzymatic reactions, and although it has later been validated experimentally for many different enzymatic reactions, the value of the model is first and foremost of theoretical nature. The status of the model relies primarily on the fact that it is developed from basic assumptions, it is simple, it gives rise to important concepts, and it provides good explanations of empirical data for some important enzymatic reactions. Moreover, the model offers a theoretical basis for characterising different enzymatic reactions by means of two well-defined parameters, and for differentiating between and quantifying different ways of inhibiting, respectively optimising enzymatic reactions.

These features explain why the model is part of the curriculum in any introductory tertiary level course in biochemistry. As we have seen, the Michaelis-Menten model relies on certain basic assumptions. These are not fulfilled for all enzymatic reactions or in all environments in which enzymatic reactions take place.

The *mathematical treatment* of the model has two different roles. The first role is to derive the final (secondary) model – the Michaelis-Menten equation – from the primary model, i.e., the system of four linked ODEs, under certain assumptions. On the assumptions made, this derivation was obtained solely by way of mathematical considerations and calculations. The second role is to draw *conclusions* from the final model and its properties, e.g. that K_M is numerically equal to the substrate concentration at which the reaction rate is half of V_{max}, or that reaction rate function is concave and asymptotically approaches V_{max} when the substrate concentrate increases (more precisely: tends to infinity). Another conclusion is that at low substrate concentrations the reaction rate varies linearly with the substrate concentration.

De-mathematisation of the Michaelis-Menten model consists of interpreting the model and its outcomes in terms of enzymatic reactions that fulfil the assumptions under which the model was constructed, and the outcomes obtained. In principle, de-mathematisation only makes sense when these conditions are satisfied. Here, the interpretation of the reaction constants and their composites, such as the dissociation constant, the Michaelis constant and the catalytic rate constant K_{cat}, forms part of the de-mathematisation.

Evaluating a theory-generating model such as the Michaelis-Menten model is a tricky task, since the model does not purport to be valid for all the cases it formally covers. This is especially the case with a model that is based on assumptions concerning the mechanisms that govern the relationships among the elements at issue and focus on the consequences of these mechanisms. There are two ways to evaluate such a model. Firstly, one can focus on evaluating the assumptions made in the construction of the model (mode 1). If these assumptions are theoretically or empirically validated the model is automatically validated as well, provided the mathematical inferences made on the basis of the assumptions are correct. Secondly, one may evaluate the model by trying to validate its outcomes (mode 2), which amounts to confronting these outcomes with empirical facts or data. If, in a given context, there is a fair degree of agreement between these facts and data and the model outcomes, this can serve as a validation of the model for this particular context. Researchers may then argue that this corroborates the assumptions on which the model relies. As to the Michaelis-Menten model, it is actually the case that for some reactions the model outcomes are in excellent agreement with empirical facts and data, whereas in others it is not. Clarifying in which cases such agreement exists gives the model an important role in research on enzymatic reactions. Application of the model outside the domain of its assumptions and conditions (mode 4) may be possible but then only empirical confrontation of the model outcomes with facts and data is a possible mode of evaluation. Here, evaluating the qualitative properties of the model (mode 3), mainly consists in evaluating the conclusions derived from the model.

What does it take to analyse and evaluate the models?

The two models presented are very different in terms of their nature and status. The Reilly model is a heuristic analogy model proposed to (possibly) capture customers' shopping behaviour. Being one of several similar models in commercial and transport geography, it does not claim to be valid let alone accurate. In contrast, the Michaelis-Menten model serves as one of the foundations of enzyme kinetics and has given rise to huge amounts of further research, especially focusing on the conditions and assumptions for the model to hold with regard to different chemical substances. For this reason, this model too does not claim to be accurate for any specific enzymatic reaction. Yet, it does purport to capture essential mechanisms in enzyme kinetics. Despite the significant differences that exist between the two models, the above analysis shows that they can in fact be analysed in much the same way, while paying attention to specific features and properties. We shall now move on to see how our analyses of the two models can assist in clarifying what it takes to analyse and critically evaluate extant models in general.

It is pretty clear that our rather extensive outline of an analysis of the Reilly and Michaelis-Menten models is somewhat demanding in several respects. Analysing the Reilly model involves both real-life considerations about commerce and geography and mathematical considerations concerning the properties of the model and the implications of these.

Analysing the Michaelis-Menten model involves a considerable pool of chemical concepts and knowledge, in addition to a variety of mathematical competencies.

In both cases, the *key steps* of the above analyses are:

- Identifying the basic elements of the model that are explicitly included in the presentation.
- Identifying, if relevant in the situation, the factual information and data quoted or invoked in the model.
- Identifying the assumptions and simplifications actually made for the construction of the model, both explicit and implicit ones. The presentations of the two models involved quite a few of both kinds.
- Identifying the mathematisation explicitly made in the model presentation, but also implicit or invisible mathematisation underpinning, or following from, the explicit parts.
- Identifying the mathematical procedures and inferences made, and the results obtained, in the model as well as the extra-mathematical conclusions drawn therefrom.
- Taking stock of the evaluation of the model as offered in the presentation, to the extent such an evaluation actually forms part of the presentation.
- Scrutinising the evaluation presented and subjecting, if relevant, the model to further evaluation, e.g. utilising the modes (1)-(4).
- Arriving at a summative conclusion about the formulation, relevance, and trustworthiness of the model.

As mentioned above, several of these steps require quite a bit of "model archaeology". It goes without saying that the model examples we have investigated here are just two out of an infinitude of very different models, ranging from "singular" or "point models", designed to deal with particular situations without any claim of generality beyond the specific situation, to more generic models supposed to cover larger classes of situations having basic features and properties in common, thus claiming some degree of generality. However, we do suggest that the steps just considered for the Reilly and the Michaelis-Menten models are, in fact, not dependent on the specifics of the models but allow for coming to grips with the crucial aspects of any model analysis. Hence, these steps are of a generic nature.

We shall now carry our analysis a step further by involving the well-known modelling cycle for active model building in capturing what is going on in our model analysis.
The main stages of constructive modelling are:

- *Pre-mathematisation* consists of preparing the extra-mathematical situation at issue for mathematisation by generating the extra-mathematical questions to be answered, by structuring the situation at issue and selecting the elements and relations to be modelled, by making simplifications, assumptions and idealisations that lead to a reduced extra-mathematical situation within which the extra-mathematical questions can be specified and formulated. Identifying or seeking factual information and data pertaining to the situation being modelled can be part of pre-mathematisation or of mathematisation (see below), depending on the circumstances.

- *Mathematisation* consists of translating the chosen elements, relations, assumptions and extra-mathematical questions into mathematical objects, relations, assumptions, and questions and problems that belong to some chosen mathematical domain.
- *Working mathematically* in order to answer the mathematical problems and questions by employing mathematical methods, such as calculations, well-known results, reasoning and inferences.
- *De-mathematising* the mathematical answers obtained, i.e., interpreting these answers in terms of answers to the extra-mathematical questions originally posed, thus yielding the outcomes of the model.
- *Validating the model outcomes* by relating them to the aims, goals, and conditions that drove the modelling enterprise in the first place.
- *Evaluating the model*, i.e., making a summative decision as to how well the model suits its purpose, everything considered. In addition to validating the model outcomes as in the previous item, evaluating a model is typically done by evaluating its structural properties, including its range and scope and sensitivity to conditions and assumptions, its quantitative features vis-à-vis the extra-mathematical situation at issue, and by comparing and contrasting the model with possible alternative models.

These stages can be depicted in diagrammatic form by way of one of the several versions of the modelling cycle, for example as in Figure 5.

It is important to keep in mind that neither the modelling stages just mentioned, nor any modelling cycle are supposed to describe in concrete terms the actual sequential steps a modeller has to, or will, undertake in practical terms. Rather it is an analytic reconstruction of the components that are necessarily present, whether explicitly or implicitly, in any modelling process.

During the last couple of decades, research has shown the importance of the so-called *implemented anticipation* (Niss, 2010) in most of the stages of the constructive modelling process. Successful modelling requires the modeller in key stages of the modelling process to anticipate later steps in it and to implement that anticipation in carrying out the current step. In other words, the modeller has to cognitively project her-himself into future modelling steps, which have not yet been made.

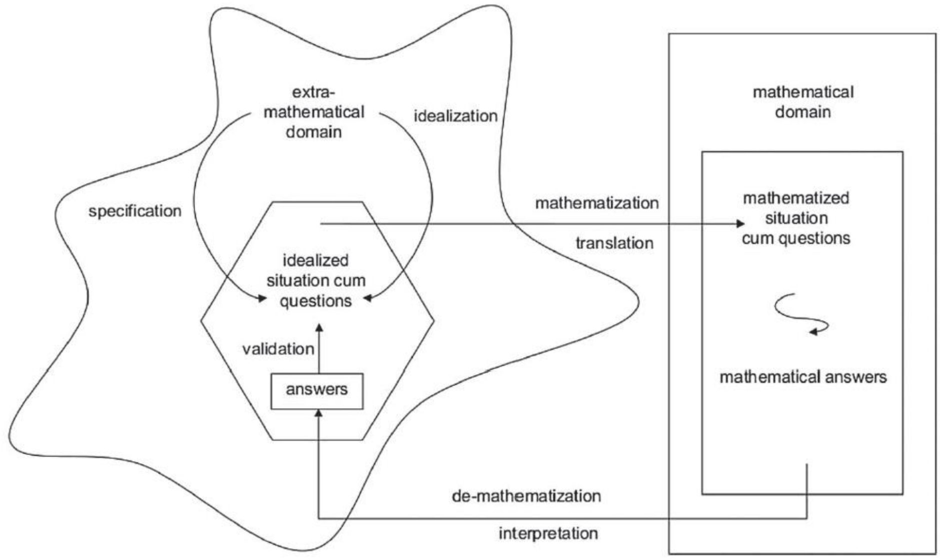

Figure 5. A Modelling cycle with all the sub-processes involved in constructive mathematical modelling (Jankvist & Niss, 2020, p. 469)

When it comes to a written or an oral presentation of a model, it is not always clear whether the presenter of the model is also the actual modeller. Sometimes, however, it is clear that the modeller and the presenter are not the same person. This is certainly the case with the Reilly and Michaelis-Menten models that were evidently not presented in WikipediA by the original modellers themselves. Nevertheless, for the *model analyst* it does not matter whether there is identity between the modeller and the presenter since the model appears extraneous to the analyst in either case. In what follows, for simplicity we shall therefore use the term "modeller" also for the presenter of the model.

We shall now show how a "mirror reflection" of each stage of the constructive modelling process, and hence of the modelling cycle, can be used to capture the analytic aspect of the modelling competency.

Reverse problem formulation

For someone who wants to critically investigate an extant model, the first step is to come to grips, if possible, with the purpose(s) for which the model has been constructed. What types of problems can be solved or investigated by means of the model? When facing a description of a mathematical model these purposes are not necessarily explicitly expressed. Neither model includes explicit statements of the questions the model was supposed to answer. Rather, these questions are implicit in the formulation of the model and in the various conclusions included in the presentations. So, it could be part of analysing a model to carry out what could be called a reverse problem formulation. In order not to be misleading, such an endeavour should involve consulting sources on possible applications of the model in different contexts and situations. This may be seen as being on the border of the analytic aspect of the modelling competency which illustrates the challenges in delimiting the scope of this aspect of the competency.

Reconstruction of the modeller's pre-mathematisation

The next step is to come to grips with the way the model has been constructed and the grounds on which the construction rests. In the constructive modelling process, a modeller begins by *carrying out* pre-mathematisation as outlined above. The first instance of implemented anticipation occurs in this stage, since the modeller, when preparing the situation for mathematisation, more or less clearly anticipates relevant mathematisation options and (perhaps) also possible mathematical treatments of the model leading to mathematical answers to the mathematised extra-mathematical questions.

In contrast, the first task of the model analyst is to *uncover* the key features of the pre-mathematisation undertaken by the modeller, which may well be a non-trivial task. It consists, firstly, of identifying and understanding the explicit choices and decisions made by the modeller. This depends strongly on the clarity of the explanations and – not least – the arguments put forward by the modeller. Even if a choice or a decision has been made explicit, the grounds on which it relies may still be obscure. As is the case with the constructive aspect of the modelling competency, when analysing a mathematical model, there is also a blurred boundary between the mathematical competency and competencies within the field in which the model is developed or (intended to be) used. This is especially true when we consider mathematical models in sciences whose basic theories are already mathematised to a large extent, as is the case with chemistry and physics. For example, the chemical reaction equation for the general enzymatic reaction is already a mathematical model in itself. The analysed Michaelis-Menten model is a further development of this model, which makes it possible to draw mathematical conclusions that can be interpreted and discussed in a biochemical context.

Next, it consists of unveiling the implicit elements of the pre-mathematisation. In addition to being tricky in and of itself, this typically requires the model analyst to make assumptions about the presence and role of implicit elements. Several examples of this were at play in the Reilly and Michaelis-Menten models. In this phase, the analyst will also attempt to uncover the extra-mathematical questions that drive the entire modelling enterprise, even though these questions may very well be non-existent or implicit, as is the case in the presentations of the two models investigated here. If the modelling questions are absent, they can often be uncovered by analysing the model outcomes and conclusions included in the presentations.

Sometimes the model analyst will have to temporarily take on the virtual role of modeller in order to understand the pre-mathematisation made. What are the choices and decisions that I, as a model analyst, would have made to approach this task had I been the modeller?

This involves comparing and contrasting what the modeller has done with what the analyst would have done.

Altogether, the model analyst is to reconstruct the modeller's pre-mathematisation. We have just seen that this can be conceptualised as a *mirror reflection*, undertaken by the analyst, of pre-mathematisation and its components. By the way, it is interesting to notice that this reconstruction does not, in general, seem to involve implemented anticipation (Niss, 2010).

Reconstruction of the modeller's mathematisation

Once the model analyst has reconstructed the pre-mathematisation involved in the model, the analyst will have to identify the mathematisation that constitutes it. Typically, the explicit parts of the mathematisation can be read off the model presentation, but implicit elements are likely to be involved as well. For example, this is the case if not all the details of the mathematisation are spelled out, perhaps because they are tacitly taken for granted by the modeller, or if the questions the model is supposed to answer are not actually translated into the mathematical domain chosen for the model. Multiple examples of implicit mathematisation elements were identified in the two models considered.

When reconstructing the mathematisation that led to the model, the analyst, once again, is producing a mirror reflection, here of the mathematization stage, but without being forced to reproduce the inventiveness that initially may have gone into that mathematisation. Similarly, this stage in the model analysis does not require implemented anticipation on the part of the analyst, even if it did for the modeller.

Hybrid – reconstructive and constructive – modelling

It is not unusual that the presentation of a model stops once the mathematisation has been completed. If so, all the subsequent stages of the modelling cycle have been left unconsidered by the modeller. However, this does not mean the model analyst will have to stop the analysis at this point. Rather, since there is no text to analyse concerning these stages, the analyst will have to change his or her role into that of a modeller undertaking (some of) the subsequent modelling steps him-herself. This means that the model analysis no longer makes use of a mirror reflection of the corresponding stages of the modelling cycle but engages in a direct version of these steps. For instance, if the model presentation does include mathematical conclusions from the model stated but only a partial – or no – demonstration of how these conclusions were obtained, the analyst will, if possible, try to derive those conclusions him- or herself, while paying attention to possible hidden assumptions or conditions that are needed for the derivation. This is what happened in the analysis of the Reilly model and partly in the analysis of the Michaelis-Menten model.

If the model presentation does *not* stop with the mathematisation, it depends on the situation which of the subsequent stages in the modelling cycle actually are activated, explicitly or implicitly, in the presentation. For each such stage, the model analyst is performing a mirror reflection of it. If, for example, the presentation shows the mathematical work done to derive consequences and conclusions from the model established, as is the case in large parts of the Michaelis-Menten presentation, the task of the analyst is to check and assess the derivations.

More generally, if all the stages of the modelling cycle are present in the exposition of the model, the entire model analysis can be perceived as a mirror reflection of the modelling cycle. For modelling stages not represented in the exposition, the model analyst will (have to) shift to the constructive modelling mode corresponding to those stages.

Summary: the process of model analysis

In contrast to the constructive modelling cycle, which is a cycle because it allows for the possibility of taking several rounds through the stages in case the original model needs to be changed or replaced by another model, this cyclicity is not at play in a model analysis. So, the modelling cycle has been replaced by a diagram for model analysis (Figure 6).

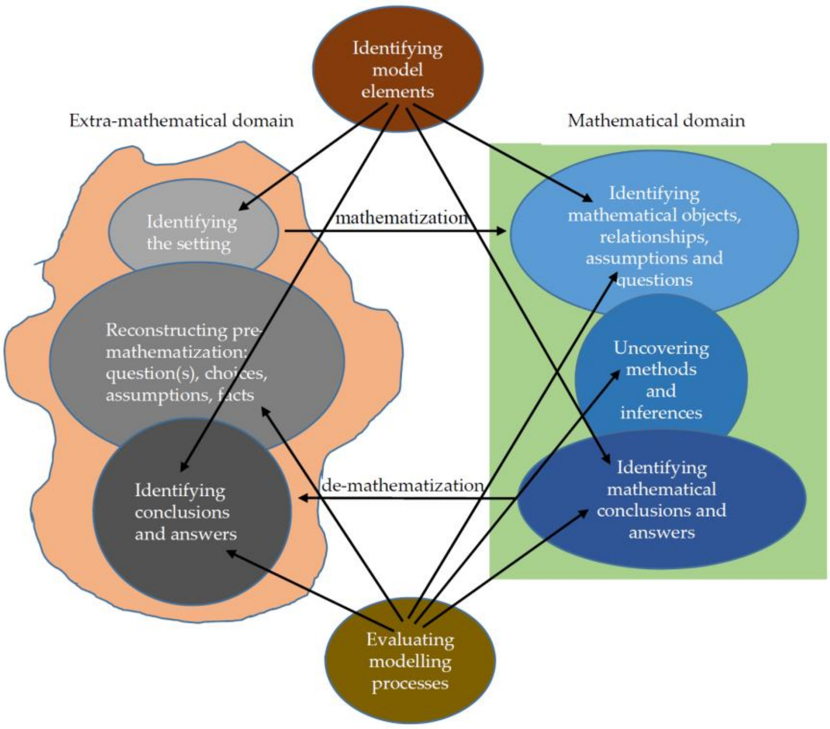

Figure 6. Diagram for model analysis

In this section, we have demonstrated how extant models can be analysed and what it takes to be able to do so. Extant models can be analysed by way of the generic analysis steps listed above and with the help of a set of mirror reflections of the respective stages of the constructive modelling process, sometimes in combination with the ability to perform (parts of) that process directly. The ability to do this represents rather high epistemological and cognitive demands on the model analyst. Undertaking “model archaeology” is a kind of detective work in which analytic and skills and the ability to combine are crucial, together with deep insight into and judgment of models and modelling processes, and together with mathematical competencies at large, in addition, of course, to competencies concerning the field being modelled In view of the fact that the model analyst will sometimes have to act as a constructive modeller her- or himself in relation to any stage of the modelling process, it is clear that the ability to analyse models is no less demanding than the ability to independently construct models, except that possible constructive sides of model analysis need not be as inventive or innovative as is typically the case with constructive modelling, especially as far as the ability to undertake implemented anticipation is concerned, since this is typically not on the agenda in model analyses.

Didactical consequences

While it is certainly essential that students develop that part of the modelling competency that consists in performing constructive mathematical modelling, it is no less important that students also develop the analytic part of the modelling competency. One may in fact argue that the majority of students in their current and future lives will encounter the presentation and use of extant models, e.g., for decision purposes, more often than they will be put in a position where they are to perform constructive modelling. Students and members of the public encounter extant models in other disciplines or practices areas and in the discussions of societal issues in different kinds of media. Being able to relate to analyse, and critically assess such models is an important competency for individuals’ private, occupational social and civic life in society. And this is exactly the analytic side of the modelling competency.

The point of departure for this paper was the somewhat surprising observation that the analytic side of the modelling competency in the sense of the KOM framework has not really been dealt with in the research and development of mathematical modelling in mathematics education. Similarly, to our knowledge critical analysis and assessment of extant models is not an activity cultivated in schools and tertiary institutions to any significant extent. There, the focus is typically on students’ learning about such models rather than on investigating them. We believe, however, that model analysis ought to be placed on the agenda of the teaching and learning of mathematics in order to foster scientific and civic education of students. In particular, we find that the analytical modelling competency is imperative in the teaching of scientific disciplines where mathematical models of different types and status are extensively used, such as for example within social science studies involving physical planning, demography, and economics, and within science domains, e.g., ecology, climate change and biochemistry.

The present paper offers a starting point for undertaking research and development work in this area. We suggest that the approach to model analysis presented here may be a means to this end. Firstly, it would be interesting for researchers to analyse a large pool of model examples with different backgrounds, theoretical foundations and characteristics along the lines suggested in this paper. Having a large reservoir of model analyses would pave the way for charting and describing the landscape of models, and possibly for identifying different significant categories of models within that landscape. Such studies could also form the basis for much-needed empirical research on students' attempt to undertake model analysis, which would allow us to better understand different sorts of opportunities and barriers involved in the analytic aspects of the modelling competency. Further down the road we would also be able to understand the relationship – causal or correlational – between these aspects of the modelling competency and the constructive ones.

As regards teaching, teachers who would like to engage students in model analysis might take their point of departure in inviting students to critically analyse familiar textbook models of well-known situations, e.g., linear, polynomial, exponential, and logistic growth models, with particular regard to uncovering the underlying assumptions and scrutinising their justification in relation to the specific domain being modelled. In further steps, student groups might be asked to build "competing models" of the same given situation and afterwards analyse and compare each other's models.

Conclusion

It is now time to return to the research question: "What are the key epistemological and cognitive components involved in the ability to handle the analytic aspects of the modelling competency?".

Aided by "model archaeology", i.e., detailed analyses of two examples of extant models, we have identified (see Section 3) the key steps in the analysis of extant models, and we have uncovered the most important epistemological and cognitive components in the analytic aspects of the modelling competency by employing a dual version of the well-known constructive modelling process and cycle consisting of mirror reflections of each stage in this process. The mirror reflection of such a stage consists of unveiling the steps that explicitly or implicitly (must) have been made in the constructive stage.

In summary, it has proven possible to outline a rational approach to analysing extant models and to identify the epistemological and cognitive demands involved in the analytic aspect of the modelling competency. Moreover, we have argued that this aspect may well be no less demanding, in terms of cognitive load and knowledge requirements, than the constructive aspect of the modelling competency. This is because the analytic aspect of the modelling competency involves reconstructing the modeller's work from explicit and implicit sources, while also involving constructive modelling work in cases where model presentations are insufficient and, above all, in performing thorough evaluation of extant models, especially vis-à-vis possible alternatives.

The findings of this paper give rise to further research and development work in two different ways. Firstly, as mentioned in the beginning, the paper is of a theoretical nature. It would be interesting to investigate to what extent the theoretical findings can be empirically confirmed with different categories of students. This opens the doors for the instigation of a larger research programme. Secondly, since model analysis doesn't figure prominently, if at all, in the teaching and learning of mathematics we propose to establish development projects to see how such analysis can be put on the agenda and be implemented in actual educational settings. The approach we have presented in this paper ought to be a helpful starting point for such projects.

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