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Correction to *New Mathematical Model for Interpreting pH-Stat Digestion Profiles: Impact of Lipid Droplet Characteristics on in Vitro Digestibility*

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Abstract

There is an inconsistency between the modeling assumptions (equations 1-6) and the main ordinary differential equation (equation 7). Indeed, the exponent in equation (7) should be 2/3 instead of 3/2, leading to several changes in subsequent equations.

In this note, we derive the corrected equations and compare them to the original ones, which show similar dynamical behavior.

Assumptions and equations from the original article

In order to make this note self-sufficient, we first recall the assumptions and equations from the original article. Numbering was kept identical to the original article, using an additional prime symbol (') for the corrected equations.

Assuming that two free fatty acid (FFA) molecules are produced per triacylglycerol molecule, the percentage of released FFA, %FFA, is given by

$$\%FFA = 100 \times \left(\frac{V_{NaOH} \times m_{NaOH} \times M_{lipid}}{2 \times w_{lipid}} \right) \quad (1)$$

where V_{NaOH} is the volume of added sodium hydroxide solution (m^3), m_{NaOH} is its molarity ($kmol.m^{-3}$), w_{lipid} is the initial mass of the triacylglycerol oil (kg) and M_{lipid} is its molar mass ($kg.kmol^{-1}$).

Assumption 1 The rate of FFA release from lipid droplets is proportional to the droplets surface area per unit volume of the emulsion, S_d ($m^2.m^{-3}$)

$$\frac{dm_d}{dt} = -k S_d V_E \quad (2)$$

where $m_d(t)$ is the number of moles of digestible FFA in the droplets, dm_d/dt is the number of moles of FFA leaving the droplets per unit time, k the rate constant ($\text{kmol.s}^{-1}.\text{m}^{-2}$) and V_E the volume of the emulsion (m^3).

Remark: it is important to notice that equation (2) has a physical meaning if and only if $m_d \geq 0$.

Assumption 2 The total number of lipid droplets remains constant and their diameter $d(t)$ decreases when the products of the lipolysis leave the droplet. The specific surface area of the droplets per unit volume of the emulsion is then given by

$$S_d(t) = n_0 \pi d^2(t) \quad (3)$$

where n_0 is the number of droplets per unit volume of emulsion (m^{-3}). n_0 is computed from the initial state of the emulsion

$$n_0 = \frac{6 \phi_0}{\pi d_0^3} \quad (4)$$

where ϕ_0 is the initial droplet volume fraction and d_0 the initial droplet diameter (m).

Assuming that all of the digested lipids leave the droplets, the ratio of the droplet volume during digestion to the initial droplet volume is given by

$$\frac{V_d(t)}{V_0} = \frac{\frac{1}{6} \pi d^3(t)}{\frac{1}{6} \pi d_0^3} = \frac{m_d}{m_0} \quad (5)$$

where m_0 is the initial number of moles of FFA in the droplets. Hence

$$d(t) = d_0 \sqrt[3]{\frac{m_d}{m_0}} \quad (6)$$

Remark: from equation (6), $d(t)$ could become negative if the nonnegativity of $m_d(t)$ is not ensured, which would lead to inconsistent results.

From this point, a discrepancy occurs between the article and the actual solution, due to a misprint in the exponent. Indeed, substituting equations (3) to (6) in equation (2), the article gives

$$\frac{dm_d}{dt} = -k \frac{6 \phi_0}{d_0} \left(\frac{m_d}{m_0} \right)^{3/2} V_E \quad (7)$$

while one should obtain

$$\frac{dm_d}{dt} = -k \frac{6 \phi_0}{d_0} \left(\frac{m_d}{m_0} \right)^{2/3} V_E \quad (7')$$

Note the modification of the exponent between equations (7) and (7'): 3/2 versus 2/3.

Analytical solutions

Equation from the original article

Corrected equation

$$\frac{dm_d}{dt} = -k \frac{6 \phi_0}{d_0} \left(\frac{m_d}{m_0} \right)^{3/2} V_E$$

$$\frac{dm_d}{dt} = -k \frac{6 \phi_0}{d_0} \left(\frac{m_d}{m_0} \right)^{2/3} V_E$$

The analytical solution writes

$$m_d(t) = \left(\frac{3 k \phi_0}{d_0 m_0^{3/2}} V_E t + m_0^{-1/2} \right)^{-2} \quad (8)$$

$$m_d(t) = \left(m_0^{1/3} - \frac{2 k \phi_0}{d_0 m_0^{2/3}} V_E t \right)^3 \quad (8')$$

which leads to

$$\Phi = 1 - \frac{m_d}{m_0} = 1 - \left(1 + \frac{3 k \phi_0 V_E t}{d_0 m_0} \right)^{-2} \quad (9)$$

$$\Phi = 1 - \frac{m_d}{m_0} = 1 - \left(1 - \frac{2 k \phi_0 V_E t}{d_0 m_0} \right)^3 \quad (9')$$

Rewriting ϕ_0 as

$$\phi_0 = \frac{w_d}{V_E \rho} = \frac{m_0 M}{2 V_E \rho}$$

with ρ the density of the triacylglycerol oil (kg.m^{-3}), it leads to

$$\Phi = \phi_{max} \left(1 - \left(1 + \frac{3 k M}{2 d_0 \rho} t \right)^{-2} \right) \quad (10)$$

$$\Phi = \phi_{max} \left(1 - \left(1 - \frac{k M}{d_0 \rho} t \right)^3 \right) \quad (10')$$

where ϕ_{max} is the asymptotic maximal percentage of released FFA.

Dynamical behaviors of the solutions

A parameter estimation has been performed on equation (10') in order to fit the equation (10). We added a condition of nonnegativity for m_d in equation (10') which then became

$$\Phi = \phi_{max} \left(1 - \max \left\{ 0, \left(1 - \frac{k M}{d_0 \rho} t \right)^3 \right\} \right) \quad (11')$$

The results are depicted in Figure 1 and show similar dynamics for both solutions (10) and (11').

Qualitatively, both solutions have a similar shape but the corrected one reaches a constant plateau more quickly.

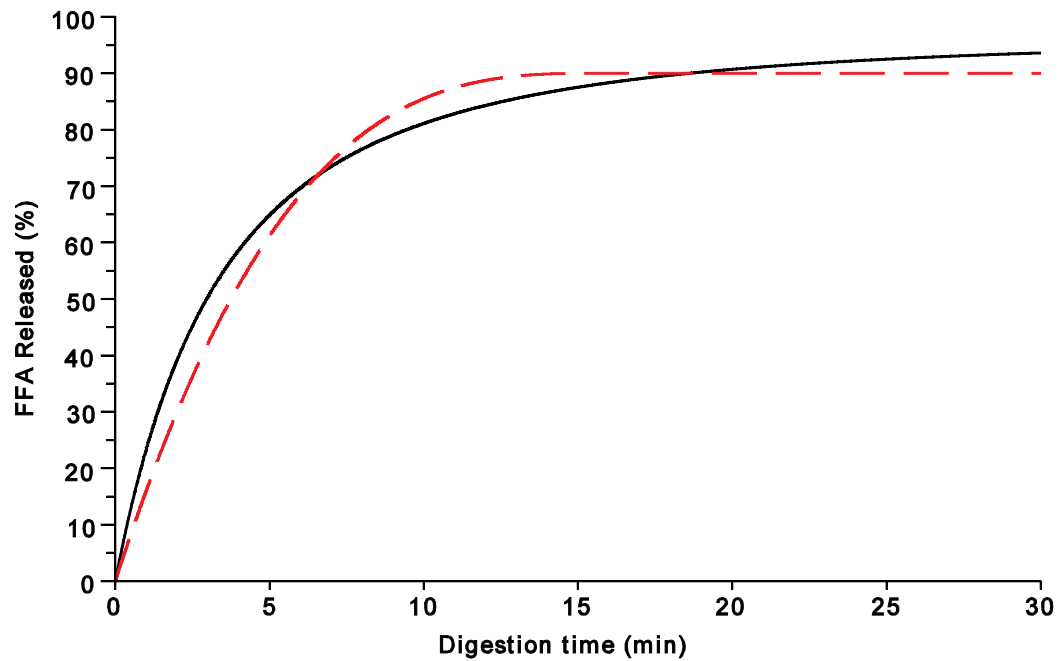


Figure 1. Comparison between original (continuous line) and corrected (dashed line) solutions. The corrected solution included a condition for $m_d \geq 0$.

If nonnegativity is not preserved, equation (10') shows a totally different behavior. Indeed, mathematically, this solution is monotonically increasing, with an inflection point, but goes to infinity (Figure 2). In contrast, the original solution, equation (10), does not need an explicit condition of nonnegativity.

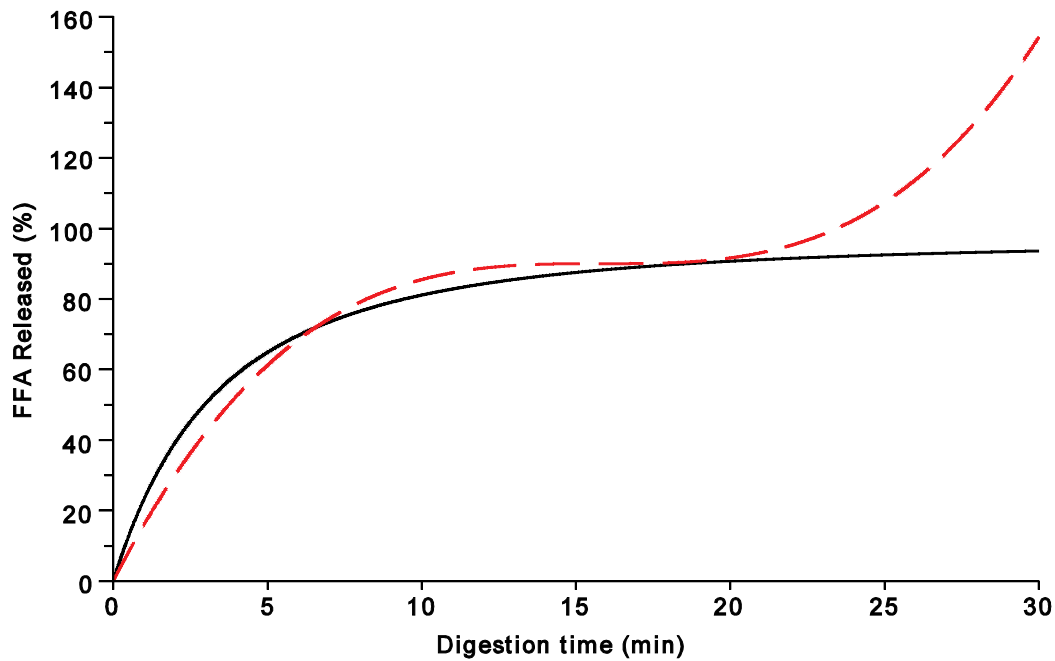


Figure 2. Comparison between original (continuous line) and corrected (dashed line) solutions when nonnegativity of m_d is not explicitly preserved.

Conclusion

Both original and corrected equations are able to fit *in vitro* lipolysis data reasonably well. The original equation (10) reproduces the observed trend of experimental data somewhat better than the corrected equation (11') and has no need to explicitly enforce the nonnegativity of number of moles (or mass) to avoid unphysical results.

Equation (10) does not correspond to the physical hypotheses described in the original article, however.