The effectiveness of using mathematical modeling in assessing the quality of food products

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Abstract. In the development of new formulations and assessment of their quality it is advisable to use mathematical modeling. The quality of any food product is determined by its characteristic properties of the quality indicator. Currently, the food industry has significantly expanded the use of mathematical methods. This is due to the fact that any technically and economically unjustified decision leads to significant material losses. In experiments, we studied the quality and safety of fat supplements with their additional introduction into the diet. As a result of the conducted research, the correlation analysis method using nonparametric methods revealed a correlation between the chemical composition of the diet and the time factor. When sunflower oil was added to the diet, a correlation was established between the activity of enzymes and the chemical composition of crude protein ($r=0.71$) and crude fat ($g=-0.62$). When palm oil was added to the diet, a correlation was found between raw fat ($r=0.55$) and organic matter ($r=-0.54$). Flaxseed oil contributed to the correlation of crude protein ($r=-0.52$) and nitrogen-free extractives ($r=-0.55$), as well as organic matter ($r=0.54$). The formulated mathematical models based on correlation allow us to take into account the time factor, diet, and individual indicators of the fat component. In addition, they allow one to develop not only a new feed recipe depending on the fat and acid composition of the diet in the presence of the specified initial data, but also to predict their effect on the quality of the product.

1. Introduction
Currently, the most important area of research in the field of animal breeding is diet compilation [1–3] and the proper functioning of an entire digestive system. [4–5]. The most energy-intensive substance entering the body is fat [6]. At present, a rather large number of works [7–9] are devoted to the issues of fat additives in a nutritious diet.

Enzymes are the key indicators of the proper functioning of the gastrointestinal tract, and biochemical blood parameters are an essential indicator of the body. Enzymes function only under certain environmental conditions. If these conditions change in a digestive canal, then enzymes reduce their activity, which leads to digestion [10–12].

To predict the functioning of a digestive system, it is necessary to develop a mathematical model capable of assessing the activity of the enzymatic system depending on the ingredient blood composition.
2. Materials and methods

2.1. Animals and feeding

The studies were performed in a laboratory of biological tests and examinations of the Federal State Budget Scientific Institution of the Federal Scientific Center for Biological Systems and Agricultural Technologies of the Russian Academy of Sciences on calves (n=3) aged 9 months with an average weight of 215–220 kg.

Animal services and experimental studies were performed in accordance with the instructions and recommendations of Russian Regulations, 1987 (Order No. 755 on January 8th, 1977 the USSR Ministry of Health) and “The Guide for Care and Use of Laboratory Animals (National Academy Press Washington, DC 1996)”. Calves were kept in a specialized cage with free access to water and feeding.

The animals were fed with regards to the main diet, compiled with the NRC recommendations (www.nap.edu/catalog/9791.html) and included the following: mixed grass (5 kg), a mixture of concentrates (2 kg), corn silage (1.5 kg), molasses (0.1 kg), fine salt (0.04 kg), vitamin and mineral premix (0.06 kg, trace elements per 1 kg of concentrates: 48 mg of Mn; 36 mg of Zn; 60 mg of Fe; 10 mg of Cu; 0.24 mg of Se; 0.12 mg of Co; vitamin content per kg of concentrate: 2640 M of vitamin A (VA); 302 IU of vitamin D (VD); 17 mg vitamin E of (VE).

The control group calves received the main diet throughout the experiment. The diet of calves of the 1st experimental group included sunflower oil, the 2nd experimental group received palm oil, the 3rd experimental group received soybean oil, and the 4th group received linseed oil. Vegetable oil was introduced in an amount of 3 % of the dry matter through the grain portion of the diet.

2.2. Observation, estimated indicators

The experiment was carried out in triplicate using the Latin square 4×4 in the laboratory of biological tests and examinations of the Federal Scientific Center for Biological Systems of the Russian Academy of Sciences. Pancreatic juice was collected from fistulated calves. A syringe was attached to the fistula by a special rubber adapter to collect chyme from an isolated segment of duodenum. Chyme was selected in the morning before feeding after 12–hour fasting and then every hour during 8 hours after feeding. The study was conducted in 3 replicates.

Blood for biochemical parameters was taken from a jugular vein into vacuum tubes with a coagulation activator (thrombin) and evaluated on an automated analyzer CS–T240 (DIRUI IndustrialCo., Ltd, China) with commercial veterinary kits (DIAKON–DS CJSC, Russia).

Amylase activity was measured by Smith Roy in the modification aimed to determine the high activity of the enzyme according to Anoson, proteases was measured by hydrolysis of purified casein according to Hammersten with calorimetric control (wavelength 450 nm), lipase were measured on a CS–T240 automatic biochemical analyzer (“Dirui Industrial Co., Ltd”, China) using commercial biochemical kits DiaVetTest for veterinary medicine (Russia).

Correlation relationships were calculated by the Spearman correlation coefficient. The obtained results of the correlation analysis suggest the existence of correlation at the 5% significance level (with a coefficient r>0.5) between the activity of enzymes in the pancreatic juice, chyme, and the chemical composition in the diet. The mathematical model was based on multiple regression dependence obtained as by applying the least squares method. In addition, the influence of the time component was singled out separately in the form of a trend model, followed by analytical inclusion in the final mathematical model.

2.3. Statistical manipulation

Statistical analysis was performed using ANOVA techniques (software package Statistica 10.0, StatSoftInc, USA) and Microsoft Excel. The significance of differences in the compared indicators was determined by the Students t–test. Valid values were considered at p≤0.05. Data are presented as the mean (M) and standard error of the mean (m). Normality testing was carried out according to Kolmogorov–Smirnov criteria. As a result, the hypothesis of the initial data normal distribution was rejected and the use of nonparametric procedures was recommended.
3. Results

A correlation analysis of the enzymes activity in a pancreas with biochemical blood parameters showed the following results: 30 minutes before feeding, no correlation was found, with the exception of a weak positive relationship between uric acid and lipase ($r=0.58$) and alkaline phosphatase and protease ($r=0.60$) as well as a negative relationship between LDH and amylase $r=-0.55$. 30 minutes after feeding, there was a correlation dependence only with lipase and urea and alkaline phosphatase ($r=0.62$ and $r=0.58$), respectively. An hour after feeding, a moderate negative correlation was noted between amylase and bilirubin as well as between glucose and lipase, where $r=-0.54$. A moderate positive relationship was observed between urea and lipase, where $r=0.54$, and AST and protease, where $r=0.55$.

Correlation values with the introduction of palm oil revealed a single moderate correlation. 30 minutes before feeding the dependence was in the form of a weak correlation between creatinine and lipase ($r=0.50$) and a moderate correlation between uric acid and protease ($r=0.67$). 30 minutes after feeding, four moderate correlations between amylase and total bilirubin ($r=0.55$), gamma–GT ($r=-0.67$), calcium ($r=0.62$) and phosphorus ($r=0.51$), as well as a positive moderate correlation between magnesium and protease ($r=0.68$) were indicated. An hour after feeding, there was only the negative correlation between AST and lipase ($r=-0.52$) and a positive one between uric acid and protease ($r=0.53$).

When soybean oil was introduced into the diet of experimental calves in the initial period, a correlation was found between total protein and lipase ($r=0.63$), as well as between protease and albumin ($r=0.54$), cholesterol ($r=-0.54$), magnesium ($r=-0.62$) and calcium ($r=0.53$). 30 minutes after feeding, the negative correlations between uric acid ($r=-0.65$), the positive correlations between glucose and lipase ($r=0.52$) and the negative correlations between albumin and protease ($r=-0.51$) were indicated. At the end of the experiment, two average positive correlations between iron and amylase ($r=0.51$) as well as between bilirubin and lipase ($r=0.62$) were found.

The introduction of linseed oil manifested itself as a weak correlation between albumin and amylase ($r=0.68$) and between total bilirubin and protease ($r=0.52$). 30 minutes after feeding, moderate correlations were found between the protease and total protein ($r=0.62$) and creatinine ($r=-0.55$). One hour after feeding, no significant correlations were found.

The revealed pairs of correlations turned out to be rather scattered, which makes their unambiguous assessment difficult. For optimal estimation of changes in functionally significant parameters, the construction of mathematical models is necessary. The revealed correlation between the characters must be interconnected, with the goal not only to identify complex interactions, but also to plan possible diet for better calves’ growth in the future.

To begin with, the influence of the time factor on the chyme key indicators should be assessed. The selection of the equation by the least squares method has led to the fact that the closest description of temporal changes for the secretory function can be given by means of polynomials of the second degree.

A set of equations describing changes in specific enzymes taking into account the diversity of the diet depending on time is given (Table 1).

All equations have a high degree of certainty. $R^2$ ranges from 0.85 to 0.95, which makes it possible to use the obtained correlation equations in the future.

Having examined the effect of a temporary factor on secretory function, we will determine the effect of the fat component on a particular enzyme depending on time. The change in enzymes was also evaluated using the least squares method, however, in the case of studying the fat component, the use of linear regression models turned out to be sufficient (Table 2).

To assess the effect of the fat component, the models were also brought to a general view. In the obtained models, the following notation was accepted:

$z_1$ is glucose;
$z_2$ is the total protein;
$z_3$ is albumin;
z4 is ALT;  
z5 is AST;  
z6 is total bilirubin;  
z7 is direct bilirubin;  
z8 is cholesterol;  
z9 is triglycerides;  
z10 is urea;  
z11 is creatinine;  
z12 is alkaline phosphatase;  
z13 is α–amylase;  
z14 is gamma–GT;  
z15 is uric acid.

**Table 1.** Assessment of time factor influence on enzymes activity with regards to diet diversity

| Oil Type     | Equation                        |
|--------------|---------------------------------|
| Sunflower oil| $y = 401.1t^2 - 18093t + 3024.6$ |
| Palm oil     | $y = -585t^2 + 2955t + 1030$    |
| Soybean oil  | $y = 811.67t^2 - 5043.7t + 9646.7$ |
| Linseed oil  | $y = 907.92t^2 - 3335.3t + 5533.2$ |

| Oil Type     | Equation                        |
|--------------|---------------------------------|
| Sunflower oil| $y = -5.93t^2 + 22.59t - 9.2733$ |
| Palm oil     | $y = 49.723t^2 - 123.36t + 127.89$ |
| Soybean oil  | $y = 178.39t^2 - 857.83t + 1053.7$ |
| Linseed oil  | $y = 8.3557t^2 - 39.958t + 68.042$ |

**Table 2.** Assessment of fat component on enzymes activity with regards to time factor

| Time       | Equation                        |
|------------|---------------------------------|
| 0–30       | $y = 1907.3l - 343.11$          |
| 30–60      | $y = 903l + 996$               |
| 60–90      | $y = 310.33l + 1929.6$         |

| Time       | Equation                        |
|------------|---------------------------------|
| 0–30       | $y = 183.46l - 221.6$           |
| 30–60      | $y = 19.723l + 8.5133$          |
| 60–90      | $y = 40.307l + 18.113$         |

| Time       | Equation                        |
|------------|---------------------------------|
| 0–30       | $y = -110.76l + 420.82$        |
| 30–60      | $y = -333.08l + 907.8$         |
| 60–90      | $y = -51.807l + 165.54$       |

A mathematical model that takes into account the effect on amylase with regards to the time factor and the fat component is as follows:

$$y = t(3734.6 - 871.84t)(0.071l + 0.919)(-498.056z_1 + 0.312z_2 - 8.113z_3 - 177.885z_4 - 0.492z_5 + 41.101z_6 + 45.392z_7 + 1726.152z_8 + 634.907z_9 - 431z_{10} + 29.147z_{11} + 3.468z_{12} - 16.391z_{13} - 10.068z_{14} - 6.433z_{15} + 11115.076).$$

A mathematical model that takes into account the effect on lipase with regards to the time factor and the fat component is as follows:
y = t(465.4−124.31t)(2009.246z1 + 10.628z2 − 11.779z3 + 231.019z4 + 1.9z5 − 32.653z6 + 43.914z7 + 3233.325z8 − 3594.539z9 + 493.462z10 + 29.477z11 − 6.677z12 + 3233.325z13 + 493.462z14 − 3594.539z15).

A mathematical model that takes into account the influence on the protease in chyme with regards to the time factor and the fat component is as follows:

A mathematical model that takes into account the influence on the protease in chyme with regards to the time factor and the fat component is as follows:

y = t(–136.7+38.75t)(–0.3l+1.527)(–4213.849z1 –25.547z2 + 182.338z3 – 217.879z4 + 18.369z5 – 82.443z6 + 1526.617z7 – 15906.433z8 + 4081.981z9 – 923.481z10 + 35.693z11 + 8.542z12 + 1.643z13 + 20.774z14 – 4.336z15 + 31086.875.

Thus, as a result of the analysis and subsequent modeling, a number of mathematical models based on correlation and regression dependences and allowing one to evaluate the effect of blood biochemical parameters, as well as the fat component and time factor on the presence of enzymes in the pancreas have been obtained. All the obtained models have a high degree of reliability (p<0.05) as well as a high degree of significance (R^2 > 0.65).

4. Discussion

Adding sunflower oil to the diet showed the following correlation between the enzymes activity in the chyme and the chemical composition in the diet 30 minutes before feeding: amylase and crude protein (r=0.71), after 30 minutes there was a negative correlation between lipase and crude fat (r=−0.62). The experimental data of a number of authors [13–14] on the determination of pancreatic enzymes activity in the duodenal chyme showed that the inclusion of sunflower oil in the diet leads to a decrease in lipase activity in the blood and significantly increases the catalytic chyme proteases activity.

With palm oil, a positive weak correlation was formed 30 minutes before feeding between amylase and organic matter r=0.53. 30 minutes after feeding a negative relationship was detected between protease and organic matter r=−0.54. A positive enzymes dependence in chyme was noted only 30 minutes after feeding between lipase and crude fat r=0.55, the correlation was low. The authors of [15–16] showed that correlations between the composition of oil with growth rates and markers of oxidative stress imply that the total polar compounds and polymerized triglycerides should be measured as an oil quality indicator with growth rates correlating with lipids in blood plasma.

A pronounced correlation between the protease and dry matter (r=0.54); lipase and crude fat (r=0.50) was most pronounced with the introduction of soybean oil. In studies [17], it was found that excessive deposition of fat causes did not only induce metabolic diseases, but also could lead to an adverse effect when consumed and affect the state of the animal’s body.

The results of the study demonstrated that when calf oil was included in the diet, there was a negative correlation between the protease and crude protein (r=0.52), namely, protease activity increased with a slight decrease in the level of crude protein. In this case, there was a lack of protease correlation, and a negative correlation was found between lipase and nitrogen–free extractive substances (r=−0.55). A number of authors [18–19] found that amylase activity in chyme obtained by feeding vegetable fats was lower compared to the control. But at the same time, there was a tendency to its increase in the period from 10 to 30 minutes. At this time, the amylolytic activity index increased by 37 %.

In the initial period, a correlation was revealed between the total protein and lipase (r=0.63) as well as between protease and albumin (r=0.54), cholesterol (r=−0.54), magnesium (r=−0.62) and calcium (r=0.53). The revealed unequal nature of enzymes activity in duodenal chyme with respect to the introduced oils is stipulated not only by the specificity of the introduced oils, but also by the influence of the microenvironment as well as functional adaptation of the enzyme system [20]. When feeding with palm fat [21,22] in an amount of 4% by weight of feed, it was found that amylase activity increased and partially stabilized proteolytic enzymes in the heterogeneous environment of the cows’ chyme.

5. Conclusion

As a result of the conducted research, the correlation analysis method using nonparametric methods revealed a correlation between the chemical composition of the diet and the time factor. When
sunflower oil was added to the diet, a correlation was found between crude protein \( (r=0.71) \) and crude fat \( (g=-0.62) \). When introducing palm oil into the diet, the relationship between raw fat \( (r=0.55) \) and organic matter \( (r=-0.54) \) was determined. Flaxseed oil contributed to the correlation of crude protein \( (r=-0.52) \) and nitrogen-free extractives \( (r=-0.55) \), as well as organic matter \( (r=0.54) \). The formulated mathematical models based on correlation allow us to take into account the time factor, diet, and individual indicators of the fat component. In addition, they allow developing not only new feed recipes depending on the fat and acid composition of the diet in the presence of the specified initial data, but also to predict their effect on the quality of the resulting products. The potential of biotechnology in this area is great and requires extensive development and implementation of new technological solutions.

Acknowledgments

The research was conducted with the financial support of the Russian science Foundation (No. 20-16-00088).

Conflict of Interest: The authors declare that they have no conflict of interest.

Ethical standards: All applicable international, national, and institutional guidelines for animal care and use have been followed.

References

[1] Kairenius P and Leskinen H 2018 Effect of dietary fish oil supplements alone or in combination with sunflower and linseed oil on ruminal lipid metabolism and bacterial populations in lactating cows *Dairy Sci.* **101**(4) 3021–35

[2] Zubtsov V A and Minevich I E 2015 The strategy of the technology development in forage production on the flax seeds and its products processing use *J. of VNIIMZH* **4**(20) 72–9

[3] Walther T C and Farese R V Jr 2012 Lipid droplets and cellular lipid metabolism *Annu. Rev. Biochem.* **81** 687–714

[4] Lebedev S V, Kvan O V, Vertiprakhov V G, Gavrish I A and Gubaidullina I Z 2019 Effects of chromium ultra–fine particles on the pancreas enzyme system of calve *IOP Conf. Ser. Earth and Environmental Sci.* **341** 012151

[5] Lebedev S, Gavrish I, Gubajdullina I and Kvan O 2019 The effect of nanoparticles on mineral metabolism in the body of laboratory animals *19th Int. Multidisciplinary Sci. GeoConf. SGEM* **1**(2) 971–8

[6] Wendlinger C, Hammann S and Vetter W 2014 Various concentrations of erucic acid in mustard oil and mustard *Food Chem.* **153** 393–7

[7] Yang HJ, Yim N and Lee KJ 2016 Simultaneous determination of nine bioactive compounds in Yijin–tang via highperformance liquid chromatography and liquid chromatography electrospray ionization–mass spectrometry *Integrat. Med. Res.* **5**(2) 140–50

[8] Lebedev S V, Gavrish I A, Shejda E V and Miroshnikov I S 2019 Effect of various fats on digestibility of nutrients in diet of calves *IOP Conf. Ser. Earth and Environmental Sci.* **341** 012066

[9] Crescenzo R, Bianco F, Coppola P, Mazzoli A, Tussellino M and Carotenuto R 2014 Fructose supplementation worsens the deleterious effects of short–term high fat feeding on hepatic steatosis and lipid metabolism in adult rat *Exp. Physiol.* **99** 1203–13

[10] Zhang G and Li C 2009 AMPK: an emerging drug target for diabetes and the metabolic syndrome *Cell Metabolism* **9**(5) 407–16

[11] Mao T, Yang L and Liu Y 2011 The mechanismof cell endoplasmic reticulum stress and glucose and lipid metabolism disorder *Chinese J. of Cell Biol.* **33**(7) 727–37

[12] Lebedev S, Sheida E, Vertiprakhov V, Gavrish I, Kvan O and Gubaidullina I 2019 A study of the exocrinous function of the cattle pancreas after the introduction of feed with a various protein source in rations *Biosci. Res.* **16**(3) 2553–62

[13] Donskova L A, Belyaev N M and Leiberova N V 2018 Fatty–Acid Composition of Lipids as
Functional *Purpose Indicator of Poultry Meat Products from: Theoret. and Pract. Aspects Food Chem. and Hygiene* **3**(1) 4–10

[14] Nakamura M, Nomura S and Yamakawa T 2018 Endogenous calcitonin regulates lipid and glucose metabolism in diet–induced obesity mice *Sci. Reports* **8** 17001.

[15] Lebedev S V, Gavrish I A, Gubajdullina I Z and Shabunin S V 2019 Effects caused by different doses of dietary chromium nanoparticles fed to broiler chickens *Agricult. Biol.* **54**(4) 820–31.

[16] Zhou J, Liu H and Zhou S 2016 Adaptor protein APPL1 interacts with EGFR to orchestrate EGF–stimulated signaling *Sci. Reports* **61** 1504–12.

[17] Xie T, Li J and Mao T 2017 Decoction Ameliorates High–Fat–Induced Nonalcoholic Steatohepatitis in Rats by Regulating JNK1 Signaling Pathway *Evidence–Based Complementary and Alternative Med.* **14** 4603701.

[18] Lebedev S V, Gavrish I A, Shejda E V, Miroshnikov I S, Ryazanov V A, Gubajdullina I Z and Makaeva A M 2019. Effect of various fats on digestibility of nutrients in diet of calves *IOP Conf. Ser. Earth and Environmental Sci.* **341** 012066.

[19] Pang J, Xi C, Huang X, Cui J, Gong H and Zhang T 2016 Effects of Excess Energy Intake on Glucose and Lipid Metabolism in C57BL/6 Mice *Dairy Sci* **11**(1) e0146675.

[20] Kvan O, Gavrish I, Lebedev S, Korotkova A, Miroshnikova E, Bykov A and Serdaeva V 2018 Effect of probiotics on the basis of Bacillus subtilis and Bifidobacterium longum on the biochemical parameters of the animal organism *Environmental Sci. and Pollut. Res.* **25**(3) 2175–83.

[21] Lebedev S, Sheida E, Vertiprakhov V, Gavrish I, Kvan O, Gubaidullina I, Ryazanov V and Miroshnikov I 2019 A study of the exocrinous function of the cattle pancreas after the introduction of feed with a various protein source in rations *Biosci. Res.* **16**(3) 2553–62.

[22] Duskaev G, Karimov I, Levakhin G et al 2019 Ecology of ruminal microorganisms under the influence of quercus cortex extract *International Journal of GEOMATE* **16**(55) 59–66.