# Modeling in Simulink Production Process of White Table Wine with Increased Biological Activity

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### Abstract

Simulation modeling is a type of computer modeling. In this case, imitation is understood to mean carrying out various experiments on computers with models that are presented as a certain set of computer programs. Currently, there are a significant number of software systems that allow using sequence calculations and graphical display of their results to reproduce (imitate) the processes of functioning of the object, subject to the impact on it of various factors. Currently, the use of mathematical modeling in economics and agriculture has become especially relevant. The activities of enterprises are carried out in a competitive environment and those who use resources most efficiently achieve success. Simulink is a block diagram environment for multidomain simulation and Model-Based Design. It supports system-level design, simulation, automatic code generation, and continuous test and verification of embedded systems. Simulink provides a graphical editor, customizable block libraries, and solvers for modeling and simulating dynamic systems. An actual direction in the development of modern winemaking is the development of technology for obtaining functional wine products with increased content of biologically active substances of grapes. The article presents simulation models of grape cultivation for the production of white table wine with increased biological activity and stastatistical results of studies of the formation of the amino acid complex of white table wine materials made in Simulink.

### **Keywords** 1

mathematical analysis, computer modeling, Simulink, biological activity, antioxidant activity, correlation dependence

# 1. Introduction

Modeling is used to understand the properties of the original by examining not the object itself, but it's model. Modeling is justified if the creation of the model is easier than the creation of the original. In principle, depending on the way the models are implemented, they can be divided into physical models and mathematical models. Physical models are identical to the original devices of reduced dimensions, which have the same physical nature. They most accurately describe the behavior of a real object, but varying their parameters is difficult, and the creation of the model itself is very expensive. Mathematical models are descriptions of an object in the form of mathematical relationships. The mathematical model that describes the behavior of an object in time is called a simulation model [1,2].

Simulink is a block diagram environment for multidomain simulation and Model-Based Design. It supports system-level design, simulation, automatic code generation, and continuous test and

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verification of embedded systems. Simulink provides a graphical editor, customizable block libraries, and solvers for modeling and simulating dynamic systems.

The biological activity of grape wines is primarily due to the qualitative and quantitative structure of the phenolic complex of wine materials [3-5]. The long-term contact of the solid and liquid components of the pulp with the ridges used for the preparation of Kakhetian-type wines promotes a significant accumulation of phenolic compounds and, as a result, an increase in the values of antioxidant activity [6-8]. An important role in the formation of the quality and biological value of white table wines is played also by other chemical compounds of wine materials, including amino acids, the composition of which depends on their content in the wort and fermentation conditions [9-10].

The purpose of this research was to delelop simulation model of production rocess of white table wine with increased biological activity. Test samples were obtained under micro-wine making conditions using the traditional "white-on-white" technological method (control) and by varying the degree of fermentation of sugars in the pulp without separating the ridges (1/3, 2/3, and complete fermentation) from their original content in the grapes. A sampling of wine materials was carried out according to GOST 31730-2012 Wine-making products [11-13]. Simulink was used to develop and to test to the model.

The qualitative and quantitative composition of amino acids was determined by high-performance liquid chromatography (HPLC) using the Agilent Technologies chromatographic system (model 1100, USA) with a diode-matrix detector according to the methods P 4.1. 1672-03. Guidelines on methods of quality control and safety of biologically active food additives. All definitions were carried out in three repetitions. The research results were processed using standard methods of mathematical statistics. The standard deviation of the measurement results did not exceed 5 % [13-16].

## 2. Main Part

At present, there are a significant number of software systems that allow, using a sequence of calculations and a graphical display of their results, to reproduce (imitate) the processes of an object's functioning under the condition of exposure to various factors. Among the computer modeling systems, the MATLAB program stands out, focused primarily on scientific and technical calculations and modeling [8,9]. The Simulink extension package of the MATLAB program allows you to perform simulation of objects consisting of graphic blocks with specified parameters

Below is an overview of the primary model created in Simulink. This Simulink model showing the relationship between vineyard/fruit area and yield (fig. 1,2).

Scope blocks are used to visualize the results of the selected function. Therefore, they have no output elements. The results of scope blocks can be used to debug functions or to visualize the results of model functioning. The model contains two blocks that contain functions for calculating yield and fruiting. The "Product" block uses data from the yield and fruiting blocks. The Saturation block sets the limit for the upper and lower data values. The result of the model's functioning is shown in Scope block 3.



#### Figure 1: Simulink model showing the relationship between vineyard/fruit area and yield



Figure 2: The results of the simulation model

The main chemical and technological indicators of the control and experimental samples of white table wine materials, corresponding to GOST 32030-2013 Table wines and table wine materials. General technical conditions. The obtained values of the antioxidant activity (AOA) of the experimental wine materials indicated an increased biological activity compared to the control sample [17-18]. As a result of the conducted studies, it was found that long-term contact of the solid and liquid parts of the pulp contributes to a significant accumulation of amino acids in the process of preparing wine materials with increased biological activity. This is because the skin of grapes and the adjacent layers of pulp contains the largest amount of nitrogenous substances that pass into the wine material when the wort is aged on the pulp [20-22].

This graph examines the dependence of the yield on the area of fruiting vineyards. In this case, the function of the sum of sines of the 6th order is taken for approximation. The maximum obtained reliability according to the R-squared criterion is 0.63. This indicates either the absence of a clear relationship between the areas of fruiting vineyards and the yields or the need for additional data analysis, taking into account other factors (fig. 2).

Studies have shown (Fig.) that when 2/3 of the sugars contained in grapes are fermented, the mass concentration of the sum of amino acids (MCA) reaches the maximum value and exceeds this indicator by 60% in wine materials prepared "in white". With the complete fermentation of sugars, the content of amino acids in the wine material decreased. 23 amino acids were identified in wine materials prepared by fermentation of pulp with ridges until complete fermentation and fermentation of 2/3 of sugars (table). Glutamic acid, serine, and alanine were not detected in the amino acid complex of the prototype and the wine material prepared by fermenting 1/3 of the sugars. The main component of the amino acid complex in all wine materials was proline, the maximum content of which was noted in samples prepared by fermenting 2/3 of the pulp sugars (fig. 3).



Figure 3: Dynamics of amino acids and antioxidant activity depending on the degree of fermentation

These wine materials were also enriched to the greatest extent with other amino acids, including essential ones (valine, leucine, isoleucine, lysine, threonine, methionine, phenylalanine). Their share in the experimental wine material with the fermentation of 2/3 of the pulp sugars was 7.9% of the total amino acid content compared to other wine materials (6.4% in the experimental sample, 6.5% with the fermentation of 1/3 of the sugars, and 5.9% with full fermentation) (fig. 4).



Figure 4: Amino acid composition of white table wine materials

Studies have shown that complete fermentation of sugars in the pulp with ridges leads to a decrease in the mass concentrations of all amino acids, which is associated with their consumption by yeast and the processes of transformation of amino acids with the formation of other compounds during fermentation (for example, higher alcohols) [7].

Mathematical processing of the data revealed a high correlation between the values of antioxidant activity in the control and experimental wine materials and the mass concentration of the sum of amino acids (r=0.74 at P=0.05). The analysis of the literature data indicates both the synergistic effect of amino acids on antioxidants [9] and the manifestation of their antioxidant activity [10].

## 3. Conclusions

Simulink is a block diagram environment for multidomain simulation and Model-Based Design. It supports system-level design, simulation, automatic code generation, and continuous test and verification of embedded systems. Simulink provides a graphical editor, customizable block libraries, and solvers for modeling and simulating dynamic systems.

The proposed model allows emulation of the production of white table wine with increased biological activity.

An actual direction in the development of modern winemaking is the development of technology for obtaining functional wine products with increased content of biologically active substances of grapes. The analysis of publications devoted to the amino acid composition and biological activity of wines is carried out. The article presents the results of studies of the formation of the amino acid complex of white table wine materials from the Rkatsiteli grape variety, the most common in the conditions among white varieties, depending on the degree of fermentation of the sugars of the pulp with ridges -1/3, 2/3 and complete fermentation. It was found that when fermenting 2/3 of the sugars contained in grapes, the mass concentration of the sum of amino acids reaches the maximum value and is 60% higher than this indicator in wine materials prepared "by white". With complete fermentation of sugars, the content of amino acids in the wine material decreases.

As a result of high-performance liquid chromatography studies, 23 amino acids were identified in white table wine materials with increased biological activity. At the main technological stages of production of control and experimental samples of wine materials, the values of antioxidant activity were determined. The established value of the correlation coefficient between the indicator of antioxidant activity and the mass concentration of amino acids (r=0.74) indicates the manifestation of antioxidant properties by amino acids. The obtained data allow us to recommend a technology for the production of white table wines with increased biological activity, which provides for the fermentation of the pulp with ridges until the fermentation of 2/3 of the sugars, followed by the separation of the solid parts of the pulp and further fermentation of the wort until complete fermentation.

# 4. References

- Ovcharova, S., Krachunov, H. Innovation activities in entrepreneurial firms: The case of Bulgaria. Entrepreneurship in the Balkans: Diversity, Support and Prospects, 2013, pp. 37-55. DOI: 10.1007/978-3-642-36577-5\_3
- [2] Krachunov, H., Sheremet, T.G. Parameters for estimate the digital national economy in the EAEU Member Countries. CEUR Workshop Proceedings, 2021, Vol-2834, (Selected Papers of the 4th All-Russian Scientific and Practical Conference with International Participation "Distance Learning Technologies", DLT 2019), pp. 219-230.
- [3] D. Harman, Aging: a theory based on free radical and radiation chemistry, J. Gerontol. Vol. 11(3), pp. 298-300 (1956), DOI: 10.1093/geronj/11.3.298.
- [4] T.G. Tsypko, N.S. Brilenok, K.S. Guschaeva, V.I. Vershinin, Determination of the total phenol antioxidants content in tea samples using different variations of FRAP assay, Analytics, and Control; vol. 23(1), pp. 143-151(2019), DOI: 10.15826/analitika.2019.23.1.011.
- [5] D. Villano, M.S. Fernandez-Pachon, A.M. Troncoso, M.C. Garcia-Parrilla, The antioxidant activity of wines determined by the ABTS(+) method: influence of sample dilution and time, Talanta. Vol. 64(2)m pp. 501-509 (2004), DOI: 10.1016/j.talanta.2004.03.021.

- [6] F. Renaud, M. de Lorgeril, Wine, alcohol, platelets and the French paradox for coronary artery disease. Lancet, vol. 339(8808), pp. 1523-1526 (1992), DOI: 10.1016/0140-6736(92)91277-f.
- [7] G.J. Soleas, E.P. Diamandis, D.M. Goldberg, Wine as a biological fluid: history, production, and role in disease prevention, J. Clin. Lab. Anal. Vol. 11(5), pp. 287-313 (1997), DOI: 10.1002/(SICI)1098-2825(1997)11:5<287::AID-JCLA6&#x0003e;3.0.CO;2-4.
- [8] J.A. Larrauri, C.Sánchez-Moreno, P. Rupérez, F. Saura-Calixto, Free radical scavenging capacity in the aging of selected red spanish wines, J. Agric. Food Chem, vol. 47(4), pp.1603-1606 (1999), DOI: 10.1021/jf980607n.
- [9] L.M.Solovyova, Y.V. Grishin, A.N. Kazak, N.N. Oleinikov, P.V. Chetyrbok, The possibility of using the potentiometric titration method to determine the antioxidant properties of wines, Journal of Physics: Conference Series, vol. 1703(1): 012048 (2020), DOI: 10.1088/1742-6596/1703/1/012048.
- [10] Y.V.Grishin, D.V. Nekhaichuk, E.A. Sergeeva, P.Shamaeva, R.R. Timirgaleeva, Prospects for the application of the traditional Medoc method of red wines production in the southern regions of Russia, V International Scientific and Practical Conference "Distance Learning Technologies", pp.349-356 (2020),
- [11] Y.V. Grishin, A.N. Kazak, N.N. Oleinikov, N.I. Gallini, P.V. Chetyrbok, Analysis of complex technologies for obtaining wine products with increased antioxidant properties, V International Scientific and Practical Conference "Distance Learning Technologies", pp. 357-364 (2020).
- [12] H.C. Budnikov, G.K. Ziyatdinova, Natural phenolic antioxidants in bioanalytical chemistry: state of the art and prospects of development, Russ. Chem. Rev. vol. 84(2), pp. 194-224 (2015), DOI: 10.1070/RCR4436.
- [13] M.N. Peyrat-Maillard, S. Bonnely, C. Berset, Determination of the antioxidant activity of phenolic compounds by coulometric detection, Talanta, vol. 51(4), pp. 709-716 (2000), DOI: 10.1016/s0039-9140(99)00331-8.
- [14] K. Schlesier, M.Harwat, V. Böhm, R. Bitsch, Assessment of antioxidant activity by using different in vitro methods, Free Radic. Res., vol. 36(2), pp. 177-87 (2002), DOI: 10.1080/10715760290006411.
- [15] M.D. Rivero-Perez, P. Muniz, M.L. Gonzalez-Sanjose, Antioxidant profile of red wines evaluated by total antioxidant capacity, scavenger activity, and biomarkers of oxidative stress methodologies, J. Agric. Food Chem., vol 55(14) (2007). DOI: 10.1021/jf070306q.
- [16] D. Gupta, Methods for determination of antioxidant capacity: A review, International Journal of Pharmaceutical Sciences and Research, Vol. 6(62), pp. 546-566 (2015), DOI:10.13040/IJPSR.0975-8232.6(2).546-66.
- [17] D. Huang, B. Ou, R.L. Prior, The chemistry behind antioxidant capacity assays, J. Agric. Food Chem., Vol. 53(6), pp. 1841–1856 (2005), DOI: 10.1021/jf030723c.
- [18] I.F. Benzie, J.J. Strain, The ferric reducing ability of plasma (FRAP) as a measure of "antioxidant power": the FRAP assay, Anal. Biochem., vol. 239(1), pp. 70-76 (1996), DOI: 10.1006/abio.1996.0292.
- [19] I.F. Benzie, J.J. Strain, Ferric reducing/antioxidant power assay: direct measure of total antioxidant activity of biological fluids and modified version for simultaneous measurement of total antioxidant power and ascorbic acid concentration, Methods Enzymol., vol. 299, pp.15-27 (1999), DOI: 10.1016/s0076-6879(99)99005-5.
- [20] G. Cao, H.M. Alessio, R.G. Cutler, Oxygen-radical absorbance capacity assay for antioxidants, Free Radical Biology and Medicine, vol. 14(3), pp. 303-311 (1993), DOI: 10.1016/0891-5849(93)90027-r.
- [21] P.T. Gardner, D.B. McPhail, A. Crozier, G.G. Duthie, Electron spin resonance (ESR) spectroscopic assessment of the contribution of quercetin and other flavonols to the antioxidant capacity of red wines, J. Sci. Food Agric., vol. 79(7), pp. 1011-1014 (1999), DOI: 10.1002/(SICI)1097-0010(19990515)79:7<1011::AID-JSFA320>3.0.CO;2-Y.
- [22] A.V. Ivanova, A.S. Petrov, E.A. Vezhlivtsev, A.I. Matern, Method of determining antioxidant activity using electron paramagnetic resonance spectroscopy method. Patent RF, No 2614365 (2015).