1. **Boyadjiev, C., & Popova-Krumova, P. (2022). Introduction in the Biotechnology Processes Modeling. *Progress in Chemical Science Research Vol. 2*, 1–13.**
https://doi.org/10.9734/bpi/pcsr/v2/1920A

Abstract: In the paper is presented a theoretical analysis of the methods for biotechnological processes modeling. The methods for modeling specific processes may be different, but in all cases, they have to bring the mathematical description closer to the real process by using appropriate experimental data. These methods are presented for biotechnology processes in column apparatuses, in the cases of multiparameter models and modeling of processes with unknown mechanism.

2. **Boyadjiev, Chr.**, **Dzhonova, D.**, **Stefanova, K.**, **Panyovska, St.**, **Popova, P.**, **Pavlenko, A., Zhukov, V., & Slesareva, E. (2020). On the phases' distribution in packed columns. Journal of Physics: Conference Series, (Vol. 1677, No. 1, p. 012054).**
IOP Publishing. ISSN: 1742-6588, doi:10.1088/1742-6596/1677/1/012054.

Abstract: Packed columns are typical apparatuses for industrial separation processes, which are important in fuel and energy production and reduction of harmful emissions in the atmosphere. The efficiency of the processes in them is strongly dependent on the regular distribution of phases. The liquid and gas maldistribution has been the subject of long intensive investigations. The formation of a liquid wall flow has been found to be one of the main factors for the large-scale radial irregularity of liquid and gas distribution. The prediction and control of this phenomenon is still unsatisfactory. Our work suggests a new approach for evaluation of the wall flow in countercurrent absorption with random packings. It uses simple mathematical apparatus and is based on experimental data of the wall flow along the column height. It allows gaining knowledge about the liquid flow and evaluating the wall flow volume as a criterion of efficiency for comparison of packings. The model is demonstrated by a case study with data for metal Pall rings.

3. **Boyadjiev, Chr.**, **Dzhonova-Atanasova, D.**, **Popova-Krumova, P.**, **Stefanova, K.**, **Pavlenko, A., Zhukov, V., & Slesareva, E. (2020). Liquid wall flow in counter-current**

column apparatuses for absorption processes with random packings. Bulg. Chem. Commun., 52, 74-79. ISSN: 0324-1130, DOI:10.34049/bcc.52.F.0013

Abstract: Absorption processes are widely applied in chemical engineering. Important modern applications are fuel production and purification of waste gases and liquids for environment protection and production of valuable substances. Packed columns are typical apparatuses for these processes. Their efficient operation is strongly dependent on the regular distribution of the liquid and gas phase. The formation of a liquid wall flow is one of the main reasons for large-scale maldistribution in packed beds. The prediction of the liquid maldistribution is needed for evaluation of mass transfer efficiency. The present work uses a new approach to model the liquid wall flow in different types of random packings. The model results, in agreement with experimental data, show the effect of important operation parameters on the wall flow development along the column. A maldistribution parameter is calculated as a base for comparison of liquid maldistribution in packings. The present method for evaluation of the wall flow is intended for further modeling of separation efficiency in packed columns.

4. **Pavlenko, A., Zhukov, V., Slesareva, E., Boyadjiev, Chr.**, **Boyadjiev, B.**, **Dzhonova-Atanasova, D., & Popova-Krumova, P. (2020). Large-scale maldistributions of local flow parameters at distillation on a structured packing. Bulg. Chem. Commun., Volume 52, 42-46.** ISSN: 0324-1130, DOI: 10.34049/bcc.52.F.0007

Abstract: The results of research and operation of industrial distillation columns with the most widely used regular packing have shown that the separation efficiency with increasing diameter can significantly decrease due to formation of large-scale nonuniformity of liquid flows, as well as concentrations along the column section, which significantly affects the performance and purity of the finished product. The experiments were carried out on a large-scale experimental setup, designed to study the integral and local characteristics of mixture separation by distillation on a structured packing. To simulate the process of separation of liquefied air, a mixture of R114/R21 freons was used. The separation of mixture was studied on a structured package Mellapack 350.Y with a diameter of 0.9 m and height of 2100 mm. We studied the efficiency of mixture separation, dynamics of formation of large-scale temperature field non-uniformity over the column cross-

section during mixture separation, and distribution of the density of local liquid flow rates at the packing outlet. The experiments were carried out at a pressure of 0.3 MPa and initial concentration of the R114 / R21 mixture of 12%. The conducted experimental studies showed that large-scale temperature maldistribution over the cross-section and height of the distillation column is formed. The conditions leading to formation of this nonuniformity are considered. The obtained experimental data will be used in the development of new approaches for numerical simulation of mass transfer and mixture separation efficiency in distillation columns with structured packing in the framework of a joint project.

5. **Boyadjiev, B.**, **Boyadjiev, Chr.**, **& Popova-Krumova, P. (2020). Convective type models of co-current absorption processes in column apparatuses. Bulg. Chem. Commun., 52, 86-94.** ISSN: 0324-1130, DOI: 10.34049/bcc.52.F.0015

Abstract: A new approach for the absorption processes modeling in co-current column apparatuses is presented in the cases of industrial conditions, where the models are convective type form. The use of experimental data for the average concentration at the column end, in the cases of highly soluble and lightly soluble gases, permits to obtain the model parameters related to the radial non-uniformity of the velocity in the gas and liquid phases. These experimental parameter values permit to obtain the mass transfer coefficient in the cases of physical and chemical absorption of the average-soluble gases.

6. **Boyadjiev, Doichinova, M., C., Boyadjiev, B., & Popova-Krumova, P. (2017). Transfer processes in industrial column apparatuses. Mathematical modeling, 1 (1), 23-27.** ISSN: 2535-0978

Abstract: The paper is a presentation of the monography “Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, Modeling of Column Apparatus Processes, Springer-Verlag, Berlin Heidelberg, 2016, pp. 313. A new approach to modeling the mass transfer processes in industrial column apparatuses, in the physical approximations of the mechanics of continua, is used for the creation of convection-diffusion and average-concentration models. The models of chemical, absorption, adsorption and catalytic processes are presented.

7. **Boyadjiev, Chr., Doichinova, M., Popova-Krumova, P., & Boyadjiev, B. (2015). On the gas purification from low SO_2 concentration. 1. Absorption processes modeling. Int. J. Eng. Res, 4 (10), 550-557.** ISSN: 2347-5013

Abstract: A theoretical analysis, of the processes for gas purification from low SO2 concentration in the thermal power plants, is presented. A new approach, for qualitative analysis (convection-diffusion type of model) and quantitative description (average concentration model) of the absorption processes in column apparatuses, is proposed. The theoretical analysis of the physical absorption, chemical absorption and absorption with two-phase absorbent is shown. The presented theoretical analysis of the methods and apparatuses for waste gases purification from SO2, using two-phase absorbent (CaCO3 suspension), shows, that the process is physical absorption practically and the mass transfer resistances in the gas and liquid phases are 44% and 56% respectively. In these conditions, a new patent is proposed, where the process optimization is realized in two-zone column, where the upper zone is physical absorption in gas-liquid drops system and the lower zone is physical absorption in liquid-gas bubbles system. The chemical reaction takes place in the column tank.

8. **Boyadjiev, Chr., Doichinova, M., Popova-Krumova, P., & Boyadjiev, B. (2015). On the gas purification from low SO_2 concentration. 2. Two-steps chemical absorption modeling. Int. J. Eng. Res, 4 (10), 557-561.** ISSN: 2347-5013

Abstract: The modeling of the gas absorption in a new column apparatus for waste gases purification from SO2, using two-phase absorbent ($CaCO_3$ / H_2O suspension) is presented. The process is realized in a three-zone column. In the upper zone, a physical absorption in gas-liquid drops system is realized and the big convective transfer in the gas phase leads to a decrease of the mass transfer resistances in this phase. In the middle zone, a chemical absorption in liquid-gas bubbles system takes place and the big convective transfer in the liquid phase leads to a decrease of the mass transfer resistances in this phase. The large volume of the liquid in the middle zone causes an increase of the chemical reaction time and as a result, a further decrease of the mass

transfer resistances in the liquid phases is realized. The third zone is the column tank, where the chemical reaction takes place only.

9. **Boyadjiev, C., Boyadjiev, B., Doichinova, M., & Popova-Krumova, P. (2015). Co-Current apparatus for gas purification from SO_2. Recent Innovations in Chemical Engineering (Formerly Recent Patents on Chemical Engineering), 8(1), 25-29.**

Abstract: A new patent co-current apparatus for gas purification from SO_2 is presented. In comparison with the counter-current gas absorbers, the gas velocity in the co-current apparatus increases 5-6 times and as a result, the column diameter decreases more than 2 times. The new approach for modeling of the column apparatuses is used for modeling the SO_2 absorption in the co-current apparatus. The convection-diffusion model for qualitative analysis and process mechanism identification is used. The average concentration model for quantitative analysis is presented.

10. **Boyadjiev, Chr., Boyadjiev, B., Popova-Krumova, P., & Doichinova, M. (2015). An innovative approach for adsorption column modeling. Chemical Engineering & Technology, 38 (4), 675-682.**

Abstract: A new method for physical and chemical adsorption modeling in column apparatuses is presented. A convection-diffusion model is obtained in the approximations of the continua mechanics, where the mathematical point is equivalent to the medium elementary volume, which is sufficiently small with respect to the column volume and the same time sufficiently large with respect to the intermolecular volumes of the medium. The created convection-diffusion type model allows performing qualitative analysis of the process and obtaining the effect of the velocity radial non-uniformity in the column. An average concentration model is applied for quantitative description of physical and chemical adsorption in the column apparatus. The methods for model equation solutions and the model parameter identification are described.

11. **Boyadjiev Chr., Doichinova M., Popova-Krumova P., & Boyadjiev B. (2014). Intensive column apparatus for chemical reactions. Open Access Library Journal, 1 (3), 1-9.**

Abstract: A solution of the intensification problem of the column chemical reactors is presented in the approximation of the mechanics of continua. The effect of the radial non-uniformity of the velocity distribution, the effect of the tangential flow and simultaneous mass, and heat transfer processes are analyzed. A theoretical analysis of the simultaneous mass and heat transfer processes in column reactors is presented.

12. **Boyadjiev, C., Doichinova, M., Popova-Krumova, P., & Boyadjiev, B. (2014). On the gas purification from low SO_2 concentration. Recent Innovations in Chemical Engineering (Formerly Recent Patents on Chemical Engineering), 7(1), 39-46.**

Abstract: The solid fuel combustion in the thermal plants, which use sulfur-rich fuels, poses the problem of SO_2 removal from waste gases. This problem is complicated by the fact, that it is required to purify huge amounts of gas with low SO_2 concentration. The huge gas amounts need big size apparatuses, which is possible to be decreased if the absorption rate is maximal. The theoretical analysis of the methods and for purification of waste gases from SO_2, using two-phase absorbent ($CaCO_3$ suspension) shows, that the process is practically a physical absorption and the mass transfer resistances in the gas and liquid phases are 44 % and 56 %, respectively. In these conditions a new patent is proposed, where the process of optimization is realized in three zone columns, where the upper zone is a physical absorption in gas-liquid drops system, the middle zone is a physical absorption in liquid-gas bubbles system and the chemical reaction takes place at the bottom of the column. The convection-diffusion type of models permits to create the average concentration models and give quantitative description of the absorption processes.

13. **Doichinova, M., Popova-Krumova, P., Boyadjiev, Chr., & Boyadjiev, B. (2014). Gas Purification from SO_2 in Thermal Power Plants. Chemical Engineering & Technology, 37 (7), 1243–1250.**

Abstract: Solid fuel combustion in thermal power plants, which use sulfur-rich fuels, poses the problem of SO_2 removal from waste gases. In addition, purification of huge amounts of gas with low SO_2 concentration is necessary. A maximum absorption rate could decrease the size of required big apparatuses. Gas purification from low-concentrated SO_2 in physical and chemical absorption is analyzed theoretically. A convection-diffusion type of models is applied for creating average concentration models and for quantitative description of the absorption processes. Theoretical analysis of methods and devices for waste gas purification from SO_2 by $CaCO_3$ suspension indicates that the process is practically physical absorption.

14. **Popova-Krumova, P., Yankova, S., & Ilieva, B. (2013, December). Mathematical modeling of glycerol biotransformation. In AIP Conference Proceedings (Vol. 1570, No. 1, pp. 74-79). American Institute of Physics.** http://dx.doi.org/10.1063/1.4854744

Abstract: A method for mathematical modeling of glycerol biotransformation by Klebsiella oxytoca is presented. Glycerol is a renewable resource for it is formed as a by-product during biodiesel production. Because of its large volume production, it seems to be a good idea to develop a technology that converts this waste into products of high value (1, 3-Propanediol; 2, 3-Butanediol). The kinetic model of this process consists of many equations and parameters. The minimization of the least square function will be used for model parameters identification. In cases of parameters identification in multiparameter models, the minimization of the least square function is very difficult because it is multiextremal. This is the main problem in the multiextremal function minimization, which will be solved on the base a hierarchical approach, using a polynomial approximation of the experimental data.

15. **Doichinova, M., & Popova-Krumova, P. (2013, December). Modeling of column apparatuses: A review. In AIP Conference Proceedings (Vol. 1570, No. 1, pp. 45-53). American Institute of Physics.** http://dx.doi.org/10.1063/1.4854741

Abstract: This paper presents a review of the modeling method on the base of the physical approximations of the mechanics of continua, which have been developed for processes in column apparatuses. This method includes diffusion type of model for modeling of mass transfer with

chemical reaction in column apparatuses with and without circulation zones. The diffusion type of model is used for modeling of scale effect in column apparatuses too. The study concluded that the proposal method is possibility for investigation the influence of radial non-uniformity of the velocity distribution on the process efficiency, influence of zones breadths on the mass transfer efficiency in the column. The method of the column apparatuses modeling can be used for modeling of physical and chemical absorption, chemical adsorption, homogeneous and heterogeneous (catalytic) chemical reactions, and airlift reactors for chemical and photochemical reactions.

16. **Boyadjiev Chr., Doichinova M., & Popova P. (2012). On the SO_2 Problem in Power Engineering. Transactions of Academenergo, 2, 44-65.**

Abstract: A theoretical analysis of SO_2 absorption with alkaline absorbents in packed bed columns in the cases of mono- and two-phases absorbents is presented. The absorption kinetics in the cases of irreversible chemical reactions on the base of a qualitative analysis of the mathematical model is analyzed. Diffusion type of model and average concentration model for modeling of gas absorption in column apparatuses are used.

17. **Popova, P., & Boyadjiev, Chr. (2010). On the modeling of moisture adsorption in a packed bed. Journal of International Scientific Publication: Materials, Methods and Technologies, 4 (2), 105-111, Sunny Beach, Bulgaria.**

Abstract: This paper presents a mathematical model, which describes process of moisture transfer from the adsorbent bed, and air filtrated through the bed. The model of the packed bed column takes into consideration mass transfer in the bed as well as water diffusion and adsorption in a new composite sorbent "$CaCl_2$/alumina". The model is applied to describe evolution of vapor concentration at the exit of experimental unit for regenerating moisture in ventilation systems, which has recently been suggested, build and tested. Sorption equilibrium of water vapor on the new sorbent has been studied to be used as input parameter in the model. Good agreement between experimental and calculation data demonstrated that the model adequately reflects main physical and chemical features of the regeneration processes. Hence, it can be used for modeling a scale-

up effect and for magnification of the unit from laboratory to larger size, e.g. single room, family house and large residential buildings.

18. **Doichinova, M., Popova, P., & Boyadjiev, Chr. (2010). Mass Transfer in counter-current flows. Transactions of Academenergo, 4, 4-22.**

Abstract: A theoretical analysis of gas-liquid counter-current flow in laminar boundary layers with flat phase boundary based on similarity variables method has been done. The obtained numerical results for the energy dissipation, mass transfer rate and their ratio are compared with analogous results for co-current flows. A diffusion type of model is proposed for modeling of the mass transfer with chemical reaction in the column apparatuses in the cases of circulation zones. The presence of rising and descending flows (the change of the velocity direction in this liquid counter-current flow) leads to using three coordinate systems. An iterative algorithm for the concentration distribution calculation is proposed. The influence of the zones breadths on the mass transfer efficiency in the column is investigated.

19. **Popova, P., & Boyadjiev, Chr. (2008). About microalgae growth kinetics modeling. Chemical and Biochemical Engineering Quarterly, 22 (4), 491-497.** https://doi.org/10.15255/CABEQ.2014.344

Abstract: A method for modeling microalgae growth kinetics is presented. The model parameters were obtained using experimental data for biomass concentration only. The relation between biomass concentration and CO2 concentration in liquid phase was obtained. The proposed model is in good agreement with the experimental data. The presented method is applicable for different photosynthetic processes.

20. **Popova P., & Boyadjiev Chr. (2008). Hierarchical approach for parameter identification of multiparameter models. Biochemical Engineering Journal, 39, 397-402.** DOI: https://doi.org/10.1016/j.bej.2007.09.014

Abstract: The problem of parameters identification in multiparameter models of the complicated kinetics processes is analyzed. In this case, the minimization of the least square function is very difficult because it is multiextremal. The problem solution needs to be obtained very well initial parameters values. A polynomial approximation of the experimental data permits to propose a hierarchical approach for obtaining initial parameters values in the global minimum area, using a consecutive approximations method. The method for parameter identification of multiparameter models is tested for modeling of fermentation systems. The model parameter values are obtained on the bases of real experimental data. The results obtained show a decrease of the model error variance on every next hierarchical level and a good agreement with the experimental data on the last level.

21. **Aristov, Yu., Mezentsev, I., Mukhin, V., Boyadjiev, Chr., Doichinova, M., & Popova, P. (2006, September). New approach to regenerate heat and moisture in a ventilation system: Experiment. In 11th Workshop on "Transport Phenomena in Two-Phase Flow" Proceedings, Bulgaria, (pp. 77-85).**

Abstract: For countries with a cold climate the large difference in winter between indoor and outdoor temperatures leads to a) large heat loses in ventilation systems; b) moisture freezing at the systems exit and c) great reduction in the indoor humidity. Here we present and discuss a new approach for regenerating heat and moisture in ventilation systems in cold climates which allows resolution of these problems. The method has been tested under climatic conditions of South Siberia (winter 2005-2006). New composite desiccant "$CaCl_2$ in alumina" was used as a water buffer and showed performance better than common adsorbents. New mathematical model of the process has been developed to describe experimental data obtained, optimize the unit operation and solve the scale-up problems. Technical, economical and social aspects of this approach are considered.

22. **Boyadjiev, Chr., Doichinova, M., Popova, P., & Aristov, Yu. (2006, September). New approach to regenerate heat and moisture in a ventilation system: 2. Modeling. In 11th Workshop on "Transport Phenomena in Two-Phase Flow" Proceedings, Bulgaria, (pp. 85-93).**

Abstract: Mathematical model of the packed bed column, which takes into consideration heat and mass transfer in the bed as well as gas chemisorption by a new composite adsorbent is presented. The diffusion type of model is used to describe, analyze and optimize a new Ventireg unit for regenerating heat and moisture in ventilation systems, which has recently been suggested. The introducing of the average concentration and temperature permits the modeling of a scale-up effect and the magnification of the unit from laboratory to larger size, e.g. single room, family house and large residential buildings. The final aim is to meet the indoor air quality and saving energy standards in such dwellings.

23. **Popova, P., & Boyadjiev, Chr. (2005, September). On the Modeling of Fermentation Systems. In 10th Workshop on "Transport Phenomena in Two-Phase Flow" Proceedings, Bulgaria, (pp. 149-158).**

Abstract: A method for modeling of fermentation systems is proposed. A polynomial approximation of the experimental data permits to use a hierarchical approach for model parameter identification. The exact model parameter values on the bases of the real experimental data are obtained.

24. **Popova, P., & Boyadjiev, Chr. (2004, September). On the regularization of the parameter identification problems, In 9th Workshop on "Transport Phenomena in Two-Phase Flow" Proceedings, Bulgaria, (pp. 145-151).**

Abstract: The solution of the parameter identification problem using a minimization of the least square function is not correct in the cases when the inverse problem is incorrect or essentially incorrect, i.e. in the cases of a solution sensibility due to errors of the "experimental" data used [1]. A comparison analysis of minimization methods shows the influence of an additional condition for solution regularization.