# Reviews of scientific publications

of Assoc. Prof. Dr. Eng. Daniela Dzhonova-Atanasova
in English

**1.** Dzhonova-Atanasova D., Tsibranska I., Vlaev S.. Flow behaviour in a membrane cross-flow filtration cell: experimental observations and CFD modelling. Chemical Technology and Metallurgy, 52, 1, 2017, ISSN: 1314-7471 (print), 1314-7978 (on-line), 58-65. SJR (Scopus):0.156 SJR, непопадащ в Q категория (Scopus) Линк

This paper presents experimental data and CFD-simulation results concerning the flow behaviour during cross-flow nanofiltration applied for concentrating antioxidants such as polyphenols and flavonoids from extracts of natural products. The effects of the cross-flow velocity and solute concentration on the permeate flux behaviour are discussed.
The first one is studied numerically and discussed in rapport with existing experimental observations in literature. The CFD modelling is focused on an experimental flat-sheet membrane cell's hydrodynamics – velocity and shear stress distribution on the membrane surface. The geometry of the cell includes tangential orientation of the feed pipe, resulting in a swirling flow in the cell, tangential to the membrane surface everywhere except for a very small region at the centre. The increase in the feed flow rate leads to greater shear forces to the membrane surface. This results in higher permeate flux attributed to reduced concentration polarization.
The effect of the solute concentration is studied experimentally using a 4 flat-sheet membrane rig for cross-flow filtration in both concentration and full recycle mode of operation. The permeate flux decline during nanofiltration of ethanolic extracts from *Sideritis ssp. L.* with membranes Duramem (molecular mass cut-off, MWCO 300 and 500 Da) is presented. It is related to concentration change and formation of a concentration polarization layer at the membrane–liquid interface, the effect being lower in case of better hydrodynamic conditions and lower feed concentrations.

**2.** Daniela B. Dzhonova-Atanasova, Iren H. Tsibranska, Stela P. Paniovska. CFD Simulation of Cross-Flow Filtration. CHEMICAL ENGINEERING TRANSACTIONS, 70, AIDIC, 2018, ISSN:2283-9216, DOI: https://doi.org/10.3303/CET1870341, p. 2041-2046. SJR (Scopus):0.273 Q3 (Scopus) Линк

The aim of the present work is to study the transfer processes in a cross-flow filtration cell, in order to determine the conditions for stable and efficient operation of a side-stream filtration module, integrated with a bioreactor.
The current interest in membrane integrated bioreactors is connected with the pursuit of energy and cost efficiency in a wide area of industrial applications, including wastewater treatment, food

industry, pharmaceutical industry, and fuel production. A numerical CFD model is employed, based on previous experience with experimental concentration of antioxidants, such as polyphenols and flavonoids from extracts of natural products by nanofiltration. The geometry under investigation is a 3D model of the experimental flat-sheet cell with tangential orientation of the feed inlet. The swirling turbulent flow in the feed channel is favourable for reducing the concentration polarization layer on the membrane surface and preventing fouling. The main factors, affecting the filtration process, are the shear stress distribution and the concentration profiles in the vicinity of the membrane surface. The CFD models of mass transfer in cross-flow nanofiltration are scarce and there are none for the reference experimental filtration cell. The present CFD simulation reveals the concentration distribution in the feed channel. It complements previous data for the flow pattern with new knowledge on the mass transfer there, directed to understanding and control of the concentration polarization phenomenon. The numerical study uses the tools of ANSYS Fluent R13, based on the finite volume method for solving the Reynolds-Averaged Navier-Stokes (RANS) equations. The obtained results are analysed in rapport with available experimental data.

**3.** Vlaev, S.D., Tsibranska, I., Dzhonova-Atanasova, D.. Hydrodynamic characterization of dual-impeller submerged membrane bioreactor relevant to single-use bioreactor options. Chemical Engineering Research and Design, Volume 132, April 2018, Pages 930-941, Elsevier, 2018, ISSN:0263-8762, DOI: https://doi.org/10.1016/j.cherd.2018.02.004, ISI IF(Web of Science):2.795 Q1 (Scopus) Линк

The flow characteristics e.g. velocity and velocity gradients in a conventional stirred sMBR with in-line tubular membrane module for integrated production and recovery of value-added material, are studied. Considering a hybrid vessel, the flow characteristics are conflicting parameters, viz. high shear is required for membrane walls and low shear required for microbial cells. Attempt is made to find a range of parameters that are balanced against known critical values. The task is resolved by numerical solution of a theoretical model of dual flat-blade impeller Biostat®5 L (T = 0.16 m, D = 6.6 cm) equipped with tubular membrane module (L = 23 cm, d = 12 mm) operating in non-Newtonian biofluid (flow index range, $0.34 < n < 0.78$). CFD for gas-liquid cross-flow (e.g. Eu-Eu model) at Re $\sim 10^3$ - $2 \times 10^4$ and mesh $10^6$ cells is employed. In a study aimed at sMBR bulk and near-wall flow proper-ties, the effect of gas flow at various tip velocity (1-2.5 m/s), sparging intensity (8-16 m/s) and rheology on shear is revealed. In a range of specific input power $10^2$-$5 \times 10^3$W/m3, the bulk shear rate varied in the range 20-60 $s^{-1}$and mean wall shear varied between 600 $s^{-1}$and 3000 $s^{-1}$. Wall shear stress non-uniformity in the range 1-30 $N/m^2$ is registered. The gas phase is found to reduce wall shear, but to increase shear uniformity. In view of preserving cells' viability, zonal shear rates of the vessel bulk and sparger openings were determined. Relating the data to similar results in single-use vessels, a correlation reported previously for bulk average shear rate $\dot{\gamma}$ versus input power [$\dot{\gamma} = C(P/V_R)^{1/3}$] is confirmed. A range of balanced bulk and wall

shear relevant to hybrid operation is determined. In view of the reported scalability of the conventional MBR design and reusable bioreactors, the data could be used for extrapolation.

**4.** Trojanowska A., Tsibranska I., Dzhonova D., Wroblewska Web of Science M., Haponska M., Jovancic P., Marturano V., Tylkowski B.. Ultrasound-assisted extraction of biologically active compounds and their successive concentration by using membrane processes. Chemical Engineering Research and Design, 147, Elsevier, 2019, ISSN:0263-8762, DOI: https://doi.org/10.1016/j.cherd.2019.05.018, p. 378-389. JCR-IF (Web of Science):3.35 Q1, не оглавява ранглистата (Web of Science) Линк

*Sideritis scardica* and *Sideritis syriaca* are considered highly valuable plant materials and their total polyphenols (TP) and total flavonoids (TF) extracts can be employed in nutraceutics and cosmetics. A two-step process was proposed consisting in the ultrasound-assisted extraction (UAE) and concentration of the biologically active compounds via nanofiltration (NF). An extensive comparison between UAE and conventional high-temperature stirring was per-formed, taking into account the effect of process parameters such as solvent, temperature and ultrasonication. In terms of radical scavenging activity and time optimization, UAE was found more effective, providing – after only 1 h – extraction yields comparable to 20 h of the conventional thermo-mechanical method. The extract was then concentrated by nanofiltration in tangential mode at 20 bar using 300 and 500 Da cut-off Duramem membranes. Permeate and rejection flux was monitored during the filtration process. The lower molecular weight membrane showed higher permeability towards TP and TF and contributed to a more stable flux and lower fouling processes. To predict operational drawbacks, computational fluid dynamic simulations were performed to model the complex rotational flow occurring during membrane filtration.

**5.** I.Tsibranska, D.Dzhonova-Atanasova, St. Panyovska. EFFECT OF VARIABLE FLUX AND REJECTION IN MEMBRANE SEPARATION OF POLYPHENOLS-CONTAINING NATURAL EXTRACTS. Journal of Chemical Technology and Metallurgy, 55, 4, University of Chemical Technology and Metallurgy, 2020, ISSN:1314-7471, 765-771. SJR (Scopus):0.19 Q3 (Scopus) https://journal.uctm.edu/node/j2020-4/12_19-170_p_765-771.pdf Линк

The present study is focused on the numerical simulation of the hydrodynamics and mass transfer in a stirred dead-end filtration cell, accounting for the concentration polarization and the supporting experimental evidence in the nanofiltration of natural extracts. The importance of mass transfer resistance in the boundary layer adjacent to the membrane is related to the velocity field in the zone between stirrer and bottom placed membrane as well as to the shear stress distribution on its surface. The effects of variable permeate flux, boundary layer thickness and rejection coefficients on the concentration profile close to the membrane surface are discussed. The

experimental evidence regarding the true and observed rejections is commented. Mass transfer coefficient is calculated in accordance with the concentration polarization theory and compared to the reported values for membrane separation of polyphenols.

**6.** S.D. Vlaev, D. Dzhonova-Atanasova, I.Tsibranska. CFD evaluation of mass transfer distribution heterogeneity along the membrane-liquid interface in stirred submerged membrane bioreactors. Chemical Engineering and Processing - Process Intensification, Volume 147, Elsevier, 2020, DOI: https://doi.org/10.1016/j.cep.2019.107738, JCR-IF (Web of Science):3.33 Q1, не оглавява ранглистата (Web of Science) Линк

The aim of the study is to reveal local mass transfer conditions along a tubular membrane module integrated in conventional stirred sMBR. The vessel comprises dual radial flow impeller and bottom gas distributor. CFD methodology is employed in simulation of a model bio-system explored previously. The solute concentration profiles near membrane surface are determined at impeller speed 400−750 rpm, gas flow rate 1–2 vvm and power law parameters $0.02<K<0.55$ Pa.sn, $0.34<n<0.78$. Boundary layer thickness δc and retention-side mass transfer coefficient km are determined; δc is most often in the range $\delta c \sim 1\cdot10^{-3}$–$2\cdot10^{-3}$ (i.e. 80−160 μm) at membrane sections facing the impellers and between $2\cdot10^{-3}$ and $8\cdot10^{-3}$ (i.e. 160−640 μm) in sections between the impellers and throughout membrane shadow. The membrane area-averaged mass transfer coefficient is found to be in the range $km \sim 3.3\cdot10^{-5}$–$5.6\cdot10^{-5}$ m/s depending on mixing intensity. Significant cross-membrane spatial variation of km between $1\cdot10^{-5}$ and $1.2\cdot10^{-4}$ m/s is discovered. The membrane performance efficiency is discussed in terms of impeller selection. Improvement of sMBR performance is foreseen in using impeller design of mixed radial-axial flow circulation.

**7.** Nurdaulet Kalassov, Daniela Dzhonova, Irene Tsibranska, Stela Panyovska, Rustem Manatbayev. APPLICATION OF INTEGRATED MEMBRANE BIOREACTORS IN RENEWABLE ENERGY INDUSTRY. Journal of Chemical Technology and Metallurgy, 55, 2, University of Chemical Technology and Metallurgy, 2020, ISSN:1314-7471, 314-323. SJR (Scopus):0.19 Q3 (Scopus) Линк

Excessive use of fossil fuel results in a rapid depletion of non-renewable fossil energy resources, a rise in fuel cost and an uncontrolled emission of greenhouse gases, which causes a severe threat to the environment. This critical state has turned the awareness to explore renewable energy resources, which include water, biomass, wind and geothermal heat. Among these possibilities, biomass based fuels, i.e. biofuels, have been proposed as a substitute for conventional diesel and gasoline. The biofuels burn cleanly, thereby reducing harmful emissions, especially in the form of carbon monoxide, unburned hydrocarbon and toxic chemicals.

This work aims at revealing the current state-of-the-art and the challenges in the application of integrated membrane bioreactors (MBRs) in biofuel production. This innovative technology is employed for production of biofuels in gaseous and liquid state, such as biohydrogen, bio crude oil, bioethanol and biodiesel.
Great opportunities for producing combustible gas mixtures open up broad prospects for integrated systems, and the low energy intensity makes them attractive for industrial developments. Coupling of bio processes and membrane filtration allows to solve the problem of producing methane and hydrogen without emission of carbon dioxide into the atmosphere.
The main advantage of a MBR system is that it can be applied using environmentally friendly technology, i.e. biotechnology based on natural processes and mechanisms of conversion of substances by enzymes and microbial cultures. The waste and by-products of these processes can also serve as additional sources of raw materials, which leads to completely waste-free production.

**8.** Tonova, K., Lazarova, M., Dencheva-Zarkova, M., Paniovska, S., Tsibranska, I., Stanoev, V., Dzhonova, D., Genova, J.. Separation of glucose, other reducing sugars and phenolics from natural extract by nanofiltration: Effect of pressure and cross-flow velocity. Chemical Engineering Research and Design, 162, October 2020, ELSEVIER, 2020, ISSN:0263-8762, DOI: https://doi.org/10.1016/j.cherd.2020.07.030, 107-116. SJR (Scopus):0.788, JCR-IF (Web of Science):3.739 Q1, не оглавява ранглистата (Scopus) Линк

This study considers the effect of cross-flow velocity and transmembrane pressure onflux and rejection behavior during nanofiltration of Eurasian water milfoil hydrolysate. Fractionation by nanofiltration was applied to obtain a glucose-rich permeate solution and a concentrated retentate solution of other sugars and phenolics. Nanofiltration was performed in a cross-flow rectangular flat-sheet cell (MaxiMem, Prozesstechnik GmbH). Membrane Microdyn Nadir$^{TM}$ NP030 with molecular weight cut-off 500 Da was used. The velocity and shear stress distribution on the membrane surface was modelled by CFD simulations. Mild hydrodynamic conditions (cross-flow velocity and pressure) are recommended based on the observed permeate flux and rejection difference between the targeted groups of compounds. The results are discussed in rapport with existing experimental observations in the literature.

**9.** Nakov, Sv. Ts., Dzhonova-Atanasova, D. B., Kolev, N. N.. Pressure drop of high performance random Intalox Metal Tower Packing. Bulgarian Chemical Communications, 44, 4, 2012, 283-288. ISI IF(Web of Science):0.328 Q4 Линк

INTALOX Metal Tower Packing (IMTP) is one of the best random packings designed especially for use in distillation operations. The advantages realized in distillation have been abundantly applied in absorption, liquid-liquid extraction and direct contact heat transfer operations as well.

There is no universal methodology for calculating the performance characteristics of this packing. The constants of the existing equations for practical calculations are obtained for each separate packing size. The present work presents and generalizes own experimental data for the pressure drop of 4 sizes of IMTP packing with nominal diameters of 25, 40, 50, and 70 mm. The experimental data for dry packing pressure drop are described by an equation with a mean deviation of 5.1%. Equations for determination of pressure drop of irrigated packing, up to the loading point and above it, are also obtained. These equations reflect not only the influence of the packing geometry, but also the column redumping.

**10.** Dzhonova-Atanasova, D., Nakov, Sv., Razkazova-Velkova, E., Kolev , N.. Pressure drop of highly efficient Raschig Super-Ring packing for column apparatuses. Bulgarian Chemical Communications, 47, 3, 2015, ISSN:0324-1130, 793-799. ISI IF(Web of Science):0.349 Q4 (Web of Science) Линк

The present work presents and generalizes own experimental data for the pressure drop of highly efficient metal Raschig Super-Ring (RSR) packing for packed columns. The contemporary demands from the chemical industry for environment protection and waste free production lead to focusing on application of these apparatuses in purification of flue gases and waste water. RSR is modern high-performance random packing of latest generation, which combines effective mass transfer, large interfacial area and uniform distribution of the phases over the column cross section. There is no universal methodology for calculating the performance characteristics of this packing. The constants of the existing equations for practical calculations are obtained for each individual packing size. The aim of the present work is to propose more precise equations for prediction of the pressure drop of RSR packing, which are common for all investigated sizes and reflect the influence of the packing geometry and the column redumping.

**11.** Dzhonova-Atansova, D., Georgiev, A., Popov, R.. Numerical study of heat transfer in macro-encapsulated phase change material for thermal energy storage. Bulgarian Chemical Communications, 48, Special Issue E, 2016, ISSN:0324-1130, 189-194. JCR-IF (Web of Science):0.229 Q4 (Web of Science) Линк

The successful development and implementation of systems using renewable energy sources, which are usually of intermittent character, require cheap and effective thermal energy storing for diurnal or seasonal heat accumulation. Thermal accumulators are also used for increasing the efficiency of conventional fuel dependent systems by storing the waste heat in low consumption periods. Much of the efforts are directed towards creation of compact solutions to replace the presently used hot water tanks requiring very large space. This is especially important for small capacity thermal systems in buildings. There are a lot of suggestions in literature using the latent

heat of phase change materials (PCM), but only a few close to commercial stage of implementation. A heat accumulator with paraffin as a PCM is a cost effective innovative solution for low grade heat storage. One of the design approaches is encapsulation of the phase change material in containers with a variety of shapes and materials. The aim of the present work is a 3D numerical simulation of the phase change process in a stainless-steel container filled with commercial E53 paraffin. This is a part of a study directed towards design optimization of a hybrid solar installation with thermal storage. The focus is on development and testing of a time effective method for numerical prediction of the thermal behaviour of the container with paraffin and assessment of the factors influencing the heat transfer process prior to the physical experiment.

**12.** Amanzholov, T., Akhmetov, B., Georgiev, A., Kaltayev, A., Popov, R., Dzhonova-Atanasova, D., Tungatarova, M.. Numerical modelling as a supplementary tool for Thermal Response Test. Bulgarian Chemical Communications, 48, Special Issue E, 2016, ISSN:0324-1130, 109-114. JCR-IF (Web of Science):0.229 Q4 (Web of Science) Линк

Nowadays, development of efficient thermal energy storage systems is becoming very important since they assist in storing gained heat from renewable energy sources at medium or large scales in an effective way with the purpose of balancing the demand and supply of energy. One of the technologies which allow thermal energy accumulation in a large-scale is Borehole Thermal Energy Storage (BTES). Such technology gives opportunity to store heat into the ground and/or groundwater in summer, and extract it during winter. To evaluate the BTES performance, the ground thermal properties must be known. One of the in situ methods for this purpose is the thermal response test (TRT). But, TRT gives an overall evaluation of the thermal properties of the ground. Therefore, for more precise evaluation, mathematical modelling is used as a supplementary tool for TRT technique. The current paper focuses on experimental TRT technique and mathematical modelling of a TRT process.

**13.** Darakchiev, R., Darakchiev, S., Dzhonova-Atanasova, D., Nakov, S.. Ceramic block packing of Honeycomb type for absorption processes and direct heat transfer. Chemical Engineering Science, 155, 22 Nov. 2016, Elsevier, 2016, ISSN:0009-2509, DOI:http://dx.doi.org/10.1016/j.ces.2016.07.028, 127-140. ISI IF(Web of Science):2.75 Q1 (Scopus) Линк

Ceramic block packing of Honeycomb type has been developed and studied for the purpose of absorption and heat transfer processes in column apparatuses. The packing design ensures high efficiency at relatively low pressure drop. The packing is easy to manufacture and the ceramic is resistant to high temperatures and chemically aggressive environments. Detailed studies on the characteristics of mass transfer and fluid flow have resulted in development of a reliable

methodology for design of packed columns for absorption processes and direct heat transfer. Their successful implementations in the chemical industry, for environmental protection, and in the power production have confirmed the validity of the methodology. The Honeycomb packing is used in an industrial system for purification of process gases from $H_2S$ in staple cellulose fiber production, which operates with a degree of absorption greater than 99%. The packing is employed in industrial systems for heat recovery of flue gases from boilers burning natural gas, which utilize up to13–15% extra heat and significantly reduce the harmful emissions. The heated and humidified air for combustion in one of the variants creates special conditions for fuel combustion such that the formation of nitrogen oxides is decreased by 3.5 times.

**14.** Seitov, A., Akhmetov, B., Georgiev, A., Kaltayev, A., Popov, R., Dzhonova-Atanasova, D., Tungatarova, M.. Numerical simulation of thermal energy storage based on phase change materials. Bulgarian Chemical Communications, 48, Special Issue E, 2016, ISSN:0324-1130, 181-188. JCR-IF (Web of Science):0.229 Q4 (Web of Science) Линк

One of the main problems related to the application of thermal energy gained from renewable energy sources is the absence of effective storage system. If we could store, for instance, solar thermal energy which is harnessed during day time, it would be possible to use it at night for space heating, ventilation, air conditioning or hot water systems. Therefore, this paper reports on the numerical analysis of heat transfer and fluid flow processes in a thermal energy storage based on phase change material designed and developed by the authors. Such study is very important in understanding of advantages and disadvantages of the design features and efficiency of the latent heat storage.

**15.** Daniela Dzhonova-Atanasova, Tatyana Petrova, Krum Semkov, Simeon Darakchiev, Konstantina Stefanova, Svetoslav Nakov, Roman Popov. Experimental Investigation of Liquid Distribution in Open structure Random Packings as a Basis for Model Refinement. Chemical Engineering Transactions, 70, The Italian Association of Chemical Engineering Online at www.aidic.it/cet, 2018, ISSN:2283-9216, DOI: https://doi.org/10.3303/CET1870347, 2077-2082. SJR (Scopus): 0.273 Q3 (Scopus) Линк

The present study aims at investigation of the liquid phase distribution in order to fill in the missing data on liquid spreading in industrial scale packing layer of metal Raschig Super-Ring (RSR) packings for development of a reliable prediction model. Our attempt to apply the well-proven dispersion model to RSR packings has faced difficulties connected with the packing open, web-like structure resulting in poor radial distribution properties and with the industrial scale of the packed column. An experimental set-up is designed so as to provide the necessary data for model parameters' identification. Special attention is paid to the uniform liquid distributor, in order to

ensure the validity of the model assumption of regular initial irrigation. The approach avoids the need of data from well-established wall flow, which can be measured at a very high (over 3 m in that scale) packing layer. Instead, it uses additional data from irrigation on the column wall, provided by a peripheral liquid distributor. The present work has obtained original data for the liquid distribution in RSR packings of different sizes addressing improvement and validation of a prediction model.

**16.** Petrova, T., Semkov, K, Dzhonova-Atanasova, D.. Modeling of Liquid Distribution in a Packed Column with Open-structure Random Packings. Chemical Engineering Transactions, 70, The Italian Association of Chemical Engineering Online at www.aidic.it/cet, 2018, ISSN:2283-9216, DOI: https://doi.org/10.3303/CET1870176, 1051-1056. SJR (Scopus):0.273 Q3 (Scopus) Линк

The scientific interest in the efficiency of packed bed columns is a part of the world-wide pursuit of sustainability of the processes. The maldistribution of the phases in the apparatus reduces the efficiency and makes difficult the prediction of process performance and scaling up. The present work aims at modeling of liquid distribution in a packed column with high performance open-structure random packings - metal Raschig Super-Rings 0.7", 1.5" and 3" and metal Pall rings 1". Some new approaches for estimation and calculation of model parameters are proposed and tested, using own experimental data for Raschig Super-Rings and published data for Pall rings. A new procedure for identifying one of the model parameters, called by us "overlapping confidential intervals" solution, is developed and illustrated for Raschig Super-Ring packing in the case of partial radial insensitivity ("plateau") of the residual variance between the model and experimental data. The obtained results show that using appropriate statistical methods of estimation, the dispersion model parameters can be successfully identified achieving a very good prediction of the experimental data. Several numerical examples and case studies are considered and discussed. For the case of Pall rings, the dispersion model predictions are in very good agreement with both published experimental data and predictions made by Computational Fluid Dynamics (CFD) modeling.

**17.** T. S. Petrova, D. B. Dzhonova-Atanasova. Flow Simulation and Identification of Important Model Parameters in Industrial Packed Beds for High-Performance Random Packings. Journal of Ecological Engineering, 20, 9, Polish Society of Ecological Engineering (PTIE), 2019, ISSN: 2299-8993, DOI: https://doi.org/10.12911/22998993/112500, 116-120. SJR (Scopus):0.312 Q2 (Scopus) Линк

The goals of this work were: first, to simulate the liquid flow distribution in a large diameter (1.2 m) packed column with an RMSR 70-5 high performance random packing (layer height up to 3

m), by a dispersion model. Second, to find and estimate the important model parameters and flow maldistribution factor, using experimental data and two different optimization approaches. A three-parameter dispersion model for prediction of radial liquid distribution and two different approaches to determine some of the model parameters from experimental data were used. In parallel, a two-parameter optimization procedure for model parameters identification was performed based on the minimum of residual variance between model and experimental liquid velocities over a column cross-section. The simulated and experimental flow maldistribution, were estimated by means of an integral estimation – a maldistribution factor. The comparison between the model and experimental liquid distribution and respective maldistribution factors at packing heights H = 1 m and H = 2.5 m for liquid load $16.6 \cdot 10^{-3}$ $m^3/m^2 \cdot s$ showed very good agreement, even for a high packing layer. In conclusion, the presented model predictions and estimations about RMSR 70-5 characteristics and behaviour will complement the information about its efficiency and operation in industrial processes.

**18.** T. St. Petrova, D. B. Dzhonova-Atanasova. Simulation of the liquid distribution in the wall zone of a packed column: case study. Bulgarian Chemical Communications, 51, F, Bulgarian Academy of Sciences, Union of Chemists in Bulgaria, 2019, ISSN:0324-1130, 91-98. SJR (Scopus):0.142 Q4 (Scopus) Линк

The maldistribution of the liquid phase in a packed column is essential for the efficiency of the mass transfer processes in it. One of the wide-spread methods to measure the liquid distribution in the packing layer includes liquid collecting device (LCD) mounted under the packed bed. The proper design of the LCD is very important for obtaining correct information about the hydrodynamics in the column. The most popular construction of LCD is composed of fixed number of concentric cylindrical sections, with equal or different cross-sectional surface areas. The number and width of these sections is determined so as to ensure enough resolution of the picture of the liquid flow. In this study an analysis and estimation of several variants for possible fragmentation of LCD are provided, based on a dispersion model simulations and calculation of the maldistribution factor. The simulation results are verified with experimental data for metal Raschig Super-Rings 1.5" (RSRM) with an improvement of the LCD. It is shown also, that model parameters identification depends on the LCD fragmentation, especially in the wall zone of the packed column. The present study defines a quantitative criterion for LCD design assessment, which is the fragmentation effect on the maldistribution factor. This solves the issue with the proper data collecting, necessary for obtaining the actual liquid distribution and for parameter identification of the dispersion model.

**19.** A N Pavlenko, V E Zhukov, E Yu Slesareva, Chr Boyadjiev, D Dzhonova-Atanasova. Studies of Freon mixture separation using a large-scale model of distillation column. Journal of

Physics: Conference Series, 1614, 012067, IOP Publishing, 2020, DOI: https://doi.org/10.1088/1742-6596/1614/1/012067, SJR (Scopus):0.227 Q4 (Scopus) Линк

The operation efficiency of distillation columns with structured packing is maximal if the distribution of countercurrent vapor and liquid film flows over the column cross-section on the mass transfer surface is most uniform. Various types of structured packing are widely used in distillation columns. Formation of the temperature field maldistribution in the column cross-section is observed in large-scale distillation columns. The sizes of large-scale maldistributions on zones are commensurate with the column diameter. The aim of this work is to obtain experimental data on the separation efficiency in large-scale distillation columns and dynamics of formation of large-scale maldistributions of local parameters of vapor and liquid in a countercurrent flow over a structured packing during mixture separation. Separation of the R114/R21 freon mixture was carried out on a structured Mellapack 350.Y packing with a diameter of 0.9 m and height of 2100 mm. The experiments were carried out under conditions of complete reflux in the range of reduced vapor velocity of $0.017 < K_v < 0.035$ m/s. Experimental data were obtained on the efficiency of mixture separation, pressure drop over the structured packing and parameters determining the formation dynamics of the large-scale temperature field maldistribution in the column cross-section. The presented experimental data will be used for the construction and verification of a new model of mass transfer and efficiency of mixture separation in large-scale distillation packed columns.

**20.** Boyadjiev, Chr., Dzhonova, D., Stefanova, K., Panyovska, St., Popova, P., Pavlenko, A., Zhukov, V., Slesareva, E.. ON THE PHASES' DISTRIBUTION IN PACKED COLUMNS. Journal of Physics: Conference Series, Volume 1677, 2020, ISSN:1742-6588, https://doi.org/10.1088/1742-6596/1677/1/012054, SJR (Scopus):0.227 Q4 Линк

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.

**21.** Boyadjiev, Chr., Dzhonova-Atanasova, D., Popova-Krumova, P., Stefanova, K., Pavlenko, A., Zhukov, V., Slesareva, E.. Liquid wall flow in counter-current column apparatuses for absorption processes with random packings. Bulgarian Chemical Communications, Volume 52, Spec. Is. F 2020, ISSN:0324-1130, DOI:10.34049/bcc.52.F.0013, 74-79. SJR (Scopus):0.14 Q4 (Scopus) Линк

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.ч

**22.** Nakov, Sv. Ts., Dzhonova-Atanasova, D. B., Razkazova-Velkova, E. N.. Dynamic hold-up of modern high-performance packings. Bulgarian Chemical Communications, 52, Special Issue F, 2020, DOI:10.34049/bcc.52.F.0005, 32-35. SJR (Scopus):0.14 Q4 (Scopus) Линк

Metal Raschig Super-Ring (RSR) and Intalox Metal Tower Packing (IMTP) are modern high-performance packings that combine efficient mass transfer, large interfacial surface area and regular phase distribution over the cross section of the column apparatus. This work presents and summarizes original experimental data of the dynamic hold-up of 4 IMTP sizes and 7 RSR sizes. Dimensionless criterion equations are proposed for both types of packings to calculate their dynamic hold-up for regimes below the loading point. The average arithmetic error of the IMTP equation is 7.5% and of the RRS equation is 4.6%. The proposed equations not only take into account the geometry of the packings, but also the effect of the dumping of the packing in the column.

**23.** Tatyana Petrova, Daniela B. Dzhonova-Atanasova, Krum A. Semkov. Comparison of experimental and model liquid distribution in large packed bed of Raflux rings 50-5. IOP Conference Series: Materials Science and Engineering (MSE), 876, IOP Publishing, 2020, ISSN:ISSN:1757-8981, E-ISSN:1757-899X, DOI: https://doi.org/10.1088/1757-

899X/876/1/012009, 012009-1-012009-5. SJR (Scopus):0.198 SJR, непопадащ в Q категория (Scopus) Линк

This work presents a continuation of our investigations on the radial liquid distribution in packed beds with open-structure random packings, by means of a dispersion model, in a scale, close to industrial one. Using experimental data for uniform initial irrigation, the optimal parameters' values of the three parameters of the dispersion model are obtained by two-parameter identification. One of the parameters (the radial spreading coefficient) is calculated independently by using experimental data for a point source initial irrigation. The dispersion model solution at optimal parameters' values is compared with both experimental and TUM WelChemCell model literature data for the liquid radial distribution in a packed column with a diameter of 1.2 m and random packing Raflux rings 50-5. The maldistribution factor of the liquid distribution is also calculated and compared. The comparison shows very good agreement between our results and the literature data and confirms the dispersion model capability to predict the liquid distribution in large columns with open-structure packings.

**24.** Pavlenko, A., Zhukov, V., Slesareva, E., Boyadjiev, Chr., Boyadjiev, B., Dzhonova-Atanasova, D., Popova-Krumova, P.. Large-scale maldistributions of local flow parameters at distillation on a structured packing. Bulgarian Chemical Communications, Volume 52, 2020, ISSN:0324-1130, DOI: 10.34049/bcc.52.F.0007, 42-46. SJR (Scopus):0.14 Q4 (Scopus) Линк

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 non-uniformity 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 *R*114/*R*21 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 *R*114 / *R*21 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 non-uniformity 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.

**25.** A. N. Pavlenko, V. E. Zhukov, E. Yu. Sukhorukova, D. B. Dzhonova-Atanasova, K. V. Stefanova. Experimental Study of Liquid Flow Maldistribution in Sulzer 500X Structured Packing and Raschig Super-Ring Random Packing. Journal of Engineering Thermophysics, 30, 171–183 (2021), DOI:https://doi.org/10.1134/S1810232821020016, 171-183. SJR (Scopus):0.402, JCR-IF (Web of Science):2.038 Q2 (Scopus) Линк

This paper presents the results of an experimental study of the formation of large-scale non-uniformity of liquid flow on a RSR metal random packing of 0.47 m in diameter and a Sulzer 500X structured packing of 0.6 m in diameter. The experiments on the RSR packing were carried out with water without vapor flow for the superficial velocity of the liquid varying as $3\ 10^{-3} < L_0 < 12\ 10^{-3}$ m/s. The experiments on the Sulzer 500X structured packing were conducted in a distillation column with separation of R114/R21 freon mixture under total reflux conditions. The superficial velocity of the liquid varied in the range $3.5\ 10^{-3} < L_0 < 6.7\ 10^{-3}$ m/s; the vapor load varied in the range $1.3 < F\text{-}factor < 2$ $\text{Pa}^{0.5}$. It is shown that the amount of liquid retained on the column wall at the outlet from the Sulzer 500X packing practically does not change in the investigated range of operating parameters. For the superficial velocity of the liquid varying as $3.5\ 10^{-3} < L_0 < 5\ 10^{-3}$ m/s, the liquid maldistribution factor for the Sulzer 500X packing is three times less than that for the RSR random packing. The resulting experimental data will help to construct and verify models for calculating the efficiency of separation of mixtures on packings in industrial column apparatus with quantitative allowance for the effect of the scale factor, which is associated with large-scale non-uniformity of local flow parameters.

**26.** A. Pavlenko, V. Zhukov, N. Pecherkin, E. Slesareva, Chr. Boyadjiev, D. Dzhonova-Atanasova. Studying the process of freons mixture separation on a structured packing Sultzer 500X. E3S Web of Conferences 258, 11008 (2021), EDP Sciences, 2021, ISSN:22671242, DOI:https://doi.org/10.1051/e3sconf/202125811008, SJR (Scopus):0.237 SJR, непопадащ в Q категория (Scopus) Линк

Structured packings are widely used in distillation columns to separate various types of mixtures. These packings have an ordered structure, which ensures more uniform conditions for interaction of counter-current flows of liquid and vapor than in the random packings and have a small hydraulic resistance. Nevertheless, in columns with a diameter of more than 0.5 m, formation of large-scale non-uniformity in distribution of liquid and vapor flow parameters over the packing cross-section is observed. In this work, experimental data on formation of large-scale non-uniformity in the temperature field over the cross-section of the Sulzer 500X packing, as well as on the efficiency of mixture separation and the pressure drop across the packing were obtained. The experiments were carried out with separation of R114/R21 freon mixture on a 10-layer

structured packing Sulzer 500X with a diameter of 0.6 m and a height of 2.2 m. Experimental data were compared with the results obtained earlier for a structured packing Mellapack 350.Y with a diameter of 0.9 m and a height of 2.1 m. The presented experimental data will be used to construct and verify a new model of mass transfer and efficiency of mixture separation in the large-scale distillation packed columns.

**27.** Dzhonova-Atanasova, D., Georgiev, A, Nakov, S., Panyovska,S., Petrova, T., Maiti, S.. Compact Thermal Storage with Phase Change Material for Low-Temperature Waste Heat Recovery—Advances and Perspectives. Energies, 15, 8269, MDPI, 2022, ISSN:1996-1073, DOI:https://doi.org/10.3390/en15218269, SJR (Scopus):0.653, JCR-IF (Web of Science):3.252 Q1, не оглавява ранглистата (Scopus) Линк

The current interest in thermal energy storage is connected with increasing the efficiency of conventional fuel-dependent systems by storing the waste heat in low consumption periods, as well as with harvesting renewable energy sources with intermittent character. Many of the studies are directed towards compact solutions requiring less space than the commonly used hot water tanks. This is especially important for small capacity thermal systems in buildings, in family houses or small communities. There are many examples of thermal energy storage (TES) in the literature using the latent heat of phase change, but only a few are commercially available. There are no distinct generally accepted requirements for such TES systems. The present work fills that gap on the basis of the state of the art in the field. It reviews the most prospective designs among the available compact latent heat storage (LHS) systems in residential applications for hot water, heating and cooling and the methods for their investigation and optimization. It indicates the important characteristics of the most cost- and energy-efficient compact design of an LHS for waste heat utilization. The proper design provides the chosen targets at a reasonable cost, with a high heat transfer rate and effective insulation. It allows connection to multiple heat sources, coupling with a heat pump and integration into existing technologies and expected future scenarios for residential heating and cooling. Compact shell-tube type is distinguished for its advantages and commercial application.

**28.** Jigar K. Andharia, Bhupendra Markam, Daniela Dzhonova, Subarna Maiti. A comparative performance analysis of sensible and latent heat based storage in a small-scale solar thermal dryer. Journal of Energy Storage 45 (2022) 103764, Elsevier, 2022, ISSN:ISSN: 2352-152X, DOI:https://doi.org/10.1016/j.est.2021.103764, JCR-IF (Web of Science):6.583 Q1, не оглавява ранглистата (Scopus) Линк

Economical and accessible thermal storage material that can store and sustain operation during off-sunshine hours is essential for small-scale solar thermal drying systems installed in households

or communities. This study presents the evaluation of two energy storage modes- sensible and latent heat storage along with a control experiment in an indigenously developed small-scale mixed-mode solar thermal dryer. Black pebble stones were used as sensible heat storage material while paraffin wax (melting temperature 58–60 ºC) was used as latent heat storage material. On a typical sunny day, under no-load condition, the maximum drying air temperatures reached were 102.30 ºC, 86.51 ºC, and 86.42 ºC for control, sensible heat, and latent heat stored units, respectively. A comparison of change in the moisture content of Indian gooseberry loaded in the units w.r.t time revealed that the berries in the latent heat stored dryer dried in 18% less time than sensible heat stored dryer. The drying air temperature of the sensible heat stored units became at-par with the control unit 2 h after sunset; however, the dryer containing paraffin wax could sustain drying for 3 more hours. CFD was employed to predict the units' airflow and temperature distribution patterns using RANS equations for natural convection. This study is expected to lead to the development of efficient small-scale solar thermal dryers for small enterprises.

**29.** Даниела Джонова-Атанасова, Константина Стефанова, Крум Семков, Татяна Петрова, Светослав Наков. Глава I. Експериментално изследване на неравномерността на течната фаза в колонни апарати с високоефективни ненаредени пълнежи. "Устойчиви процеси, устойчиви системи, устойчива околна среда", Издателство на БАН "Проф. Марин Дринов", 2020, ISBN:978-619-245-056-4, 17-43 Линк

Packed columns are typical apparatus for separation processes in gas-liquid systems. They are widely used for absorbing harmful substances from waste gases from the energy and chemical industries, for distillation in the production of fuels, food and pharmaceutical products, and for the recovery of waste heat from combustion plants (Kolev, 2006; Langa et al., 2017; Dzhonova et al., 2013). An important element in the construction of a heat or mass exchange column apparatus is the choice of the type of filling, which ensures the efficiency of the processes taking place in it. Recently, structured fillers or disordered fillers with an open-to-flow structure, i.e. third or fourth generation according to the Schultes (2003) classification, are mostly used in industry. Modern high efficiency non-stacked packings with an open structure provide efficient mass transfer by creating a large interfacial area and turbulating the flows while maintaining a low hydraulic resistance. A typical representative of these fillings is a Raschig Super-Ring (RSRM) metallic unordered filling - fourth generation. In contrast to structured fillings, it is much less studied, especially the distribution of phases in and after such a layer of filling, as well as the factors that influence it.

**30.** Татяна Петрова, Даниела Джонова-Атанасова, Крум Семков. Глава II. Математическо моделиране на процесите на неравномерност на течната фаза в колони с пълнеж, методи за идентификация на моделните параметри, методи за определяне на

оптимален дизайн на устройствата в проблемните зони. "Устойчиви процеси, устойчиви системи, устойчива околна среда", Издателство на БАН "Проф. Марин Дринов", 2020, ISBN:978-619-245-056-4, 44-86 Линк

The performance of packed columns is strongly influenced by the uniform distribution of phases in it. Nonuniform distribution, especially of the liquid phase, can reduce mass transfer efficiency by up to 50% (Stichlmair and Stemmer, 1987). The distribution of the liquid in the column is highly dependent on the initial uniformity of the liquid introduction and its uniform distribution before the packing bed. Correct prediction of the concentration or temperature distribution of the substances involved in a column is possible based on a detailed knowledge of the hydrodynamics and structure of the flow(s) within it.
Adequate modeling of mass transfer is possible only by considering the effects of column flow non-uniformity (radial and/or axial). From the research done on the subject, it appears that there are several types of models for predicting liquid distribution in packed columns. The first is the random walk model (Tour and Lerman, 1939), describing the distribution of liquid in a packed column of infinite radius, followed by the dispersion model (Cihla and Schmidt, 1957), subsequently supplemented by other authors to account for wall flow (Staněk and Kolář, 1965; 1968a; 1968b; 1973; Semkov et al., 2000; Petrova et al., 2002). There is also a series of works on the use of the dispersion model in the modeling of the liquid phase in the presence of additional devices (reflector rings) to correct the non-uniformity created by the wall flow and finding their optimal placement and spacing axially in the column (Staněk et al., 1985; Semkov et al., 1987; 1987a; 1987b). The models described have been tested and work very well on traditional disordered packings such as Raschig rings, Pall rings, Intalox saddles, spheres, etc., but have not been tested on modern high-performance packings with an open-to-flow structure where there are characteristic sizes smaller of the nominal fill size.

**31.** Tsibranska I., Vlaev S.D., Dzhonova D., Tylkowski B., Panyovska S., Dermendzhieva N.. “Chapter 8. Modeling and assessment of the transfer effectiveness in integrated bioreactor with membrane separation”. Theoretical and Computational Chemistry: Applications in Industry, Pharma, and Materials Science, De Gruyter, 2021, ISBN:978-3-11-067815-4, DOI: https://doi.org/10.1515/9783110678215-008, pp. 227-252 (Scopus): Линк
Also in: Physical Sciences Reviews, 7, 8, De Gruyter, 2020, ISSN: eISSN 2365-659X, ISSN 2365-6581, DOI: https://doi.org/10.1515/psr-2020-0063., 877-900. SJR (Scopus):0.21 Q3

Integrating a reaction process with membrane separation allows for effective product removal, favorable shifting of the reaction equilibrium, overcoming eventual inhibitory or toxic effects of the products and has the advantage of being energy and space saving. It has found a range of applications in innovative biotechnologies, generating value-added products (exopolysaccharides, antioxidants, carboxylic acids) with high potential for separation/ concentration of thermosensitive

bioactive compounds, preserving their biological activity and reducing the amount of solvents and the energy for solvent recovery. Evaluating the effectiveness of such integrated systems is based on fluid dynamics and mass transfer knowledge of flowing matter close to the membrane surface – shear deformation rates and shear stress at the membrane interface, mass transfer coefficients. A Computational Fluid Dynamics (CFD)-based approach for assessing the effectiveness of integrated stirred tank bioreactor with submerged membrane module is compiled. It is related to the hydrodynamic optimization of the selected reactor configuration in two-phase flow, as well as to the concentration profiles and analysis of the reactor conditions in terms of reaction kinetics and mass transfer.

**32.** J. Patel, J. Andharia, A. Georgiev, D. Dzhonova, S. Maiti, T. Petrova, K. Stefanova, I. Trayanov, S. Panyovska. Chapter 8. Modeling and Simulation of Phase Change Material Based Thermal Energy Accumulators in Small-Scale Solar Thermal Dryers. Modeling and Simulation in Chemical Engineering Project Reports on Process Simulation (ed. Ch, Boyadjiev), Springer, 2022, ISBN:Print ISBN 978-3-030-87659-3, Online ISBN 978-3-030-87660-9, DOI: https://doi.org/10.1007/978-3-030-87660-9_8, 36, 155-191 Линк

Solar thermal energy is of intermittent and dynamic character and the necessity to use this energy during non-sunshine periods has led to the development of thermal energy accumulators. The need of compact solutions have prompted researchers towards using latent heat storage. Phase change materials as thermal energy storage are attractive because of their high storage density and characteristics to release thermal energy at constant temperature corresponding to the phase transition temperature. The chapter overviews the recent state-of-the-art small-scale solar thermal dryers integrated with phase change material as an energy accumulator. This is an intensive field of investigation for more than 30 years with importance for the agriculture and the food industry especially in hot climate. A variety of commercial small-scale solar dryers are offered as a low-cost, zero-energy solution for small farmers. And yet, there are no commercial systems using latent thermal storage because at the present level of development this unit will increase unacceptably the price of the system. The solution needs very simple design, accessible materials, and optimal conditions for operation.
The aim of the present work is to make an overview of the methods for theoretical evaluation and prediction, which are used to design and assess this devices and to point out the most appropriate of them for this new solution. The models enable to distinguish the most cost- and energy-effective solar dryer systems with thermal storage among the great number of designs, devices, and materials. The resulting conclusions from the collected and compared information will serve as a base for a novel solution of a cost-effective thermal energy storage for a small-scale solar dryer, which will lead to improved efficiency of the drying process, due to controlled temperature and longer operational time. This information might serve also in the development of the wider field

of thermal energy storage, which is an important part of the technologies of renewable and waste energy conversion.

**33.** Полезен модел: КОЛОНЕН АПАРАТ ЗА ИНТЕНЗИВНО МАСОПРЕНАСЯНЕ В ТРИФАЗНИ СИСТЕМИ
Стела Пламенова Паньовска, Константина Владимирова Стефанова, Даниела Боянова Джонова - Атанасова, Боян Христов Бояджиев, Петя Георгиев ПОПОВА-КРУМОВА, Христо Боянов Бояджиев,
Reg. No. 3609, Приоритет 03/02/2020, https://portal.bpo.bg/bpo_online/-/bpo/utility-model-detail

The column apparatus is used in the chemical industry, biotechnologies and thermal energy for carrying out countercurrent absorption and extraction processes, non-stationary adsorption processes and heterogeneous catalytic reactions. It ensures the maximum rate of mass transfer in gas or liquid phase when they pass through a stationary bed of solid-phase fillers or solid-phase particles. The column apparatus consists of a cylindrical column (5) forming a working zone, an inlet pipe (1) for a gas or liquid phase, mounted directly in the lower part of the working zone and located tangentially to the cylindrical column (5), an outlet (2) for gas or liquid phase located at the top of the cylindrical column (5). According to the useful model, in the working area of the column apparatus there is a stationary layer of solid-phase packing bodies (4) when conducting countercurrent absorption or extraction processes, or solid-phase adsorbent particles (4) when conducting non-stationary adsorption processes, or solid-phase catalyst particles (4) when conducting heterogeneous catalytic reactions.