



### **WORKSHOP**

### "Challenges in Chemical and Biochemical

### Technologies and Environmental Protection"

dedicated to the 85th anniversary of

Professor Christo Boyanov Boyadjiev

### **Book of Abstracts**

25 - 27 October, 2021 Sofia, Bulgaria

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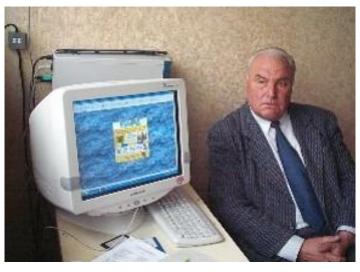
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#### **SCIENTIFIC TOPICS**

- 1. Chemical processes.
- 2. Bioprocesses
- 3. Separation technologies
- 4. Absorption processes.
- 5. Adsorption processes.
- 6. Chemical and Biocatalysis.
- 7. Environmental Protection,
- 8. Green Technologies, Energy Resources and Energy Efficiency
- 9. Fundamental transport phenomena theory and applications.
- 10. Two-phase and multi-phase flows and heat transfer; Heat transfer enhancement.



Проф. Христо Боянов Бояджиев, дтн

Професор Емеритус

40 години Професор

60 години в БАН

60 години от първия математичен модел

65 години от първата научна работа

85 години - философията на химичното инженерство

85 години представляват основната част от живота на човека и му позволяват да си изгради жизнената философия. От тях: 65 от първата ми научна работа, 60 в БАН и 40 Професор в областта на химичното инженерство. За тези години става срастване на жизнената ми философия с философията на химичното инженерство.

#### Пътят в науката

Моят път в науката представлява последователност от етапи:

- 1. Трети курс студент първа научна работа 1957;
- 2. Дипломант (1960 първи математичен модел) Оптичен модел на текстилен плат, публикуван като "Аналог на закона на Беер за отразената светлина от текстилен плат" в К. Dimov, Chr. **Bojadgiev**, Ein Analogon zum Gesetz von Beer uber das reflektierte Licht von gefarbten Textilmaterialien, **Zeitschr. fur Physikalische Chemie**, **219**, 106-113, 1962;
- 3. Първи изследвания в областта на химичното инженерство (1963) Хидродинамика и масопренасяне в тръба на Вентури. Патент за едновременно улавяне на прах и серен двуокис в отпадни газове, внедрен през 1965 в Медодобивния завод в Елисейна;
- 4. Начало на теоретичните изследвания в областта на химичното инженерство (1965) Хидродинамика и масопренасяне в стичащи се филми. Успешно сътрудничество с В. Бешков, В. Крилов, В. Левич. Резултатите публикувани в монографиите Chr. **Boyadjiev**, V. Beschkov, "Mass Transfer in Liquid Film Flows", **Publ. House Bulg. Acad. Sci.**, Sofia, 1984, 128 рр. и Хр. **Бояджиев**, В. Бешков, "Массоперенос в движущихся пленках жидкости", **Изд.** "Мир", Москва, 1988, 137 с..
- 5. Начало на теоретичните изследвания в областта на нелинейното масопренасяне и хидродинамичната устойчивост (1983). Резултатите са публикувани в монографиите В. С. Крылов, Хр. Бояджиев, "Нелинейный массоперенос", Институт теплофизики,

**Новсосибирск**, 1996, 232 с. и Chr. **Boyadjiev**, V. N. Babak, "*Non-Linear Mass Transfer and Hydrodynamic Stability*", **Elsevier**, Amsterdam, 2000, 500 pp.;

- 6. Използваната широка база от теоретични техники става основа на монографиите Хр. Бояджиев, "Основи на моделирането и симулирането в инженерната химия и химичната технология", ИИХ-БАН, София, 1993, 253 с. (Modeling and Simulation in Chemical Engineering and Chemical Technology Bulgarian), Chr. Boyadjiev, "Theoretical Chemical Engineering. Modeling and simulation", Springer-Verlag, Berlin Heidelberg, 2010, 594 pp. и Хр. Бояджиев, "Основи на моделирането и симулирането в химичната промишленост", Изд. БАН "Проф. Марин Дринов", София, 2017, 120 с. (Modeling and Simulation in Chemical Industry Bulgarian);
- 7. Системотехника (1976). Проф. Еленков инициира изследванията в областта на Инженернохимичната системотехника (Process systems engineering),т.е. моделиране на съвкупността на процесите в технологични схеми (технологии). Интересно направление със собствен математичен апарат (матрични методи). Това щастливо съвпадна с появата на възпитаниците на катедра "Химична кибернетика" на акад. Кафаров от Менделеевския институт – Р. Статева, Т. Желев, Н. Банчева, Д. Филипова, а след това и на Б. Иванов. Бяха проведени широкомащабни изследвания в областта на моделирането и оптимизацията на химикотехнологичните системи (ХТС):
- 7.1. Зони на въздействие и програма за структурен анализ на XTC;
- 7.2. Декомпозиционен метод за оптимизация и програмна система за оптимизация на многоасортиментни XTC;
- 7.3. Оптимална топлинна интеграция и оптимален синтез на система от топлообменници;
- 7.4. Оптимални разписания на многоасортиментни XTC;
- 7.5. Автоматизирано оптимално проектиране на многопродуктови XTC;
- 7.6. Реновация на XTC.

След тези първи стъпки аз нямах физическата възможност да продължавам работата си в тази област и я оставих в ръцете на сътрудниците си, което не беше фатално защото всички станаха професори (без Дагмар, която си отиде от този свят много рано);

8. Нов подход за моделиране и симулиране на масопренасяне в колонни апарати (2006). Създаване на конвективно-дифузионни и средно-концентрационни модели на процеси в колонни апарати (химични реакции, абсорбция, адсорбция и хетерогенен катализ). Резултатите са публикувани в монографиите Chr. **Boyadjiev**, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, "Modeling of Column Apparatus Processes", **Springer-Verlag**, Berlin Heidelberg, 2016, 313 pp. и Chr. **Boyadjiev**, M. Doichinova, B. Boyadjiev, P. Popova-Krumova,

"Modeling of Column Apparatus Processes" (Second edition), **Springer-Verlag**, Berlin Heidelberg, 2018, 456 pp.

Така натрупания научен опит стана основа за редица обобщения.

#### Основни проблеми на химичното инженерство

Целта на химичното инженерство е решаването на основните проблеми в химичната промишленост (биотехнологиите, топлоенергетиката и други сродни производства), които са свързани с оптималното проектиране и управление, т.е., с минимизирането на инвестиционните и експлоатационните разходи. Тези проблеми се решават чрез оптималното проектиране на нови апарати и оптималното управление на действащи процеси, т.е. чрез минимизиране на габаритите на апаратите в нови производства и максимизиране на производителността на процесите в съществуващи производства. И в двата случая това се постига чрез увеличаване на скоростта на процесите. За целта е необходимо създаване на методи и алгоритми за моделиране и симулиране на скоростта на промишлените процеси.

#### Скорост на промишлените процеси

Процесите в химичната промишленост (биотехнологиите, топлоенергетиката) са резултат от отклонението на системите от тяхното термодинамично равновесие. Една система не е в термодинамично равновесие, когато концентрациите на компонентите (веществата) и температурата в отделните точки във фазите са различни. Тези разлики са резултат на реакции, т.е. на процеси, които създават или консумират вещество и (или) топлина.

Реакциите в промишлеността протичат в обема на фазите (хомогенни) или на границата между две фази (хетерогенни). Хомогенните реакции са обикновено химични, докато хетерогенните реакции са химични, хетерогенно-каталитични, физична и химична адсорбция, междуфазно масопренасяне газ-течност и течност-течност (на фазовата граница вещество изчезва от едната фаза и се появява в другата фаза).

Скоростите на промишлените процеси се определят от реакционната кинетика и нейното, моделиране и симулиране и позволява решаването на основните проблеми в химичната промишленост (биотехнологиите, топлоенергетиката).

#### Моделиране и симулиране

Основите на моделирането и симулирането в химичното инженерство, като част от човешкото познание и науката, са свързани със съчетанието на интуицията и логиката, които имат различни форми и съчетания в отделните науки. В математиката интуицията е аксиомата

(безусловна истина, която не подлежи на доказване), а логиката е теоремата (логичните следствия от аксиомата), като логиката преобладава над интуицията.

В природните науки (физика, химия, биология) аксиомите имат обикновено условен характер (принципи, постулати, закони), но логиката също преобладава над интуицията. Съчетанието на логиката и интуицията има различни степени на приближения - термодинамично, хидродинамично и молекулярно, където химичното инженерство използва основно хидродинамичното приближение (механиката на непрекъснатите среди).

#### Хидродинамично приближение

Хидродинамичното ниво използва приближенията на механиката на непрекъснатите среди. Тук математичната точка съответства на елементарен обем от фазата, който е едновременно достатъчно малък по отношение на целия разглеждан обем на фазата в апарата, и в същото време достатъчно голям по отношение на междумолекулните обеми във фазата. В тези приближения молекулите не са различими, както това се прави в следващото молекулно ниво на детайлизация на Болтцман (Boltzmann) при идеалните газове.

Химичното инженерство използва хидродинамичното ниво, съчетавайки в себе си химията, физиката и математиката, и гради своите логични построения на три основни "аксиоми":

- 1. Постулатът на Стокс (Stokes) за линейната връзка между напрежението и скоростта на деформацията, който стои в основата моделите на хидродинамиката на Нютоновите течности;
- 2. Първият закон на Фик (Fick) за линейната връзка между масовия поток и градиента на концентрацията, който стои в основата на моделите на линейната теория на масопренасянето;
- 3. Първият закон на Фурие (Fourier) за линейната връзка между топлинния поток и градиента на температурата, който стои в основата на моделите на линейната теория на топлопренасянето.

Тези три основни "аксиоми" имат условен характер при реалните газове и течностите и могат да се разглеждат като следствия от кинетичната теория на идеалния газ на Болтцман, където това са три "теореми", които произтичат от аксиомата за "еластичния удар" (при удар между две молекули се променят скоростите и посоките им, но сумарната кинетична енергия се запазва), а скоростните коефициенти се определят теоретично в зависимост от средната скорост и средния свободен пробег на молекулите.

#### Механизъм на влияние на реакционната кинетика

В химичната промишленост (биотехнологиите, топлоенергетиката) процесите протичат в движещи се фази (газ, течност, твърдо). Реакциите (реакционните процеси) водят до различни концентрации (и температури) в обема на фазите и на фазовите граници. В резултат, към

реакционните процеси се присъединяват хидродинамичните процеси, дифузията и топлопроводността. При тези условия се проявяват различни форми на масопренасяне (топлопренасяне), които биват конвективни (в резултат на движения във фазите) и дифузионни (в резултат на концентрационни (температурни) градиенти във фазите).

Конвективното масопренасяне (топлопренасяне) може да бъде ламинарно или турбулентно (в резултат на крупномащабните турбулентни пулсации).

Дифузионното масопренасяне (топлопренасяне) може да бъде молекулярно или турбулентно (в резултат на дребномащабните турбулентни пулсации). Дифузионното топлопренасяне представлява (на български) топлопроводността.

Математичните модели на промишлените процеси целят определянето на концентрацията на веществата (температурите на потоците) във фазите.

Математичните модели представляват материален (топлинен) баланс в елементарен (малък) фазов обем, който е еквивалентен на математична точка. Те съдържат математични оператори (функции и производни), които са математични описания на отделни физични и химични ефекти. Компоненти в този баланс са скоростите на конвективното масопренасяне (топлопренасяне), дифузионното масопренасяне (топлопренасяне) и хомогенните реакции (топлинния ефект на реакциите). Хетерогенните реакции участват в граничните условия на уравненията в моделите на масопренасяне (топлопренасяне). На тази основа са създадени моделите на класическата теория на масопренасянето.

#### Теория на масопренасянето

Ако една фаза (газ, течност) се движи по отношение на своята подвижна или неподвижна фазова граница, наличието на разлика в концентрацията на компонент (вещество) в обема на фазата и на фазовата граница води до пренасяне на вещество от по-високата към по-ниската концентрация за достигане на термодинамичното равновесие (равенство на концентрациите). В резултат се получава изменение на концентрацията в тънак слой около фазовата граница, така наречения дифузионен граничен слой.

Съвременната теория на масопренасянето се основава на теорията на дифузионния граничен слой (Ландау, Левич). Този подход замества (физически обосновано) елиптичните частни диференциални уравнения с параболични частни диференциални уравнения, което улеснява тяхното математическо решение и предлага математично описание на физичните процеси със свободни (не предварително определени) граници. Теорията на дифузионния граничен слой се развива в случаите на капки и мехурчета (Левич, Крилов), филмови течения (Левич, Крилов, Бояджиев, Бешков), нелинейно масопренасяне и хидродинамична устойчивост (Крилов, Бояджиев, Бабак).

Предложеният до тук теоретичен анализ показва възможността за определяне на скоростта на сложните процеси при известен механизъм, т.е., известен набор от елементарни (прости) процеси и взаимодействията между тях. В противен случай е необходим специален подход.

#### Модели на процеси в колонни апарати

Механизмът на сложните процеси в колонните апарати е известен, но не са известни разпределенията на скоростите във фазите и фазовите граници и практически няма възможност за тяхното теоретично или експериментално определяне. Предвид на това е неприложима теорията на масопренасянето и е предложен нов подход (Хр. Бояджиев, М. Дойчинова, Б. Бояджиев, П. Попова- Крумова). Повърхностните реакции на фазовите граници (междуфазно масопренасяне, адсорбция, катализ) са заменени с еквивалентни обемни реакции и експериментално определяеми параметри. Така получените конвективно-дифузионни модели се използват за качествен анализ (определяне на механизма на процеса) и получаване на средно-концентрационни модели за количествен анализ чрез заместване на скоростите и концентрациите със средните им стойности по сечението на колоната. Ефектът на скоростите във фазите се въвежда чрез експериментално определяеми параметри. Тези модели са полученни за случаите на химични реакции, правоточна (противоточна) физична (химична) абсорбция, нестационерна физична (химична) адсорбция, хетерогенен катализ с физичен (химичен) адсорбционен механизъм.

#### Модели на сложни процеси с неизвестен механизъм

За целта се използва комбинация от аксиоми и теореми при определяне на математичния модел на скоростта на процеса. От аксиомата "Матаматичната структура на количественото описание на реалните (промишлените) процеси не зависи от измерителната система на величините, които участват в тях" следва аксиомата "Математичните модели на реалните (промишлените) процеси са инвариантни по отношение на метрични преобразования", където "Метричните преобразования" представляват получаването на нови величини, получени от старите, умножени с положителни константи. Тези операции се наричат от Гухман "Подобни преобразования". Той формулира понятието "Хомогенна функция", когато тя е инвариантна по отношение на подобни преобразования. На тази основа Гухман доказва теоремата "Ако математичната структура е инвариантна по отношение на подобни преобразования, тя може да се представи като степенен комплекс", където "степенен комплекс" представлява произведение от величините, повдигнати на степени. От казаното до тук следва теоремата "Математичната структура на количественото описание на реални процеси може да се представи като степенен комплекс", чието доказване използва доказателството на теоремата

на Гухман. Използването на степенните комплекси като математични модели на скоросттите на сложни реални процеси, след определяне на степенните показатели от експериментални данни, разкрива огромни практически възможности.

От изложеното стана ясно какъв е пътят ми в науката, извървян за 85 години. Не стана ясно обаче: **КОГА МИНАХА ТЕЗИ 85 ГОДИНИ???** 

#### **PROGRAM**

Monday / October 25 2021			
	Wioliday / October 25 2021		
9:00 - 9:30	Registration		
9.00 - 9.30	Registration		
9:30 - 10:00	Opening Ceremony		
7.30 - 10.00	opening ceremony		
	Chairman: Assoc. Prof. Dr. E. Razkazova-Velkova		
	Chairman Association Division Razhazo (a. Vento (a.		
10:00 - 11:00	Chr. Boyadjiev A NEW APPROACH TO MODELING AND SIMULATION OF		
	INDUSTRIAL PROCESSES		
	(plenary lecture)		
	T		
11:00 - 11:30	Coffee Break		
11:30 - 12:30	Venko Beschkov		
	MATHEMATICAL MODELING OF MICROBIAL PROCESSES (plenary lecture)		
12:30 - 13:30	DISCUSSION		
13:30 - 14:30	LUNCH		
14:30 - 16:00	POSTER SESSION 1		
	Tuesday / October 26 2021		
	Chairman: Assoc. Prof. Dr. D. Dzhonova-Atanasova		
9:00 - 9:30	Tatyana Petrova		
	MODELING, ESTIMATION AND METHODS FOR REDUCING		
	LARGE-SCALE LIQUID PHASE MALDISTRIBUTION IN COLUMNS WITH OPEN STRUCTURE PACKINGS		

(plenary lecture)

0.20 10.00	III T	
9:30 - 10:00	Iliyan Trayanov	
	ASSESSMENT OF THE FUNDAMENTAL CFD CALCULATION METHODS IN SMALL PIPES	
	METHODS IN SMALL FIFES	
10:00 - 10:30	Coffee Break	
10:30 - 11:00	Evgeniy Ganev	
	OPTIMAL SYNTHESIS AND MANAGEMENT OF SUPPLY CHAINS	
	FOR PRODUCTION AND UTILIZATION OF BIOGAS	
11.00 11.00		
11:00 - 11:30	Apostol Apostolov, Dragomir Yankov, Yulia Tsareva, Maria Petyaeva	
	DEVELOPMENT, DIGITALIZATION AND IMPLEMENTATION OF	
	THE ROTATING FILM PERTRACTION METHOD FOR SELECTIVE	
	SEPARATION OF COMPOUNDS	
11:30 - 12:00	DISCUSSION	
11.30 - 12.00	DISCUSSION	
12:00 - 13:00	LUNCH	
12.00 10.00	Lenen	
12.00 17.00	POCETIP CHCCAOA	
13:00 – 15:00	POSTER SESSION 2	
	Wednesday / October 27 2021	
	Wednesday / October 27 2021	
10:00 - 12:00	POSTER SESSION (exhibition and discussion of all posters)	
10.00 12.00	1 OSTER SESSION (Cambition and discussion of an posters)	
	DISCUSSION	
12:00	Official ceremony in honor of the 85 <sup>th</sup> anniversary of	
	Professor Christo Boyadjiev	
	CLOSING the WORKSHOP	
"Challenges in Chemical and Biochemical Technologies and Environmental Protection"		
	Sofia'2021	

#### **POSTER SESSION 1**

	Monday October 25 2021		
P1	Microalgae as a feedstock for high-value compounds		
	Flora Tsvetanova, Dragomir Yankov		
P2	Analysis of optimization methods for improving the energy efficiency of		
	wastewater treatment plants		
	Rayka Vladova, Natasha Vaklieva-Bancheva		
P3	Preliminary results on the extraction of verbascum thapsus (great mullein)		
	S. Boyadzhieva, G. Kalotova, D. Yankov, R.P. Stateva		
P4	Study of the potential applications of thermophilic microorganisms at various		
	operating conditions in mfcs		
	Nadya Armenova, Dragomir Yankov, Stefan Stefanov, Elena Razkazova-Velkova		
P5	A multi-objective approach toward optimal design of sustainable dairy supply		
	chain taking into account the preferences of all network participants		
	Elisaveta Kirilova, Natasha Vaklieva-Bancheva, Tatyana Petrova, Rayka Vladova		
P6	Review of CFD simulations of fluid flow for development of an innovative bubble-		
	cap tray column for so <sub>2</sub> removal		
	Konstantina Stefanova, Daniela Dzhonova-Atanasova, Elena Razkazova-Velkova		
P7	Modeling of absorption-adsorption process		
	Chr. Boyadjiev, B. Boyadjiev, P. Popova-Krumova, E. Razkazova-Velkova		
P8	Air flow quality management in a residential bathroom by cfd method		
	Konstantina Stefanova, Maria Georgieva, Desislava Mehandzhijska		
P9	Composition determination and evaluation of Eurasian water milfoil		
	M. Lazarova, Konstantza Tonova		
P10	Recovery of valuable phenolics from Eurasian water milfoil		
	M. Lazarova, Konstantza Tonova		

#### POSTER SESSION 2

	Tuesday October 26 2021		
P11	Membrane processing alternatives for the production of natural grape extracts		
	M. Lazarova		
P12	In vitro assessment viability and activity of candidate -probiotic lactobacilli under		
	x-ray treatment		
	Lili Dobreva, Kristina Kostova, Hristina Sbirkova-Dimitrova, Svetla Danova		
P13	Flux and rejection behaviour in nanofiltration with mixed solvents		
	Maria Zarkova-Dencheva, Dragomir Yankov, Julia Genova, Iren Tsibranska		
P14	Mathematical modelling of 1,2-dibromoethane biodegradation in electric field		
	Petya Popova-Krumova, Venko Beschkov, Evgenia Vasileva, Tsvetomila Parvanova-		
	Mancheva		
P15	Investigation of membrane separation with an integrated model by the methods		
	of computational fluid dynamics		
	S. Panyovska, D. Dzhonova, I Tsibranska		
P16	Carbon materials for Sulphur oxidation/reduction reactions		
	George Pchelarov, Dzamal Uzun, Alexander Tsanev, Adriana Gigova, Marinela		
	Dimitrova, Ognian Dimitrov, Nadezhda Dermendzhieva, Elena Razkazova-Velkova,		
	Konstantin Petrov		
P17	Investigation of gas purification from SO <sub>2</sub> by absorption-adsorption process		
	Stela Panyovska, Daniela Dzhonova-Atanasova, Elena Razkazova-Velkova		
P18	Extraction of some organic acids by means of different ionic liquids. Comparison		
	of own and other results		
	Svetlana Zhivkova		
P19	Current state of immobilized microbial consortia application in the second		
	bioreactor of two-phase anaerobic digestion (tpad) of lignocellulosic materials		
	Jeny Miteva-Staleva, Rumyana Eneva, Lyudmila Dimitrova, Nikoleta Boteva, Venelin		
	Hubenov		
P20	Application of Microbial Electrolysis Cells (MECs) in Hydrogen production		
	Tsvetomila Parvanova-Mancheva, Evgenia Vasileva, Venko Beschkov		

A NEW APPROACH TO MODELING AND SIMULATION OF INDUSTRIAL

**PROCESSES** 

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Abstract

In the paper are presented theoretical analysis of the methods for industrial processes modeling and a

new approach to modeling and simulation of industrial processes in cases of lack of information on

the mechanism of the process.

**Prelude** 

The main problems in the industry are the optimal design of new devices and the optimal control of

active processes, i.e., minimization of the investment and operating costs. These problems are solved

by modeling methods [1].

The creation of the mathematical model begins with the formulation of the physical model of the

complex process, i.e., the definition of the simple (elementary) processes that make it up and the

interactions between them. The second step is to define simple processes that have mathematical

descriptions (equivalent mathematical operators). The other simple processes are introduced into the

mathematical model through quantitative information obtained from experimental data, which brings

the mathematical model as close as possible to the real process. The experiment brings mathematics

closer to physics (reality).

The optimal design and control in the chemical industry is uniquely related to processes rates, so all

mathematical descriptions of processes are linked to algorithms to determine these rates, i.e.,

processes kinetics.

**Keywords:** modeling, simulation, chemical engineering, industrial processes

# MODELING, ESTIMATION AND METHODS FOR REDUCING LARGE-SCALE LIQUID PHASE MALDISTRIBUTION IN COLUMNS WITH OPEN STRUCTURE PACKINGS

#### Assoc. prof. PhD Tatvana Stefanova Petrova

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#### **Abstract**

This lecture is a summary of the theoretical model research and the results obtained under Activities  $1.2 \div 1.4$  of the project "Sustainable processes, sustainable systems, sustainable environment", contract with BNSF No DN 07-14 / 15.12.2016, which ended at the end of 2020.

The possibilities of the dispersion model for the modeling of the radial distribution of the liquid phase after a layer of packing with open structure in a packed column are presented. The parameters of the model are analyzed and new methods for their determination in different situations are proposed, depending on the available experimental data and the conditions under which they are obtained. The estimation of the non-uniformity of the liquid phase is quantified by the integral characteristic - the maldistribution factor.

The problem areas (with large-scale maldistribution of liquid phase) in a pilot column installation (own data) have been identified, which are the reason for reducing the efficiency of the processes in it: the irrigation device (above the packing layer) and the collecting device (below the packing layer). Structural changes have been proposed in their design, which significantly reduces the unevenness of the installation. A theoretical methodology for determining the optimal geometric configurations of the devices in the problem areas is proposed.

The verifications of the model and of the methods for identification of its parameters, as well as the verification of the methodology for optimal geometric configuration of the collecting devices were performed successfully with own and other literature data in columns of semi-industrial and industrial size (0.47m, 0.6 m and 1.2 m) and random open structure packings (RSRM 0.7, 1.5 and 3 '', 25 mm metal Pall rings (Yin, 1999); RMSR 70-5 and Raflux rings 50-5) (Hanusch et al., 2018, 2019).

# ASSESSMENT OF THE FUNDAMENTAL CFD CALCULATION METHODS IN SMALL PIPES

#### Chem. Eng. Iliyan Trayanov

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#### **Abstract**

Nowadays we face large variety of CFD software packages and suites, but meanwhile we cannot trust the results from them as a real assessment of the designs we explore in them. With my presentation I will expose my work and my suggestions about the reliability of the calculation methods in one of the most used CFD programs: ANSYS. Large calculation times with 16 cores for 22+ days do not give us sufficiently reliable results, but on the other hand the fast calculations for just under an hour give us good ideas about changes in the design that can be executed.

**Acknowledgment:** This work was partially supported by the Ministry of Education and Science through the National Program "Young Scientists and Postdoctoral Students", approved by DCM # 577 / 17.08.2018

OPTIMAL SYNTHESIS AND MANAGEMENT OF SUPPLY CHAINS FOR PRODUCTION

AND UTILIZATION OF BIOGAS

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**Abstract** 

The continuous increase in greenhouse gas emissions due to the rapid development of technical

progress, as well as the growing needs for electricity requires serious attention to the so-called "green

energy" to meet permanently the needs of modern human society along with reducing emissions from

greenhouse gases. Even without human intervention, significant amounts of gases (mainly methane)

are generated with the most serious greenhouse effect, In this context, on the other hand, as a result

of human vital activity, biodegradable waste is generated both from everyday life and from industry,

i.e. from agriculture, forestry, animal husbandry, municipal wastewater treatment plants and others.

These activities reinforce the generation of putrefactive gases on an extremely large scale and promote

the need to create technologies and optimally design the flows in order to achieve sustainable

development in modern conditions. This research focuses on the problem of studying biogas

production technologies, the evaluating raw materials and products, carefully studying and evaluating

all possible flows of raw materials and products, and assessing the environmental impact of this

activity. Based on the above study, an optimization model will be created through mixed integer linear

programming (MILP) to determine potential locations and optimal parameters, as well as transport

flows of existing and potential initiatives within the Republic of Bulgaria.

Keywords: integrated biogas supply chain; optimal design; life cycle analysis; GHG emissions; solid

waste use; economic, environmental and social criteria

Acknowledgement: The authors would like to thank the HITMOBIL Center of Competence for the

financial support received under project BG05M20P001-1.002-0014

DEVELOPMENT, DIGITALIZATION AND IMPLEMENTATION OF THE ROTATING FILM PERTRACTION METHOD FOR SELECTIVE SEPARATION OF COMPOUNDS

Apostol Apostolov<sup>1</sup>, Dragomir Yankov<sup>1</sup>, Yulia Tsareva<sup>2</sup>, Maria Petvaeva<sup>2</sup>

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Abstract

Due to the increasing needs of specified chemicals with a high analytical grade, new methods for extraction are developing - one of them is the pertraction method of separating compound. The current work describes the rotating film pertraction method. It also considers to create a roadmap for scaling and implementing pertraction technology. Because of this other fields of science, technology, work organization and management are put on discussion here. Using the powerful tools of the digital era and computational methods, the test time and the probable implementation can be shortened.

**Keywords:** chemical engineering, chemical process design, extraction, pertraction, prototyping, digital modelling, computational fluid dynamics, additive manufacturing, scaling-up

Acknowledgements: The work is supported by National Research Fund grant KP-06- Russia-10

MICROALGAE AS A FEEDSTOCK FOR HIGH-VALUE COMPOUNDS

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Abstract

Microalgae are photosynthetic autotrophs, inhibiting saltwater and freshwater. They range widely

from prokaryotic single cell cyanobacteria to more complex multicellular eukaryotic algae.

They are considered as a sustainable feedstock for wide spectrum of bioactive compounds like lipids,

high-quality proteins, carbohydrates, dyes, carotenoides, vitamins for the food industry. Moreover,

some of the species have a good potential for biofuels production, like biohydrogen, biomethane,

biodiesel. In addition to the secretion of commercially valuable cellular metabolites, microalgal

production systems can be used for environmental- protecting technologies as wastewater treatment

and greenhouse effect diminishing.

Microalgal biomass offers numerous advantages as an object to work with. A very important factor

is that it does not requires a special fertile land to grow on, as it can be grown on a land which is

unsuitable for other purposes, even on domestic wastewater. Moreover, microalgae are resistant to

various contaminants. As they normally live in natural reservoirs, their utilization is cost-effective.

Also, microalgae build biomass rapidly. As for the disadvantages, a common problem is the low

biomass production and the small size of cells. To address these problems, some optimizations have

to be taken into account, like the temperature, the light intensity, the growth phase. There are two

possible ways for microalgal cultivation- in open pond and in photobioreactors.

For the bioproducts extraction, first have to be performed cellular disruption in order to be released

and purified the cellular contents. Then different strategies can be employed, like mechanical

extraction, chemical extraction using solvents or supercritical carbon dioxide, physical extraction,

enzymatic lysis.

**Key words**: microalgae, cultivation, valuable bioactive compounds, products extraction

Acknowledgements The authors thank to the Scientific Fund, Republic of Bulgaria, as this work was

financially supported by the  $K\Pi$ -06- $O\Pi P$  04/1 project.

ANALYSIS OF OPTIMIZATION METHODS FOR IMPROVING THE ENERGY

EFFICIENCY OF WASTEWATER TREATMENT PLANTS

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Abstract

Overcoming environmental problems and climate change are one of the main priorities in the policies

of the 21st century. Reducing energy costs and improving energy efficiency helps companies and

enterprises in the industrial sector on the path to sustainability. Sustainable operation is characterized

by the use of less materials and energy, improvement of processes by closing the cycle and utilization

of waste streams. One of the major energy consumers in the municipal sector is wastewater treatment

plants (WWTPs). Efficient wastewater treatment is associated with high energy consumption, which

represents a significant part of labor costs. Improving the energy efficiency of this type of facilities

would reduce both operating costs and the amount of greenhouse gases emitted into the atmosphere.

One way to achieve this goal is to apply optimization methods. In this paper, optimization methods

for improving the energy efficiency of WWTPs are presented.

**Keywords:** Energy efficiency, Optimization, Modeling, Wastewater treatment plants.

Acknowledgments: This work has been supported by the Bulgarian Ministry of Education and

Science under the National Research Programme "Young scientists and postdoctoral students"

*approved by DCM # 577 / 17.08.2018.* 

# PRELIMINARY RESULTS ON THE EXTRACTION OF VERBASCUM THAPSUS (GREAT MULLEIN)

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#### **Abstract**

*Verbascum thapsus* (Great mullein) is a biennial medicinal plant of the family *Schrophulariaceae*, which is widespread throughout the world. Due to the rich variety of bioactives present in the herb-saponins, flavonoids, phenolic acids, fatty acids, triterpenes and polysaccharides – it is used for the treatment of spasmodic cough, asthma, inflammation, various types of cancer and heart disease.

Dried areal parts of the leaves, stem, and blossom of Mexican Mullein, known as Gordolobo, were purchased from a pharmacy in Aguascalientes, Mexico. In our study we examined the influence of liquid to solid phase ratio, and solvents (ethanol, and water/ethanol mixtures) on the yield, and total phenolic content (TPC) of the extracts recovered from the different parts of the plant, and from their mixture. For this purpose, atmospheric extractions at 70 °C in a flask were performed. Firstly, liquid to solid phase ratio was changed from (20 to 50) ml/1g. It was determined that solvent volume of 30 ml was enough to dissolve all soluble substances from 1 g of any of the four plant matrices. Therefore, all subsequent experiments on the influence of the solvent ethanol, and hydroalcoholic mixtures with ethanol compositions from (25 to 96) %, on the yield and TPC of the extracts recovered were performed at the optimum solid-liquid ratio. The results obtained showed that the highest yield (13.6 %) was obtained from the leaves with 70 % ethanol, while with 48 % the yield was 12.6 %. As regards the TPC, the highest values were achieved with 48 % ethanol, the leaves extracts being the richest in polyphenols (TPC = 39.6 mg GAE/g rm). Extraction of a mix of the three matrices at the optimal extraction conditions determined were also performed. The yield achieved was 10 %, and the TPC - 23.9 mg GAE/g rm.

The optimal operating parameters established assure a maximum yield with a minimal use of raw material and energy, and will be applied in our future studies on the recovery of bioactives from Gordolobo.

**Keywords**: Gordolobo, atmospheric extraction, polyphenols

**Acknowledgement:** The authors acknowledge the funding received from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 778168.

STUDY OF THE POTENTIAL APPLICATIONS OF THERMOPHILIC MICROORGANISMS AT VARIOUS OPERATING CONDITIONS IN MFCS

Nadya Armenova, Dragomir Yankov, Stefan Stefanov, Elena Razkazova-Velkova

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Abstract

Bulgaria is among the leaders in Europe in the number of thermal mineral springs with varying

temperatures (from 45 to 100 °C) and pH values. Thermophilic microorganisms are widely distributed

around the high-temperature ecosystems in nature and they can develop their own physiology and

characteristic membrane structures. For this reason, thermophiles have been applied to various

industrial areas such as food and paper industry, detergents, drugs, toxic wastes removal, and starch

industry.

Thermophilic microorganisms thrive in high temperature conditions and have high metabolic rate.

Their accelerated biochemical processes lead to increased electron production during their lifecycle

- a trait that can be beneficial when applied in high-temperature microbial fuel cells (MFCs). The

thermophilic microorganism-based MFCs may be useful in different applications for electricity

generation by an environmental friendly approach.

In this study a microbial consortium obtained from the thermal spring "Rupite", Bulgaria, is being

used for oxidation of sulfide-contaminated waters in the anodic compartment of a membraneless

MFC, while sulfate-contaminated waters are used in the cathodic compartment. Additional

experiments are carried out with and without microorganisms in the cathodic compartment. The

results of the power output and oxidation rate are compared to a chemical FC under the same

conditions.

**Key words:** Thermophilic microbes, MFC, Membraneless fuel cell, Sulfide, Sulfate;

Acknowledgements: This work has received funding from the National Research Program "Low

Carbon Energy for the Transport and Household (E<sup>+</sup>)" and by the National Research Programme

"Young Scientists and Postdoctoral students" approved by DCM # 577 / 17.08.2018 both granted by

the Bulgarian Ministry of Education and Science

# A MULTI-OBJECTIVE APPROACH TOWARD OPTIMAL DESIGN OF SUSTAINABLE DAIRY SUPPLY CHAIN TAKING INTO ACCOUNT THE PREFERENCES OF ALL NETWORK PARTICIPANTS

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#### Abstract

The production of dairy products is related to water and energy costs and generation of large amounts of pollutants in air and water. Improving the sustainability of this type of product production can be achieved by optimizing all activities throughout the supply chain: from milk suppliers through production itself to end-users who meet environmental, economic and social criteria, while meeting the preferences of all network participants. The present study proposes a multi-objective modelling approach for optimal design of three-echelon supply chain for production of dairy products according to different recipes where all aspects of sustainability – economic, environment and social and the preferences of milk suppliers, dairies and markets are taken into consideration. The approach includes models for the production of dairy products along with the economic, environmental and social impact of the considered supply chain. The approach was implemented on a real case study from Bulgaria. Three optimization problems are defined and solved at different optimisation criteria representing the preferences of all participants in the supply chain. They are solved using General Algebraic Modeling System (GAMS) software. The first solution is related to the supply of such quantities of raw materials that lead to exceeding the market demands. This is the solution with the largest economic and social costs and lowest production profit. The second solution is related the lowest economic costs and largest production profit. In the third solution, full satisfaction of market demands was achieved. The obtained solutions can be used in the decision-making process.

**Keywords:** Optimal design, Dairy supply chain, Sustainability improvement, Preference satisfaction

REVIEW OF CFD SIMULATIONS OF FLUID FLOW FOR DEVELOPMENT OF AN INNOVATIVE BUBBLE-CAP TRAY COLUMN FOR SO<sub>2</sub> REMOVAL

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**Abstract** 

A waste-free innovative installation for SO<sub>2</sub> removal, combining two separation methods - adsorption and absorption, is considered for design improvement by CFD methods. The present work is a short review of CFD modeling of fluid flow in bubble-cap tray columns for the purpose of development of a simulation model using ANSYS Fluent. The Initial dimensions of a model of the laboratory installation are specified according to the established dependencies for the design of a bubble-cap tray. It is proposed to compare the fluid flow pattern obtained by ANSYS Fluent methods with the observations of the gas phase distribution, as demonstrated in literature for a bubble column using

high-speed cameras with high resolution.

**Keywords:** Desulfurization, purification of waste gas, bubble cap tray, mathematical modeling, CFD

simulation

**Acknowledgments:** This work has received funding from the Bulgarian National Science Fund project No KP-06-N37/11/ 06.12.2019 "Integrated absorption-adsorption process for waste free decontamination of gases from sulfur dioxide".

MODELING OF ABSORPTION-ADSORPTION PROCESS

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Abstract

The proposed mathematical model of the absorption-adsorption process uses an absorption-

adsorption column and makes it possible to create a waste-free technology for waste gases

purification from sulfur dioxide by means of regenerable adsorbent, where the system for the

regeneration of the adsorbent is similar to the regeneration system in the patent. The efficiency of the

processes is increased in an absorption-adsorption apparatus, where the absorption is realized in co-

current flows and the adsorption takes place in the flexible adsorbent. For this is proposed a new

absorption-adsorption column apparatus with bubbling plates.

In the proposed absorption-adsorption method for waste gases purification from sulfur dioxide, the

absorption is realized in the counter-current absorber (where practical gas velocity does not exceed 5

m.s<sup>-1</sup>) and the adsorption is carried out in a fixed bed adsorber. The efficiency of the process can be

increased if the absorption is realized in co-current flows and the adsorption takes place in the flexible

adsorbent. For this it can use a new absorption-adsorption apparatus with bubbling plates.

A new method for waste gas purification is realized in two steps: physical absorption of SO<sub>2</sub> with

water and chemical adsorption of HSO<sub>3</sub><sup>-</sup> from the water solution by synthetic anionite particles. The

adsorbent regeneration is made with NH<sub>4</sub>OH solution. The obtained (NH<sub>4</sub>)<sub>2</sub>SO<sub>3</sub> (NH<sub>4</sub>HSO<sub>3</sub>) is used

(after reaction with HNO<sub>3</sub>) for production of concentrated SO<sub>2</sub> (gas) and NH<sub>4</sub>NO<sub>3</sub> (solution).

Convection-diffusion and average concentration models of the absorption and adsorption processes

are presented.

Keywords: Absorption, adsorption, gas purification, SO<sub>2</sub>, convection-diffusion model, average

concentration model.

**Acknowledgments:** This work has received funding from the National Research Fund project No KP-

06-H37/11/06.12.2019 "Integrated absorption-adsorption process for waste free decontamination

of gases from sulfur dioxide".

# AIR FLOW QUALITY MANAGEMENT IN A RESIDENTIAL BATHROOM BY CFD METHOD

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#### Abstract

To ensure an effective ventilation in the residential bathroom the fan must be properly positioned according to the space of the room. The location of all furniture is essential for the correct positioning of the fan. In this work are shown how the different location of the fan in a bathroom can contribute to achieve the desired healthy environment. The quality of ventilation was improved using a software simulation by Ansys Fluent. Two cases are presented: 1) first, the fan is standard mounted in the chimney on the wall according to the technical project; and 2) second, the fan place is on the ceiling, so its position should be in front of the sink. The results show that the proposed ceiling position has a visible reduction of stagnant areas which are favorite place of uncontrolled mould growth.

Keywords: air flow, fan ventilation, bathroom, humidity, CFD

COMPOSITION DETERMINATION AND EVALUATION OF EURASIAN WATER

**MILFOIL** 

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Abstract

Eurasian water milfoil, EWM, is a worldwide spread weed, considered one of the most aggressive

species that invades almost all kinds of communities of submerged aquatic plants and displaces most

other plants. It is still unstudied as a potential source of bioenergy and valuable chemicals.

EWM biomass composition was characterized by determining the monosugar and lignin content, ash

and extractives. Carbohydrates weighed 44.70% of the submerged body of the plant. It was found

that glucose, Glu, monomer dominates in EWM carbohydrates, about 32%, based on a dried plant

weight,. Fructose, Fru, is the second monosugar in weight, but its availability is about 5-times lower

than the glucose content. Other monosugars represent 5.43% all together. This means that the

saccharification of this plant could reach a high yield of pure glucose.

Acid insoluble lignin, AIL, was evaluated to be 11.17%. Acid insoluble ash, 1.22%, contained mainly

biogenic silica as it was determined by X-ray diffraction. The total amount of ash in the studied

biomass was 7.11%. The nature of the remaining material was supposed to be nitrogenous material

which condensed into the acid insoluble residue and might comprise of polypeptides and nucleic

acids.

The total polyphenols, TPH, extracted following the procedure for determination of extractives in

biomass were 2.31%. In addition, the acid soluble lignin, ASL, extracted according to procedure was

estimated to be 5.48%.

RECOVERY OF VALUABLE PHENOLICS FROM EURASIAN WATER MILFOIL

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**Abstract** 

The growth form, low requirements of nitrogen and phosphorus, and high vegetative reproductive capacity of the aquatic plant Eurasian water milfoil, EWM, are among the factors determining its wide invasion success, but also the increased polyphenols' release is thought to stabilize the

macrophyte-dominated state of shallow lakes. For this reason, the phenolics of EWM first attracted

the researchers' attention.

Eurasian water milfoil extractives contain beneficial phenolic compounds, which health-related properties are currently a subject of intensive research. The aim of this study was to develop an

appropriate extraction treatment in order to recover valuable phenolics from EWM biomass.

First, the effect of different solvents and pHs on the total polyphenols, TPH, extraction was checked.

The presence of ethanol caused the most significant effect on the TPH recovery, which was further

enhanced by adding acid or base. Using the acidified water-ethanol mixture seemed the most

appropriate way to extract more TPH from the EWM matrix.

Next, the impact of autoclaving the EWM prior to the extraction was studied. Autoclaving increased

twofold the TPH liberated in the liquid phase compared to the result at room temperature. As a whole,

the total phenolics released from the plant autoclaved with acids exceeded those from the raw plant.

Considering that the above pre-treatment would cause simultaneous release of carbohydrates, for the

purpose of separating phenolics from sugars a raw EWM should be primarily used for extraction of

TPH. The extracted material obtained from the raw EWM is characterized in respect to TPH,

anthocyanins' content and antioxidant capacity. 50% ethanol of moderate acidity, 0.1 kmol m<sup>-3</sup> HCl,

could be considered an appropriate solvent for recovery of valuable TPH and anthocyanins from

EWM.

### MEMBRANE PROCESSING ALTERNATIVES FOR THE PRODUCTION OF NATURAL GRAPE EXTRACTS

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#### **Abstract**

Vast amounts of by-products are released during the winemaking process. Grape pomace usually constitutes about 20% of the processed wine grape weight. Its chemical composition includes dietary fibers, lipids, proteins, and a wide diversity of phenolic compounds. Traditionally, winemaking by-products are used as animal feedstock or fertilizer, but in the last decade they are considered as low-cost and rich source of valuable phenolics, which have very high market value as nutraceuticals, food additives and cosmeceuticals, due to their biological activity.

The recovery approach of these biologically active compounds is directed towards the production of natural grape extracts with the desired composition and free of detrimental constituents. This can be achieved when unharmful solvents and mild operating conditions are applied which do not lead to biological activity loss. The production scheme of grape extracts includes: wine by-products pretreatment, phenolics extraction, purification by adsorption and drying by evaporative process to obtain a product with specified characteristics. Membrane processes, such as ultrafiltration, nanofiltration and reverse osmosis, can substitute adsorption in the purification/fractionation step and become a powerful alternative for the production of natural grape extracts. Membrane processes offer significant advantages over traditional processes: variety of membrane materials and structures which can be used to obtain products enriched in diverse target compounds or diverse molecular mass fractions, and products for specific applications; much greater degree of control of hazardous contaminants in the final product; the use of lower solvent quantity and operation under milder conditions (temperature and pressure).

# IN VITRO ASSESSMENT VIABILITY AND ACTIVITY OF CANDIDATE -PROBIOTIC LACTOBACILLI UNDER X-RAY TREATMENT

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#### **Abstract**

Probiotics (*Pro-for and bio-life*) are live microorganisms which, when administrated in appropriate dose, possessed positive health effects. Lactic acid bacteria (LAB) are well-known probiotic bacteria, with beneficial role in gut homeostasis. Thus, several investigations have focused on behavior of lactobacilli in different habitats and variety of physical/chemical factors. A limited information exists on radiation exposure of LAB and related changes on the microbiome. In the same time, ionizing radiation is used as a therapeutic option in the treatment of certain neoplasm. The therapeutic doses of radiation employed often result in adverse effects. Some of them are based on changes of beneficial microbiota, during the treatment. The short-term effects on radiation exposure of LAB bacteria, however, remain unknown. With this aim we estimated viability of multibacterial formula with different candidate – probiotic strains. They are with dairy and human origin, belonging to our laboratory collection. Selected lactobacilli are exposed to X-ray treatment (Cu LLF ceramic tube operating at 45 kV and 40 mA) for 30 and 60 min. Survival decrease to zero was not demonstrated for any of the tested strains. The growth and biofilm-formation are monitored up to 72 h after irradiation. An interesting change in Lactobacillus biofilm formation during the cultivation, have to be pointed. Therapeutic doses of radiation do not significant affect the growth of lactobacilli. In the same time irradiated samples are able to delay the exponential growth of out-patient strain Escherishia coli.

**Acknowledgment:** Gratitude to prof. Boris Shivachev from IMC-BAS for experimental help. This work is a part of joint project with prof. Koltovaya, Lab. Radiation biology - JINR-Dubna, Russia

#### FLUX AND REJECTION BEHAVIOUR IN NANOFILTRATION WITH MIXED SOLVENTS

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#### Abstract

Membrane processes meet the requirements for efficient and cost-effective separation methods, although they still have to solve challenges such as insufficient selectivity. The quality of separation is a problem particularly relevant to mixed solvents (ex. water-alcohol mixtures) given their numerous applications, such as: extraction of bioactive molecules from renewable sources (plants, seaweed, by-products from the agro-food industry); separation of ethanol from water-ethanol systems. Achieving high flux and rejection is a major challenge for the membrane separation in view of alcohol recovery, production of low alcohol beverages and others.

This article presents a brief overview of research in the field of mixed solvents nanofiltration, the experimental evidence and theoretical interpretation of the observed effects. Own results with NADIR NP030 P membrane are presented. Model water-alcohol mixtures as well as red wine (Mavrud) nanofiltration are investigated in view of flux and rejection behavior relative to ethanol. Lower flux is observed with water-ethanol mixtures as compared to water. Transmembrane pressure affects both the permeate flux and the separation efficiency towards ethanol.

### MATHEMATICAL MODELLING OF 1,2-DIBROMOETHANE BIODEGRADATION IN

**ELECTRIC FIELD** 

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Abstract

The main goal of this study is to model the biodegradation process of 1,2-dibromoethane with

Bradyrhizobium japonicum 273 cells. Different processes of dehalogenation were carried out in a

laboratory bioreactor in presence and absence of constant electric field. The influence of electric field

was investigated. Complete biodegradation was observed corresponding to the stoichiometric

concentration of bromide ions in the medium.

Mathematical model describing this biodegradation process is composed and used for kinetic

parameter estimation on the base of least square function minimization, using own experimental data.

It is demonstrated that the dibromoethane biodegradation to bromoethanol and bromide ions by the

Bradyrhizobium japonicum 273 cells is successfully described by the composed model.

**Keywords:** 1,2-Dibromoethane (DBE), processes in presence and absence of constant electric field,

modeling, parameter evaluation

Acknowledgments: This work was supported by grant DN 17/4/2017 by the Fund for Scientific

Research, Republic of Bulgaria.

# INVESTIGATION OF MEMBRANE SEPARATION WITH AN INTEGRATED MODEL BY THE METHODS OF COMPUTATIONAL FLUID DYNAMICS

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#### Abstract

This work is part of a research on integrated bioreactors with membrane separation. Mass transfer associated with concentration polarisation phenomenon in spiral-wound and plate-andframe nanofiltration (NF) modules is mainly influenced by both the hydrodynamics in the feed channel and the solute transport inside the membrane.

The aim of the present study is to compare and evaluate different approaches to modeling processes in a filtration cell. To achieve this goal, CFD analysis will be performed to improve the hydrodynamic model and develop a model for simultaneous simulation of fluid flow and mass transfer across the membrane, using ANSYS Fluent techniques with UDF functions, at an acceptable computational time.

The present work complements previous results on mass transfer coefficient and their validation with data from literature.

**Acknowledgement:** This work was partially supported by the Bulgarian Ministry of Education and Science under the National Programme "Young scientists and postdoctoral students" approved by DCM # 203/19.09.2018.

CARBON MATERIALS FOR SULPHUR OXIDATION/REDUCTION REACTIONS

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**Abstract** 

Novel electrocatalyst carbon materials are used for oxidation of S<sup>2</sup>- and SO<sub>3</sub><sup>2</sup>-. The characterization

of the electrocatalysts were conducted by phisicochemical methods (SEM, X-ray diffraction, XPS

and BET) as well as electrochemical tests. Polarization curves of electrodes with incorporating higher

and fullerenes C<sub>60</sub>/C<sub>70</sub> were recorded. The experiments showed that higher fullerenes and C<sub>60</sub>/C<sub>70</sub>

fullerene catalysts convert SO<sub>3</sub> to SO<sub>4</sub> electrochemically. The oxidation products do not poison the

electrodes. The higher fullerenes play a major role in the synthesis of more effective catalysts. The

electrodes built by incorporating catalysts containing higher fullerenes and manganese oxides are

most promising in the effective electrochemical decontamination of industrial and natural waste

water.

**Keywords:** high fullerenes, C<sub>60</sub>/C<sub>70</sub>, DWCNTs

**Acknowledgements:** This work has received funding from the National Research Program "Low

Carbon Energy for the Transport and Household (E<sup>+</sup>)" granted by the Bulgarian Ministry of

Education and Science.

INVESTIGATION OF GAS PURIFICATION FROM SO2 BY ABSORPTION-

ADSORPTION PROCESS

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Abstract

The increasing content of SO<sub>2</sub> in the atmosphere needs new engineering solutions and cost-effective

methods for its reduction. Computational Fluid Dynamics (CFD) is an indispensable tool in solving

and analyzing problems that involve fluid flow.

The subject of the present work is investigation of a new approach and equipment for purification of

waste gasses from SO<sub>2</sub>. It includes a column with bubble-cap trays. As part of an extensive study of

the bubble-cap tray hydrodynamics, the present work is aimed at the specific two-phase flow pattern

on the novel tray proposed. A simplified 3D model of a cylindrical compartment was composed.

Different geometries and regimes were simulated in order to improve the design of the bubble-cap

tray for optimal gas-liquid mixing. Gas holdup has been considered as basic performance parameter.

The equations were solved using a CFD software ANSYS FLUENT (R13) based on the finite volume

technique.

**Keywords:** CFD, modeling, hydrodynamics, gas-liquid, bubble columns, tray columns

**Acknowledgements:** This work is supported by the National Science Fund of Bulgaria, contract KP-

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EXTRACTION OF SOME ORGANIC ACIDS BY MEANS OF DIFFERENT IONIC LIQUIDS. COMPARISON OF OWN AND OTHER RESULTS

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Abstract

A huge number of compounds found in nature are organic acids. When they are produced

microbiologically it is necessary for the end product to be removed so as to reduce the product

inhibition. They are often present in industrial waste water, from where they must be removed and

used. One way of removing organic acids from aqueous solutions is through liquid-liquid extraction.

The liquid-liquid extraction process is a highly selective method and one of the most versatile

procedures used for the extraction, separation and concentration of a variety of organic and inorganic

components from various aqueous media, and a process with the lowest cost for obtaining a high

quality ends products. In the last decade aqueous two-phase systems (ATPS) based on ionic liquids

(ILs) have been successfully implemented in a wide range of extraction and separation processes. IL

has the advantage of removing the acid in greater measure which makes them more effective.

The aim of this research is to look at the quantitative characteristics of some organic acid extraction

processes in using ionic liquids based on the different mechanisms of the extraction process as well

as in using kosmotropic salts instrumental in forming ATPS and their impact on increasing extraction

efficiency.

**Key words:** organic acids, liquid-liquid extraction, ionic liquids, aqueous two-phase systems.

# CURRENT STATE OF IMMOBILIZED MICROBIAL CONSORTIA APPLICATION IN THE SECOND BIOREACTOR OF TWO-PHASE ANAEROBIC DIGESTION (TPAD) OF LIGNOCELLULOSIC MATERIALS

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#### **Abstract**

Globally, more than 1.3 billion tons of organic waste materials per year are produced from agricultural production, during processing and transportation, in distribution and consumption. One of a number of technologies that can be used to reduce their quantity, to decrease global warming and waste management problems is anaerobic digestion.

The separation of the biological chain of acetogenesis and methanogenesis into two different bioreactors is not a new approach to anaerobic digestion. This idea was first suggested in 1984 (2). Separation of the natural ecology and metabolism of an anaerobic bacteria consortium into different classes: H<sub>2</sub>-producing bacteria (*Clostrium*) and H<sub>2</sub>-consuming methanogens (*Archaea*) underlie the two-stage bioreaction. In the first acidic step, pH conditions are selected in order to favor the production of H<sub>2</sub>. The liquid metabolites produced at this stage consist of volatile fatty acids such as: VFA, mainly acetic and butyric, and alcohols which are readily metabolized by methanogens. The second stage under conditions of neutral pH provides conditions for methanogenesis with CH<sub>4</sub> production. The two-phase anaerobic digestion process, which produces hydrogen gas in the first phase, followed by methane production in the second phase, has many advantages. However, the process of biohydrogen production is much faster than biomethane formation, which requires selection of the respective volumes of the two bioreactors. A possible approach for reducing the difference in the hydraulic retention time of the two processes and hence the reduction of the volume of the second bioreactor is the use of immobilized microbial cells in the second stage of the integrated system.

The use of immobilized organisms in modern biocatalysis allows the acquisition of many positive effects. Anaerobic sludge cells are capable of self-immobilization via formation of granules and biofilms. The study of microbial species and the possible interactions between them will allow the development of new strategies to increase methane and hydrogen yield by varying the factors affecting the development of particular groups of microorganisms in the integrated system of two laboratory bioreactors for biomethane and biohydrogen production. Recent years the culture-independent genomic approach to elucidate the structure and functioning of the microbial community became more accessible and promising.

Acknowledgements: This study is funded by the Bulgarian National Science Fund under contract KII-06-M 26/5 "Innovative two-stage system for production of hydrogen and methane using immobilized microbial anaerobic community".

# APPLICATION OF MICROBIAL ELECTROLYSIS CELLS (MECS) IN HYDROGEN PRODUCTION

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#### **Abstract**

Microbial electrolysis cells (MECs) are a relatively new, advanced technology in which hydrogen is produced simultaneously with wastewater treatment. It is a young generation technology for bioenergy that possesses a tremendous potential. The use of the battery as external power source is generally considered, but the use of renewable power generated from solar, wind, MFCs and waste heat can be seen too.

Biological production of hydrogen in anaerobic conditions, using bacteria, is a promising and advantageous area, especially when hydrogen is gained from a variety of renewable resources. Substantial factors like availability and cost are highly important in the selection of waste materials to be used in hydrogen production with fermentative bacteria.

Hydrogen can be produced biologically by bio-photolysis (direct and indirect), photo-fermentation and dark-fermentation or by combination of these processes (such as integration of dark- and photo-fermentation (two-stage process), or biocatalyzed electrolysis, etc

**Key words:** microbial electrolysis cells (MFCs), biotechnolo gy, renewable energy sources, biohydrogen

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