PROCESS SYSTEMS ENGINEERING – BRAZIL – 2022

II CONGRESSO BRASILEIRO DE ENGENHARIA DE SISTEMAS EM PROCESSOS

CRONOGRAMA GERAL & RESUMOS
GENERAL SCHEDULE & ABSTRACTS

Curitiba, Brazil
2022

CRONOGRAMA GERAL/ GENERAL SCHEDULE[1]

DAY #01 – WEDNESDAY – MAY 11th, 2022

OPENING SECTION & LECTURES
8.30 a.m. – 12.00 a.m.

ORAL PRESENTATIONS
1.30 p.m.-5.00 p.m.

POSTER PRESENTATIONS
5.30 p.m.-7.00 p.m.

DAY #02 – THURSDAY – MAY 12th, 2022

ORAL PRESENTATIONS
8.30 a.m.-11.30 a.m.

ORAL PRESENTATIONS
1.30 p.m.-5.00 p.m.

POSTER PRESENTATIONS
5.30 p.m.-7.00 p.m.

DAY #03 – FRIDAY – MAY 13th, 2022

ORAL PRESENTATIONS
8.30 a.m.-11.30 a.m.

ORAL PRESENTATIONS
1.30 p.m.-3.30 p.m.

PSEBR-2022 AWARD LECTURE
4.00 p.m.-5.00 p.m.

CONFERENCE CLOSING
5.00 p.m. – 5.30 p.m.

[1] : Click to access futher details/ : Clique para acessar detalhes

NOTAS/NOTES

🖱 : Clique para acessar mais detalhes / 🖱 : Click to access futher details

Apresentações Orais: Um dos autores terá 15 minutos para apresentar o trabalho e depois haverá 5 minutos para perguntas.
Oral Presentations: One of the authors will have 15 minutes to present the work and then there will be 5 minutes for questions.

Apresentação de Pôster: Às 17h30 um dos autores de cada poster deverá comparecer à sala de seu respectivo poster e aguardar os participantes para a discussão/apresentação. Os membros da comissão organizadora visitarão todos os pôsteres. A comissão organizadora sugere que o autor do poster ou prepare um poster virtual ou uma apresentação com 3-5 slides para mostrar o trabalho aos participantes que entrarem na sala de seu poster. Lembramos que o autor do poster poderá compartilhar a tela de apresentação e que cada poster tem seu link especifico.
Poster Presentation: At 5:30 pm, one of the authors of each poster must appear in the room of their respective poster and wait for the participants for the discussion/presentation. Members of the organizing committee will visit all posters. The organizing committee suggests that the poster author either prepare a virtual poster or a 3-5 slide presentation to show the work to participants who enter their poster room. We remind you that the poster author will be able to share the screen and that each poster has its own link.

Caso o autor de uma apresentação oral queira participar da seção de pôsteres do mesmo dia para dar continuidade às discussões, basta entrar em contato com a comissão organizadora pelo e-mail psebr2022@gmail.com .
If the author of an oral presentation wants to participate in the poster section of the same day to continue the discussions, just contact the organizing committee by e-mail psebr2022@gmail.com .

O evento será realizado pela plataforma Microsoft Teams.
The event will be held by the Microsoft Teams platform.

DAY #01

WEDNESDAY – MAY 11th, 2022
MORNING

OPENING SECTION & LECUTRES
8.30 a.m. – 12.00 a.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_MTY2M2I3YjYtZWFhNi00Mjg5LWE0NTMtOTM3M2Q2NDE0NTZi%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

8.30 a.m. - 9.00 a.m.
Opening & Reception

9.00 a.m. – 10.30 a.m.
Lecture
NEURAL NETWORKS: ON THE PURSUIT OF ROSENBLATT'S DREAM
Prof. Mauricio Bezerra de Souza Jr. - Universidade Federal do Rio de Janeiro, Brazil

10.30 a.m. – 12.00 a.m.
Lecture
ENERGY SYSTEM OF THE FUTURE: SOCIAL ISSUES IN THE ENERGY TRANSITION
Prof. Mariano Martín – University of Salamanca, Spain

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DAY #01

WEDNESDAY – MAY 11th, 2022
AFTERNOON

ORAL PRESENTATIONS

1.30 p.m.-5.00 p.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_ZWNmZDkzMmMtNDAxZi00NjBiLWEwZGUtYzZmMDJjNzUyMzU4%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

1.30 p.m.-1.50 p.m. - Oral Presentation 1
MODELING AND ECONOMIC OPTIMIZATION OF AN INDUSTRIAL COMPLEX FOR NATURAL GAS PROCESSING
Tayná Souza1, Argimiro R. Secchi, Letícia Cotia

1.50 p.m.-2.10 p.m. - Oral Presentation 2
DIGITAL TWIN DE OPERAÇÕES DE CARGA/DESCARGA DE GNL
Jacques Niederberger, Márcio dos Santos Novaes Filho

2.10 p.m.-2.30 p.m. - Oral Presentation 3
CATALYTIC REACTOR DESIGN OPTIMIZATION USING SET TRIMMING AND SMART ENUMERATION
Andre L. M. Nahes, Miguel J. Bagajewicz, André L. H. Costa

2.30 p.m.-2.50 p.m. - Oral Presentation 4
MODELING AND SIMULATION OF A CONTINUOUS KRAFT PULP DIGESTER
Isabela Barreto Correa, Maurício Bezerra de Souza Jr., Argimiro Resende Secchi

2.50 p.m.-3.10 p.m. - Oral Presentation 5
APLICAÇÃO DE MODELOS ACÚSTICOS PARA DETERMINAÇÃO DE DISTRIBUIÇÃO DE TAMANHO DE GOTAS DE EMULSÕES DE ÁGUA EM ÓLEO USANDO A TÉCNICA DE ESPECTROSCOPIA ULTRASSÔNICA
Carlos Adriano Moreira da Silva, Samuel Victor Saraiva, Darlan Bonetti, Rosiane Lopes da Cunha, Luiz Octavio Vieira Pereira, Flavio Vasconcelos da Silva, Ana Maria Frattini Fileti

3.10 p.m.-3.30 p.m. - Oral Presentation 6
FUZZY LINEAR PARAMETER-VARYING MODEL-ORIENTED MPC APPLIED TO AN ESP-LIFTED OIL WELL SYSTEM
Victor S. Matos, Thiago P. Chagas, Márcio A. F. Martins

3.30 p.m.-4.00. p.m. – BREAK/INTERVALO

4.00 p.m.-4.20 p.m. - Oral Presentation 7
MINLP MODEL FOR WORK AND HEAT EXCHANGE NETWORKS SYNTHESIS CONSIDERING UNCLASSIFIED STREAMS
Lucas F. Santos, Caliane B. B. Costa, Jose A. Caballero, Mauro A. S. S. Ravagnani

4.20 p.m.-4.40 p.m. - Oral Presentation 8
A CFD STUDY ON THE G-EQUATION MODEL OPTIMIZATION FOR A SPARK-IGNITION ENGINE FUELED WITH ETHANOL
Mikael Maraschin, Jean Lucca Souza Fagundez, Nina Paula Gonçalves Salau

4.40 p.m.-5.00 p.m. - Oral Presentation 9
AVALIAÇÃO DE DESEMPENHO DE CONTROLADORES PREDITIVOS MULTIVARIÁVEIS EM UMA PLANTA DE CAPTURA DE CO_2
José C. D. Filho, Antônio F. S. Netto, Humberto G. L. Fernandes Jr, Arioston A. Morais Jr

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POSTER PRESENTATIONS

5.30 p.m.-7.00 p.m.

POSTER 1

SIMULAÇÃO DO EQUÍLIBRIO DE FASES E CINÉTICA NA TRANSESTERIFICAÇÃO DE ÓLEO DE SOJA E METANOL

Bruno Kohlemann Tanque1, Luís Fernando Novazzi1

Link

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POSTER 2

MODELING THE OXIDATIVE COUPLING OF METHANE PROCESS VIA MACHINE LEARNING

Gabriela F. P. D. Silva, Andréa P. Parente, Leonardo D. Souza Netto, Amanda L.T. Brandão
Pontifícia Universidade Católica do Rio de Janeiro - PUC-Rio, Rio de Janeiro - RJ,

Link

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POSTER 3

OPTIMIZATION OF REACTIVE DISTILLATION FOR PRODUCING ETHYL LACTATE AND ITS OLIGOMERS USING MATLAB LINKED WITH ASPEN PLUS

Murielk S. Valvassore, Caliane B. B. Costa

Link

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POSTER 4

MODELAGEM HÍBRIDA BASEADA EM REDES NEURAIS FISICAMENTE INFORMADAS (PINN) APLICADA A SISTEMAS DE ELEVAÇÃO ARTIFICIAL DE PETR´OLEO POR BOMBEAMENTO ELÉTRICO SUBMERSÍVEL (BCS)

Taniel S. Franklin,, Leonardo S. Souza, Raony M. Fontes, Márcio A. F. Martins

Link

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POSTER 5

SIMULAÇÃO DE CONVECÇÃO NATURAL EM CAVIDADE CÚBICA CONTENDO MEIO POROSO HETEROGÊNEO: EFEITO DA RAZÃO DE CONDUTIVIDADE K*

Bruna Sgarlate, Éliton Fontana

Link

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POSTER 6

PREDICTING ASPECT RATIO OF MICRO/NANOCELLULOSE FIBERS USING MACHINE LEARNING TECHNIQUES

Giovana Signori Iamin, Marcos Lúcio Corazza, Quim Tarrés, Marc Delgado-Aguilar, Alexandre Ferreira Santos

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POSTER 7

ANALYSIS OF BIOGAS REFORMING PROCESS TO SYNGAS VIA DRY REFORMING AND BI REFORMING

Nadia Maria do Valle Ramos, Luiz Fernando de Lima Luz Júnior, Marcos Lúcio Corazza1

Link

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POSTER 8

OPTIMIZING CO2 EMISSIONS FOR A BIOGAS-TO-METHANOL PROCESS PLANT

Rafael O. Santos1, Diego M. Prata2 , Argimiro R. Secchi1

Link

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POSTER 9

LEARNING FROM SUB-OPTIMAL DEMONSTRATIONS WITH DDPG ALGORITHM AND OFF-POLICY DISCRIMINATOR: AN OPTIMAL CONTROL PROBLEM

Ruan de Rezende Faria, Bruno Didier Olivier Capron, Argimiro R. Secchi, Maurício Bezerra de Souza Jr.

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POSTER 10

MULTI-LAYER HEALTH-AWARE OPERATION AND CONTROL OF SUBSEA OIL LIFT SYSTEMS SYSTEMS

Nathália Teles Gomes Machado, Argimiro R Secchi, Maurício B de Souza Jr.

Link

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POSTER 11

OPTIMIZATION OF A MICRO-PHOTOCATALYTIC REATOR USING A CFD-ANN-GA HYBRID METHOD

Jéssica Oliveira de Brito Lira, Humberto Gracher Riella, Natan Padoin, Cíntia Soares

Link

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POSTER 12

KINETIC MODELLING CONSIDERING PHASE EQUILIBRIA THE NON-ISOTHERMAL ESTERIFICATION REACTION FOR THE DI(2-ETHYLHEXYL) TEREPHTHALATE PRODUCTION

Leoni Brondani, Dian Celante, Lisiane O. Diehl, Cezar A. Bizzi, Fernanda de Castilhos

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POSTER 13

MODELLING CONSIDERING COMPOUNDS' VOLATILIZATION INFLUENCE FOR TRANSESTERIFICATION REACTIONS FROM FFA AND METHYL ACETATE AT HIGH TEMPERATURE AND PRESSURE

Leoni Brondani, Luiz Jardel Visioli, Fernanda de Castilhos

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POSTER 14

AVALIAÇÃO DA SELETIVIDADE DE MECANISMOS DE HIDROTRATAMENTO PARA OBTENÇÃO DE HVO POR MEIO DE SIMULAÇÃO DE MODELOS CINÉTICOS

Lucas Sudré dos Santos, Nina Paula Gonçalves Salau

Link

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POSTER 15

SIMULAÇÃO DA GASEIFICAÇÃO DE BIOMASSA POR MODELO DE EQUILÍBRIO

Felipe Moro, Rodolfo Rodrigues

Link

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POSTER 16

DEVELOPMENT OF VAPOR COMPRESSION SYSTEM DYNAMIC MODELS FOR CONTROL AND SIMULATION PURPOSES USING MOVING BOUNDARY APPROACH

Breno Saldanha Sousa, Ana Maria Frattini Fileti

Link

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POSTER 17

ASSESSMENT OF CO2 HYDROGENATION TO FORMIC ACID USING TERNARY AMINE AND DIOL SOLVENTS

Abner Luiz da Silva, Murilo Leite Alcantara, Antônio Ésio Bresciani, Rita Maria Brito Alves.

Link

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DAY #02

THURSDAY – MAY 12th, 2022
MORNING

ORAL PRESENTATIONS

8.30 a.m.-11.30 a.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_YjBhYzAzNDgtN2NiNy00NmRmLWJmZDItNzdmNjM5ZTMzZDBi%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

8.30 a.m.-8.50 a.m. - Oral Presentation 10
ANALYSIS OF OPTIMAL CONTROL MODELS FOR BIOPROCESSES BASED ON DYNAMIC FLUX BALANCE ANALYSIS
Caroline S. M. Nakama, Johannes Jäschke

8.50 a.m.-9.10 a.m. - Oral Presentation 11
LIFE CYCLE ASSESSMENT OF CELLULOSE NANOCRYSTALS PRODUCTION IN SUGARCANE BIOREFINERIES
Gustavo Batista, Cristiane Sanchez Farinasa, Antonio José Gonçalves da Cruz

9.10 a.m.-9.30 a.m. - Oral Presentation 12
DESEMPENHO DE REATORES CONTÍNUOS PARA A PRODUÇÃO DE ÁCIDO LEVULÍNICO A PARTIR DA PALHA DE SOJA
Julio César de Jesus Gariboti, Leticia Mayuri Aiacyda de SouzA, Marina Gontijo Souza Macedo, Eliezer Ladeia Gomes, Emília Savioli Lopes, Melina Savioli Lopes, Romilda Fernandez Felisbino, Laura Plazas Tovar

9.30 a.m.-9.50 a.m. - Oral Presentation 13
GLOBALLY OPTIMAL DESIGN OF DISTILLATION COLUMNS USING SMART ENUMERATION
Alice Peccini, Lucas F. S. de Jseus, Argimiro R. Secchi, Miguel J. Bagajewicz, André L. H. Costa

9.50 a.m.-10.10 a.m. - Oral Presentation 14

DECISION SUPPORTED BY DIGITAL TWIN AND MACHINE LEARNING ALGORITHMS IN THERMAL POWER PLANT WITHCOMBUSTION ENGINES

Bruno Deon, Kleyton Pontes Cotta, Robson Felipe Viana da Silva, Camilla Barros Batista, Flavio Leite Loução Junior, Rodrigo José Silva de Almeida, Carlos Antonio Alves de Araujo

10.10 a.m.-10.30 a.m. - Oral Presentation 15

ANN ARCHITECTURES FOR THE PREDICTION OF DRYING KINETICS OF RED HUSK RICE

Piazzi A. C. F., Gasparetto H., Salau N. P. G.

10.30 a.m.-10.50 a.m. - Oral Presentation 16

EXPERIMENTAL VALIDATION OF A MULTIPHYSICS MODEL FOR THE MICROWAVE-ASSISTED PASTEURIZATION OF APPLE JUICE

Tamires K. Oishi, Eduardo V. S. Pouzada, Jorge A. W. Gut

10.50 a.m.-11.10 a.m. - Oral Presentation 17

AUDIO SIGNALS AND ARTIFICIAL NEURAL NETWORKS FOR CLASSIFICATION OF PLASTIC RESINS FOR RECYCLING

Letícia Tessarini, Ana Maria Frattini Fileti

11.10 a.m.-11.30 a.m. - Oral Presentation 18

A SET-POINT TRACKING CONTROL PROBLEM USING A MULTI-AGENTACTOR-CRITIC ALGORITHM

Ruan de Rezende Faria, Bruno Didier Olivier Capron, Argimiro R. Secchi, Maurício Bezerra de Souza Jr.

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DAY #02

THURSDAY – MAY 12th, 2022
AFTERNOON

ORAL PRESENTATIONS

1.30 p.m.-5.00 p.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_NTYxMmRmYzgtMTE1Zi00ZGJiLWE5OWMtYTk1YTZiNjg5OTM2%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

1.30 p.m.-1.50 p.m. - Oral Presentation 19
BIOPROCESS ONTOLOGY FOR SOFTWARE DEVELOPMENT
Priscila M. da Paz, Caroline S. M. Nakama, Galo A. C. Le Roux

1.50 p.m.-2.10 p.m. - Oral Presentation 20
XGBOOST MODEL OF STEAM REFORMING OF METHANE IN A MEMBRANE REACTOR
Mariana Almeida1, Andrea Parente, João Gonçalves Neto, Amanda Lemette

2.10 p.m.-2.30 p.m. - Oral Presentation 21
STABLE NMPC WITH ZONE CONTROL AND OPTIMIZING TARGETS
Guilherme A. S. de Souza Bruno F. Santoro, Darci Odloak

2.30 p.m.-2.50 p.m. - Oral Presentation 22
A RECURRENT NEURAL NETWORKS-BASED APPROACH FOR CONTROLLING THE SOLUTE CONCENTRATION OF A CRYSTALLIZATION PROCESS
Fernando Arrais R. D. Lima, Marcellus G. F. de Moraes, Maurício B. de Souza Jr.

2.50 p.m.-3.10 p.m. - Oral Presentation 23
ESTIMATIVA DA COMPOSIÇÃO ELEMENTAR DO CARVÃO MINERAL DE CANDIOTA–RS POR REDE NEURONAL ARTIFICIAL
Bruno Pasa, Nina Paula Gonçalves Salau, Rodolfo Rodrigues

3.10 p.m.-3.30 p.m. - Oral Presentation 24

ADDRESSING MACHINE LEARNING-BASED FAULT DETECTION AND DIAGNOSIS IN SOUR WATER TREATMENT UNITS UNDER PRE-FAULT AND FOULING SCENARIOS

Guilherme F. Pitanga, Júlia do N. P. Nogueira, Príamo A. Melo, Maurício B. de Souza Jr.

3.30 p.m.-4.00. p.m. – BREAK/INTERVALO

4.00 p.m.-4.20 p.m. - Oral Presentation 25

APLICAÇÃO DE ANÁLISE WAVELET PARA DETECÇÃO DE INSTABILIDADES FLUIDODINÂMICAS EM UM PROCESSO DE UMEDECIMENTO DE PARTÍCULAS EM LEITO DE JORRO

Vinicius Seferian Scheffer Machado, José Junior Butzge, Carlos Alexandre Moreira da Silva

4.20 p.m.-4.40 p.m. - Oral Presentation 26

FORECASTING FIXED-BED COLUMN SOYBEAN OIL EXTRACTION THROUGH ADAPTIVE NEURO-FUZZY INFERENCE SYSTEM (ANFIS)

Henrique Gasparetto, Ana Carolina Ferreira Piazzi, Fernada de Castilhos, Nina Paula Gonçalves Salau

4.40 p.m.-5.00 p.m. - Oral Presentation 27

A MATHEMATICAL MODEL TO SOLVE THE CAPACITATED VEHICLE ROUTING PROBLEM FOR MUNICIPAL SOLID WASTE COLLECTION AND TRANSPORTATION

Thales Rossi Spartalis, Leandro Vitor Pavão, Caliane B. B. Costa

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POSTER PRESENTATIONS

5.30 p.m.-7.00 p.m.

POSTER 18

TREE-BASED MACHINE LEARNING MODELS FOR OCM PROCESS: A CORRELATION STUDY OF HARD-TO-PREDICT PROCESS VARIABLES

Bruna de Abreu Camargo, Andréa Pereira Parente, Leonardo D. Souza Netto, Amanda Lemette T. Brandão

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POSTER 19

IMPLEMENTAÇÃO EM ASPEN CUSTOM MODELER DE UM MODELO CINÉTICO DE POLPAÇÃO KRAFT

Ana Carolina Ornellas Sardou, Jeiveison Gobério Soares Santos Maia, Argimiro Resende Secchi

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POSTER 20

APLICAÇÃO DA METODOLOGIA DE BOUND CONTRACTION EM SÍNTESE DE REDE DE TROCADORES DE CALOR

Eduardo Henrique Bender Pacola, Carolina Borges de Carvalho, Esdras Penêdo de Carvalho

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POSTER 21

INFLUÊNCIA DO COPROCESSAMENTO NA INDÚSTRIA CIMENTERIA EM RELAÇÃO AO ABATIMENTO DAS EMISSÕES DE NOX

Victor Jorge Prigol Rodrigues, Maribel Valverde Ramirez

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POSTER 22

SYNTHESIS OF PROPYL ETHANOATE BY SULFATED ZIRCONIA: KINETICS AND MECHANISM MODELING

Geovana S. Marques, Vinícius F. Bregenski, Giovana G Dusi, Fabiane Hamerski,Vítor R. Silva

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POSTER 23

A NEW FRACTIONAL MODEL APPLIED TO DESCRIPTION OF THE VISCOELASTIC CREEP BEHAVIOR OF TWO BRAZILIAN OILS AND THEIR W/O EMULSIONS

Wesley P. do Carmo, Alexandre F. Santos, Marcelo Kaminski Lenzi, Montserrat Fortuny, Ervin K. Lenzi

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POSTER 24

PERFORMANCE MONITORING AND DIAGNOSIS OF FILTERED SMITH PREDICTOR FOR SISO SYSTEMS WITH DOMINANT TIME DELAY

Sergio Andres Castaño Giraldo, Príamo A. Melo, Argimiro R. Secchi

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POSTER 25

FAULT DETECTION AND DIAGNOSIS BASED ON NEURAL NETWORKS IN THE TENNESSE EASTMAN PROCESS

Fernando Arrais R. D. Lima, Marcellus G. F. de Moraes, Maurício B. de Souza Jr.

Link

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POSTER 26

MODELAGEM DINÂMICA BASEADA EM APRENDIZADO DE MÁQUINA: APLICAÇÃO À INDÚSTRIA DO ÓLEO E GÁS

Thiago Dopazo Rey Simões, Felipo Doval Rojas Soares, Mauricio Bezerra de Souza Jr

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POSTER 27

CUSTO DO RSU COMO MATÉRIA-PRIMA PARA PLANTA DE WTE

Júlia P. Oliveira, Joana P. Pereira, Pedro R. R. Rochedo, Argimiro R. Secchi

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POSTER 28

CODEQ: ENSINO DE PROGRAMAÇÃO NA ENGENHARIA QUÍMICA VIA PLATAFORMA INTERATIVA

Luiz Emanuel Nicola, Thiago Reschützegger, Nícolas Anése, Bruno Pasa, Paulo Morgado, Nina Paula Gonçalves Salau, Christian Luiz da Silveira

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POSTER 29

USO DO SIMULADOR EMSO EM AULAS DE OPERAÇÕES UNITÁRIAS PARA PROJETO DE TROCADORES DE CALOR E EVAPORADORES

Rodolfo Rodrigues

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POSTER 30

STATISTICAL COMPARISON BETWEEN ARTIFICIAL NEURAL NETWORKS AND ADAPTIVE NEURO-FUZZY INFERENCE SYSTEMS TO PREDICT BREAKTHROUGH CURVES IN ADSORPTION SYSTEMS

Henrique Gasparetto, Ana Carolina Ferreira Piazzi, Nina Paula Gonçalves Salau

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POSTER 31

PREDICTING EXTRACTION EFFICIENCY OF METHYL ACETATE IN PRESSURIZED LIQUID EXTRACTION OF CRAMBE SEED OIL USING DECISION TREES REGRESSION

Piazzi A. C. F., Gasparetto H., Salau N. P. G.

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POSTER 32

TREATMENT OF EVAPORATED WATER FROM CONDENSED MILK PRODUCTION

Paulo Alves da Costa Filho, Guilherme Peixoto

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POSTER 33

FROM MISCONCEPTIONS TO ADVANCES ON THE THERMO-KINETIC STUDY OF BIOMASS PSEUDO-COMPONENTS DECOMPOSITION USING MODEL-FREE METHODS: IMPACT ON THE PRETREATMENT PROCESSES BY A MULTI-STAGE MODELING

Juliana O. Bah, Julio César de Jesus Gariboti, Eliezer Ladeia Gomes, Romilda Fernandez Felisbino, Rubens Maciel Filho, Laura Plazas Tovar

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POSTER 34

THERMODYNAMIC STABILITY OF FORMIC ACID UNDER AQUEOUS SOLVENTS: A PERSPECTIVE OF DFT CALCULATIONS AND MOLECULAR DYNAMICS SIMULATIONS

Raphael da Silva Alvim, Antonio Esio Bresciani and Rita Maria Brito Alves

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DAY #03

FRIDAY – MAY 13th, 2022
MORNING

ORAL PRESENTATIONS

8.30 a.m.-11.30 a.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_YTgxMzhiZGQtOWU4ZC00ZWJiLTk4NTgtMWQ2ZjhjMzdkZmE0%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

8.30 a.m.-8.50 a.m. - Oral Presentation 28
COMPARATIVE ANALYSIS OF MACROSCOPIC MODELLING AND SIMULATION APPROACHES FOR COAL COMBUSTION IN A FLUIDIZED BED
Carla N. M. dos Santos, Thiago F. de Aquino, Natan Padoin, Cíntia Soares

8.50 a.m.-9.10 a.m. - Oral Presentation 29
MODELAGEM E SIMULAÇÃO DO PROCESSO QUÍMICO DA TENNESSEE EASTMAN UTILIZANDO REDES NEURAIS ARTFICIAIS COM A LINGUAGUEM DE PROGRAMAÇÃO PYTHON
Gabriel F Xavier, Fabio M Cavalcanti

9.10 a.m.-9.30 a.m. - Oral Presentation 30
DEVELOPMENT AND IMPLEMENTATION OF A LINKAGE BETWEEN MODEL PREDICTIVE CONTROL AND REINFORCEMENT LEARNING
José R. Torraca, Argimiro R. Secchi, Bruno D. Capron

9.30 a.m.-9.50 a.m. - Oral Presentation 31
COMPARAÇÃO DA PRODUÇÃO DE DIMETIL ÉTER VIA REAÇÃO DIRETA ATRAVÉS DE DOIS SIMULADORES DE PROCESSOS
Natanael Casarin da Rosa, Christian Luiz da Silveira, Rodolfo Rodrigues

9.50 a.m.-10.10 a.m. - Oral Presentation 32

FLOW ASSURANCE IN OFFSHORE PIPELINES: KINETIC AND THERMODYNAMIC ASPECTS OF HYDRATE FORMATION AND DISSOCIATION IN OIL-DOMINATED SYSTEMS

Tamires de S. A. da Silva, Thamires A. L. Guedes, Iuri S. V. Segtovich, Argimiro R. Secchi, Príamo A. Melo

10.10 a.m.-10.30 a.m. - Oral Presentation 33

EMPREGO DE REDES NEURAIS RECORRENTES PARA PREDIÇÃO DA DINÂMICA DE REMOÇÃO DE TURBIDEZ EM UM PROTÓTIPO DE FLOTAÇÃO POR AR DISSOLVIDO

Felipe Sousa, Ana Souza, Newton Ferreira, Ana Fileti, Flávio Silva

10.30 a.m.-10.50 a.m. - Oral Presentation 34

MODELLING AND PARAMETER ESTIMATION OF METHYL METHACRYLATE DISPERSION POLYMERISATION IN SUPERCRITICAL CARBON DIOXIDE

Fabricio Machado, Kristoffer Kortsen, Ana A. C. Pacheco, Vincenzo Taresco, Steven M. Howdle

10.50 a.m.-11.10 a.m. - Oral Presentation 35

A NUMERICAL AND EXPERIMENTAL INVESTIGATION OF A FIXED BED CO2 ADSORPTION PROCESS USING PHASE CHANGE MATERIAL

C.S. Beraldo, M.M. Seckler

11.10 a.m.-11.30 a.m. - Oral Presentation 36

REDE NEURONAL ARTIFICIAL PARA MODELAGEM E OTIMIZAÇÃO DA SÍNTESE DE ACETATO DE ISOPROPILA CATALISADA POR ÓXIDO DE NIÓBIO

Aline C. M. Trindade, Heveline Enzweiler, Nina P. G. Salau,

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DAY #03

FRIDAY – MAY 13th, 2022
AFTERNOON

ORAL PRESENTATIONS

1.30 p.m.-3.30 p.m.

Link

https://teams.microsoft.com/l/meetup-join/19%3ameeting_ZDlmNjRlODEtZDJkZi00NDE1LTk1NjQtYzM5Y2VjM2ZkOWQ5%40thread.v2/0?context=%7b%22Tid%22%3a%22c37b37a3-e9e2-42f9-bc67-4b9b738e1df0%22%2c%22Oid%22%3a%22f8a39651-7ac7-4c13-8316-11b74cb90e5e%22%7d

1.30 p.m.-1.50 p.m. - Oral Presentation 37
ANALYSIS OF THE INTERFACIAL FORCE EFFECT ON SIMULATED OXYGEN TRANSFER OF A BUBBLE COLUMN BIOREACTOR USING COMPUTATIONAL FLUID DYNAMICS
Ana Carolina Borges Silva, Gustavo Batista, Mateus Nordi Esperança, Alberto Colli Badino, Rodrigo Béttega

1.50 p.m.-2.10 p.m. - Oral Presentation 38
NLP REFORMULATION OF A SYSTEM OF DIFFERENTIAL ALGEBRAIC EQUATIONS WITH EMBEDDED OPTIMIZATION
Rafael D. de Oliveira, Galo A.C. Le Roux, Radhakrishnan Mahadevan

2.10 p.m.-2.30 p.m. - Oral Presentation 39
COMPARISON OF MULTISTEP METHANOL PRODUCTION PROCESSES FROM BIOGAS USING ASPEN HYSYS
Guilherme Vieira Espinosa, Amanda Lemette T. Brandão

2.30 p.m.-2.50 p.m. - Oral Presentation 40
DYNAMIC FLUX BALANCE ANALYSIS APPROACH FOR THE OPTIMIZATION OF BIOPROCESSES
Willians O. Santos, Galo A. C. Le Roux, José G. Gomez

2.50 p.m.-3.10 p.m. - Oral Presentation 41
SYNTHESIS OF HIGHER ALCOHOLS FROM AN ETHANOL SOURCE ON A PFR
Rogério Pazetto, Leonardo Dantas, Amanda Lemette

3.10 p.m.-3.30 p.m. - Oral Presentation 42
APPLICATION OF A PREDICTIVE Q-LEARNING ALGORITHM IN A SUGARCANE ETHANOL BIOREFINERY MULTIPLE-EFFECT EVAPORATOR
Erick Y. Emori, Mauro A.S.S. Ravagnani, Caliane B.B. Costa

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PSEBR-2022 AWARD LECTURE

4.00 p.m.-5.00 p.m.
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UMA BREVE HISTÓRIA DA ENGENHARIA DE SISTEMAS DE PROCESSOS NO BRASIL
Prof. Dr. Evaristo Chalbaud Biscaia Junior
Universidade Federal do Rio de Janeiro

CONFERENCE CLOSING
5.00 p.m. – 5.30 p.m.

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RESUMOS
ABSTRACTS

LECTURES
PALESTRAS

LECTURE

NEURAL NETWORKS: ON THE PURSUIT OF ROSENBLATT'S DREAM

Prof. Maurício Bezerra de Souza Jr.
Universidade Federal do Rio de Janeiro, Brazil

In 1958, a young Cornell Professor, Frank Rosenblatt, presented the perceptron, "a machine", he claimed, "capable of perceiving, recognizing and identifying its surroundings without any human training or control." Despite his optimism, Professor Rosenblatt died a few years later (in 1971), during the so-called AI-winter, a period in which neural networks were ostracized due to the limitations of his perceptron, a one-layer neural network. Today, fifty years after the announcement of that ancestral learning machine, the success of artificial neural networks (ANN) in different areas of applications seems to have vindicated at least partially Rosenblatt's expectations. Out from this history, this talk will reflect on the ANN's role in the present industrial scenario, which is favorable to using data-based approaches due to the recent gains in capturing, transmitting, storing, managing, and analyzing data. Additionally, improved computational power and more efficient algorithms to deal with large amounts of data are available nowadays. Some areas of Process System Engineering (PSE) may particularly benefit from this situation, like fault detection and diagnosis (FDD) and advanced process control (APC). So, one challenge now is to bring ANN and other machine learning (ML) approaches to the realm of chemical industrial processes and systematically apply them. In this context, some tasks considered in the literature as technologically "easy" still need to be more disseminated in the industries; an example could be the development of soft sensors directly based on neural network models. Other challenges, presumably more "difficult" through the same point of view, involve the synergistic use of ANN with laws of physics providing hybrid models for monitoring and control. Finally, the routine use of Watson-like "questioning machines" for chemical industrial processes will probably take longer to become a reality. In this presentation, particular attention will be given to new paradigms based on deep learning, including convolutional and recurrent neural networks, and also to Physics-Informed Neural Networks (PINN). Comparisons with standard approaches will provide a reference basis. With EPQB/UFRJ's and PEQ/COPPE/UFRJ researchers, the author has a consolidated contribution to developing artificial intelligence (AI) based tools in Brazil, so applications for chemical and Oil & Gas industries will be presented to provide a comprehensive panorama. The talk intends to show that Rosenblatt's dream of creating autonomous machines based on ANN still provides an evergreen motivation for developing AI-based PSE applications.

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LECTURE

ENERGY SYSTEM OF THE FUTURE: SOCIAL ISSUES IN THE ENERGY TRANSITION

Prof. Mariano Martín
University of Salamanca (Spain)

With the expected growth in energy consumption and the current trend towards a sustainable and renewable power system a number of challenges must be addressed including the production of power from alternative sources and the need for backup when solar and wind energy are not available. Process engineering can provide the tools for the optimal integration of processes at different scales and their operation to mitigate the absence and/or variability in solar and wind. In addition, the production of a portfolio of chemicals that can be stored in a medium and long term for power production at demand is a solution to be added to the system as well as the need to produce renewable utilities including steam. In this talk we go over several examples presenting the design challenges of integrated facilities from facility level to system integration including the power to chemicals initiative (methane, methanol, ammonia, or metal hydrides production) and the possibilities in terms of wealth and job generation when coal or even nuclear plants are substituted by renewable based facilities to provide base load in the energy transition and the power system of the future.

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PSEBR-2022 AWARD LECTURE

UMA BREVE HISTÓRIA DA ENGENHARIA DE SISTEMAS DE PROCESSOS NO BRASIL

Prof. Dr. Evaristo Chalbaud Biscaia Junior
Universidade Federal do Rio de Janeiro, Brazil

O principal objetivo desta apresentação é apresentar um breve relato do estabelecimento e consolidação da área de engenharia de sistemas de processos no Brasil baseado em minha vivência como espectador e coparticipante dos primórdios da área. O surgimento desta área de ensino e pesquisa está intimamente relacionada ao início da pós-graduação em Engenharia Química no país, que ocorreu em 1963 no então Instituto de Química da Universidade do Brasil (atualmente Universidade Federal do Rio de Janeiro), capitaneada pelo Prof. Alberto Luiz Coimbra. Já em 1964 foi defendida a primeira dissertação de mestrado de cunho computacional do Prof. Carlos Augusto Guimarães Perlingeiro (Configuração do Escoamento Axissimétrico por Computador Digital) sob orientação do Prof. Coimbra. Com a criação do curso de mestrado em Engenharia Mecânica em 1965 foi então estabelecido o Orgão Suplementar do Centro de Tecnologia da Universidade denominado: COPPE – Coordenação dos Programas de Pós-Graduação e Pesquisa de Engenharia. O prosseguimento de pesquisas de natureza computacional em Engenharia Química só ocorreu em 1970 com o retorno do Prof. Perlingeiro de seu doutorado nos Estados Unidos versando sobre estabilidade dinâmica de reatores tanque contínuos. Com um programa de estudos multidisciplinar adequado organizado pelo Prof. Perlingeiro iniciei o curso de mestrado sob sua supervisão neste ano, tendo defendido a dissertação de mestrado em 1972 intitulada Funções de Liapunov e o Controle Ótimo de Reatores Tanque Contínuos.Os recursos computacionais nesta época eram ainda bastante precários, contando a UFRJ com apenas um computador monousuário da IBM (IBM 1130) para atender à toda sua comunidade). A computação analógica era também um recurso disponível na época, porém de natureza bastante limitada. Mesmo antes de concluir mestrado fui contratado como Auxiliar de Ensino do PEQ em 1971, ficando responsável pela área de Controle de Processos do programa ministrando disciplinas no curso de mestrado e na graduação da Escola de Química, tendo orientado nesta época quatro dissertações de mestrado. As numerosas atividades docentes e a inscrição em inúmeras disciplinas de doutorado atrasaram a complementação da minha formação acadêmica, a total liberação destas atividades e o estabelecimento de um programa conjunto com a Universidade de Leeds permitiu concluir meu doutoramento sob a supervisão do Prof. Colin McGreavy. No início da década de 80 o aprimoramento dos recursos computacionais atráves de estações de trabalho e do computador pessoal produziu uma revolução na área, criando grupos de pesquisa de alta qualidade na área em vários cursos de pós-graduação do país. Desde então, nestes 40 anos, a área de engenharia de sistemas de processos no Brasil consolidou-se como uma área de pesquisa sólida e consistente com uma formidável formação de recursos humanos e de pleno reconhecimento internacional.

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ABSTRACTS

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APRESENTAÇÕES EM FORMATO ORAL

ORAL PRESENTATION 1

MODELING AND ECONOMIC OPTIMIZATION OF AN INDUSTRIAL COMPLEX FOR NATURAL GAS PROCESSING

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The objective of this work is to develop an integrated simulation-optimization model to determine the optimum economic operating point of an industrial complex for natural gas processing with multiple process units and feedstock. Natural gas industrial facilities have the intrinsic characteristic of dealing with dynamic scenarios, with daily and intraday changes in inlet feed conditions. For being in midstream, it is not possible to have control over raw inlet gas, which leads the plant to suboptimal conditions. This scenario is intensified in the long term with comissioning and decomissioning of natural gas production sources, what might lead to incorporation of new process units within an existing business facility. Historically, natural gas processing plants have been looked at as facilities which the role was to give a destination to associated raw gas, making oil extraction feasible. Process and economical optimization were not key parameters to be looked at. However, this scenario is changing as market is getting more competitive and demanding. Even though onshore gas processing modeling and optimization has become a field of growing attention, as literature works point out, most previous efforts on optimization are still limited to: 1) recovery enhancement in natural gas production/processing, 2) natural gas transportation and 3) natural gas market. However, product price changes play an important role in gas processing plant optimization4 – the high frequency of those changes is such that optimizing liquid recovery does not always lead to the highest profit. In this context, an integrated modeling-optimization framework was proposed, using Aspen HYSYS for process simulation, Python for optimization and Microsoft Excel as data transfer interface. Process model comprises of three slug catchers, three liquid fractionating units, compression systems and auxiliary equipment, as well as simplified representation of gas treating units (mercury, CO2 and H2S removal). It also includes MEG injection and regeneration cycle, plus molecular sieve dehydration and regeneration. Simulation (and optimization) was performed in an Intel ® Core*TM* i5 10210U processor with 1.60 GHz with execution time ranging from 40-60 seconds to 2.5 min, depending on inlet input conditions. The objective function was built based on the maximum business profit, given by revenue minus operating expenses (OpEx) – revenue comes from selling the four products Sales Gas, LPG (liquified petroleum gas), NGL (natural gas liquid) and C5+ (natural gasoline) and OpEx was calculated by adding electricity and fuel gas costs. An augmented objective function was defined to incorporate, as penalty functions, inequality and equality constraints: product specifications, logistic bottlenecks and plant limits. Optimization model was validated against actual industrial data from an industrial facility, chosen as case study and responsible for processing over one quarter of all natural gas used in Brazil. The MINLP (Mixed-Integer Nonlinear Programming) optimization problem was broken down into an NLP (Nonlinear Programming) contribution, solved by Nelder-Mead algorithm, added to a MIP (Mixed Integer Programming) problem, solved by Branch and Bound method. Preliminary simulation results indicate good agreement with plant data. The NLP problem was successfully executed for ten normalized decision variables with 0.005 absolute tolerance in 1.5 to 2 hours and indicated a potential increase of 6.4 % in variable profit, as well as the existence of local minimums in the optimization space.

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ORAL PRESENTATION 2

DIGITAL TWIN DE OPERAÇÕES DE CARGA/DESCARGA DE GNL

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A questão das mudanças climáticas vem assumindo uma importância cada vez maior. Algumas nações e muitos atores econômicos em geral já possuem ou estão elaborando seus planos de descarbonização e uma das premissas dos processos de redução de emissões de gases geradores de efeito estufa é o emprego de um combustível fóssil de transição. O Gás Natural, composto majoritariamente por metano, foi considerado como o combustível de transição para a economia de baixo carbono, devido à sua característica de queima mais limpa (Lee et al, 2012). Diante deste cenário, o gás natural tem assumido importância crescente, e as operações com GNL têm ocorrido com mais frequência no país, batendo recordes históricos. Em 2019, a capacidade instalada global de liquefação de gás natural cresceu cerca de 42,5 MTPA, elevando a capacidade mundial para 430,5 MTPA. Esse acréscimo representa um aumento de 11% em relação ao ano de 2018 (International Gas Union, 2020). O transporte de Gás Natural em curtas distâncias é feito através de gasodutos, mas a maneira mais viável de movimentar grandes volumes entre pontos distantes entre si é na forma de GNL, gás natural liquefeito (Eden et al, 2018), transportado em navios projetados e construídos para este fim, conhecidos como “navios metaneiros”. O GNL é mantido líquido nos tanques dos navios a cerca de -160 oC e a pressões ligeiramente superiores à atmosférica (em torno de 1,2 bar). Durante o deslocamento dos metaneiros, devido à temperatura ambiente e ao balanço da embarcação, ocorre vaporização de parte da carga. Este vapor é denominado BOG - *boiloff gas*, e deve ser gerenciado adequadamente de forma a não pressurizar os tanques de armazenamento de GNL. Como o volume específico do gás natural em estado gasoso é 600 vezes maior do que o volume específico no estado líquido, quantidades relativamente pequenas de vapor podem causar elevações drásticas de pressão. Nas operações de carregamento do GNL nos navios de transporte e nas operações de descarregamento e recarregamento deste GNL também ocorre intensa geração de BOG em função da troca de energia entre o GNL e o meio externo. Neste contexto, um modelo dinâmico de transferência de GNL entre navios que permita prever e mitigar possíveis problemas operacionais decorrentes destas operações se mostra como uma ferramenta extremamente útil, principalmente no que tange ogerenciamento do BOG gerado nestas transferências, além de permitir a otimização das operações de carga/recarga de GNL (Contreras & Ferrer, 2005). Este trabalho descreve o desenvolvimento e a implantação de um modelo dinâmico de operações de transferência de GNL entre navios elaborado no software Aspen Hysys (Aspen Technology, 2020). Foram modelados um navio de transporte de GNL, também denominado *metaneiro* um terminal e um navio do tipo FSRU – *Floating, Storage and Regasification Unit*. O modelo foi validado contra os dados de uma transferência real e os aspectos relevantes da validação serão apresentados.

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ORAL PRESENTATION 3

CATALYTIC REACTOR DESIGN OPTIMIZATION USING SET TRIMMING AND SMART ENUMERATION

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We address the problem of the design of fixed-bed catalytic reactors. The goal is to determine the geometry needed to achieve a minimum production while limiting the pressure drop to minimize the catalyst volume. The solution of this problem is attained using a new technique involving Set Trimming followed by Smart Enumeration. Set Trimming employs the inequality constraints of the problem to reduce the number of candidates. After this step, the solution is found through an enumeration procedure applied to the remaining search space organized in an ascending order of the objective function (Smart enumeration). The proposed approach always identify the global optimum and do not present convergence problems. The solution scheme is applied successfully to the design of a methanol production reactor. A comparison with Genetic Algorithms and Particle Swarm Optimization show that the proposed approach can attain better solutions.

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ORAL PRESENTATION 4

MODELING AND SIMULATION OF A CONTINUOUS KRAFT PULP DIGESTER

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An extended Purdue model was developed and implemented in EMSO software to simulate a continuous kraft pulp digester. The axial transport mechanism was approximated through a series of continuous stirred-tank reactors. Mass, energy, and momentum balances were applied for each phase considered in the system (solid and entrapped liquor phases forming the wood chip, and free liquor phase). Unlike most works, we considered the formation of hexenuronic acids from methylglucuronic acids in hardwoods and the dissolution of both compounds. As an innovation, we proposed the addition of the syringyl/guaiacyl ratio influence on the delignification rate of hardwoods, by using experimental data obtained from several works. The steady-state profiles and dynamic responses behaved as expected. By performing a sensitivity analysis, the blow-line kappa number proved to be very sensitive to variations in the syringyl/guaiacyl ratio.

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ORAL PRESENTATION 5

APLICAÇÃO DE MODELOS ACÚSTICOS PARA DETERMINAÇÃO DE DISTRIBUIÇÃO DE TAMANHO DE GOTAS DE EMULSÕES DE ÁGUA EM ÓLEO USANDO A TÉCNICA DE ESPECTROSCOPIA ULTRASSÔNICA

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O objetivo do trabalho foi aplicar o princípio de medição baseado na espectroscopia ultrassônica para estimar a distribuição de tamanho de gotas de emulsões de água em óleo de girassol. Foi desenvolvido um sistema experimental baseado em medições acústicas na faixa de frequência de 4-14MHz, utilizado modelos físicos de propagação de ondas ultrassônicas em sistemas heterogêneos para interpretar os espectros de atenuação experimental. Por meio de um procedimento de inversão matemática e um algoritmo de otimização não linear é possível estimar os parâmetros que descrevem uma função de distribuição de probabilidade. Os resultados dos espectros de atenuação experimental foram comparados com as previsões dos modelos teóricos. Concluiu-se que a abordagem desenvolvida neste trabalho apresenta boa concordância com a obtida pela técnica da difração a laser. Os resultados indicam que a metodologia empregada neste estudo é adequada para a caracterização do tamanho de partícula polidispersa para concentrações moderadas de até 20%.

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ORAL PRESENTATION 6

FUZZY LINEAR PARAMETER-VARYING MODEL-ORIENTED MPC APPLIED TO AN ESP-LIFTED OIL WELL SYSTEM

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This work presents an application of a fuzzy infinite horizon model predictive control (FIHMPC) strategy to an ESP-lifted oil well system. The proposed scheme is based on a fuzzy model to approximate the nonlinear behavior to a linear parameter-varying model and incorporate into an infinite horizon MPC with feasibility guarantee by considering slacked terminal constraints and zone control strategy to handle time-varying ESP operating envelope constraints. The fuzzy identification process was based on commonly measured variables data only. Nonlinear mismatch scenarios with unmeasured disturbances show the effectiveness of the proposed controller over multiple operating conditions comparing to static model approach.

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ORAL PRESENTATION 7

MINLP MODEL FOR WORK AND HEAT EXCHANGE NETWORKS SYNTHESIS CONSIDERING UNCLASSIFIED STREAMS

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The optimal synthesis of work and heat exchange networks (WHENs) is deeply important to achieve simultaneously high energy efficiency and low costs in chemical processes via work and heat integration of process streams. This paper presents an efficient MINLP model for optimal WHENs synthesis derived from a superstructure that considers unclassified streams. The derived model is solved using BARON global optimization solver. The superstructure considers multistaged heat integration with isothermal mixing, temperature adjustment with hot or cold utility, and work exchange network for streams that are not classified a priori. The leading advantage of the present optimization model is the capability of defining the temperature and pressure route, i.e. heating up, cooling down, expanding, or compressing, of a process stream entirely during optimization while still being eligible for global optimization. The present approach is tested to a small-scale WHEN problem and the result surpassed the ones from the literature.

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A CFD STUDY ON THE G-EQUATION MODEL OPTIMIZATION FOR A SPARK-IGNITION ENGINE FUELED WITH ETHANOL

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The paper presents a CFD simulation for a Ricardo Proteus engine operated with ethanol. To model the experimental combustion process, a G-equation model was applied with US San Diego reaction mechanism. The reaction rates multiplier was optimized in a range of ×10 to ×30 as a way to validate experimental combustion data, finding the best value at ×20 to fit the in-cylinder pressure profile, IMEPgross, and combustion duration. Finally, at the best reaction multiplier value the mesh indecency was tested at 20mm, 10mm, 7mm and 5mm, only the 20mm mesh presented inconsistent simulated values compared with experimental values. Results pointed out that the mesh can be considered independent at values from 10mm and lower.

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AVALIAÇÃO DE DESEMPENHO DE CONTROLADORES PREDITIVOS MULTIVARIÁVEIS EM UMA PLANTA DE CAPTURA DE CO_2

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As plantas de captura de carbono (PCC) têm ganhado notoriedade nos últimos anos, haja vista que é uma alternativa viável quando acopladas em usinas de geração de energia. Os processos de absorção química com regeneração do solvente por desabsorção são, sem dúvida, a tecnologia mais consolidada de PCC. Entretanto, algumas desvantagens estão associadas a esses processos, por exemplo, alto consumo de energia, dinâmica altamente não linear, variáveis de difícil controle, acoplamento de variáveis e sistema multivariável. Assim, esse trabalho propôs uma metodologia para inserir dois controladores PID (Proporcional-Integral-Derivativo) e controladores preditivos multivariáveis baseados em modelo (MPC) em uma PCC. A partir da identificação do processo foi possível obter as funções de transferência do sistema MIMO (múltiplas entradas e múltiplas saída), projetar duas malhas de controle realimentação com ações PID, efetuar a sintonia e avaliar seus desempenhos. Para suprir a desvantagem se ter um controlador para cada malha de controle e não tratar das restrições do problema, foram propostos os controladores: controle preditivo multivariável linear sem restrições (MPCLSR) e controle preditivo multivariável linear com restrições (MPCLSR). Os controladores PID's, em comparação com o MPCLSR e MPCLCR, apresentaram menor desempenho frente às perturbações e mudanças de setpoint.

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ORAL PRESENTATION 10

ANALYSIS OF OPTIMAL CONTROL MODELS FOR BIOPROCESSES BASED ON DYNAMIC FLUX BALANCE ANALYSIS

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The use of optimal control in bioprocess can be an important strategy to increase efficiency and improve quality satisfaction of bioproducts. This type of control is based on a mathematical model of the bioprocess and is usually implemented using unstructured models, which rely on fixed parameters to characterize the metabolism of the microorganism, such as specific growth and yields. An issue with unstructured models is that they are only valid for narrow ranges of process conditions and cellular behavior [1]. One way to overcome this limitation is to use a more comprehensive model that can describe, for example, changes in the active metabolism. Dynamic flux balance analysis (dFBA) is a suitable modeling technique in this scenario as it is based on the metabolic network of microorganisms and can describe distinct physiological states and changes among them. dFBA models are composed of a differential algebraic system of equations that describes the dynamics of the process variables, such as substrate and product concentrations, and the exchange between the microorganism and medium. To describe the internal metabolism of the cell, dFBA models also comprise a linear program (LP) that calculates the internal flux distribution for the metabolic network [2]. Due to the presence of the LP, an optimal control model based on dFBA is a bi-level optimization problem, which can be challenging to solve. Since the inner optimization model is linear, a possible approach is to substitute the LP with its first-order optimality condition (KKT conditions), resulting in a nonlinear program (NLP) with complementarity constraints due to the relationship between the inequalities and their corresponding Lagrange multipliers. To use standard NLP solvers to solve this optimal control problem, these complementarities need to be relaxed to become smooth expressions. Interior point solvers are NLP solvers that are suitable to handle large problems with many degrees of freedom and inequalities, but they have the disadvantage of compromised convergence when dealing with ill-posed models [3]. Optimal control models based on dFBA have both characteristics; therefore, in this work, we analyze them and the challenges that may arise when employing an interior point solver, specifically IPOPT [4], to solve them. To perform this analysis, we work on a case study that implements both open- and closed-loop formulations for the optimal control problem of finding the optimal feed profile for a fed-batch bioreactor in which the goal is to maximize growth of *Escherichia coli* on glucose. Limitations due to the use of IPOPT are discussed and we show that the stoichiometry matrix should be carefully assembled so it is full row rank to avoid convergence issues. We also compare two common reformulation approaches for the complementarities: the penalty term method and the relaxation method. The former discards complementarities of the form $a^T b = 0$ and adds a weighted penalty term $\pi a^T b$ to the objective function, while the later replaces each complementarity $a_i b_i = 0$ with an inequality $a_i b_i \leq \varepsilon$ with ε being a small positive value. We concluded that both reformulation approaches are suitable for solving the model considered in the case study using IPOPT; however, they present some differences that are worth mentioning. The relaxation method can control the degree of complementarity satisfaction since it sets a maximum value for it, while the penalty-term approach can converge faster when a good variable initialization for the model is not available.

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LIFE CYCLE ASSESSMENT OF CELLULOSE NANOCRYSTALS PRODUCTION IN SUGARCANE BIOREFINERIES

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Growing environmental concerns on a global scale make the development of environmentally sustainable processes a priority. Life Cycle Assessment (LCA) is a standardized tool to quantify the environmental sustainability performance of emerging technology products. The purpose of using LCA in this work was to evaluate the cellulose nanocrystals (CNCs) production in sugarcane biorefineries, identifying hotspots that can drive to process design changes to reduce environmental footprint. Modeling and simulation of an incremental unit for CNCs production from sugarcane bagasse (the main residue from the sugarcane industry) was performed. The production route considered steps as organosolv delignification with ethanol, acid hydrolysis with H2SO4, and downstream processes such as centrifugation, dialysis and drying of CNCs, which were obtained in 95% purity by mass. In order to proceed the LCA, an inventory of raw-materials, products and emissions was made. The analysis employed the cradle-to-gate approach, and the functional unit was considered as 1 kg of CNCs produced. In addition to the Global Warming Potential (GWP) metric, other environmental assessment categories were also evaluated, as the CML-IA 2000 Baseline method was selected in the SimaPro® software and using the EcoInvent v.3.3 database. Energetic allocation was carried out as the distribution factor of environmental impacts to the products and by-products. LCA results showed that daily production of 7.73 ton of CNCs occurred with accumulated GWP of 23.6 tons of CO2 equivalents. Ethanol from organosolv pretreatment, sulfuric acid from hydrolysis, and sugarcane bagasse burning for steam and energy generation were the main contribution inputs for GWP. An estimated GWP of 0.23 kg of CO2 equiv. per kg of dry equiv. CNCs were accounted after energetic allocation. This result corresponds to 13.43 g of CO2 equiv. per MJ of process outputs. In other impact categories aside from GWP, the environmental impacts of H2SO4 were generally the most relevant, especially in the abiotic depletion.

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DESEMPENHO DE REATORES CONTÍNUOS PARA A PRODUÇÃO DE ÁCIDO LEVULÍNICO A PARTIR DA PALHA DE SOJA

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O ácido levulínico (AL), promissor das biorrefinarias, é utilizado em diversos segmentos das indústrias, como farmacêutico, combustíveis, têxtil, entre outros. Este trabalho objetivou a consolidação de um mecanismo cinético para obtenção do AL a partir da palha de soja definindo-se condições operacionais adequadas para obtenção de uma alta conversão de celulose em reatores contínuos. A síntese do sistema reacional para a despolimerização catalítica da celulose, determinou que o uso de reatores de fluxo pistonado leva a maiores rendimentos de AL (45%) em comparação a reatores de mistura perfeita (35%), ambos operando a 463,15 K e 5% m/v H_2SO_4.

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ORAL PRESENTATION 13

GLOBALLY OPTIMAL DESIGN OF DISTILLATION COLUMNS USING SMART ENUMERATION

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Distillation is the most important unit operation for separation of mixtures employed in the chemical industry. The design problem of distillation columns involves the identification of the number of distillation stages and the feed tray to obtain an stream according to the desired specifications of purity and recovrey. This paper addresses the solution of the optimal design of distillation columns, seeking for the minimization of the total annualized cost (TAC). The technique employed to solve this problem is Smart Enumeration, which circumvents the limitations observed in other techniques employed in the literature, such as mathematical programming and metaheuristic methods. The proposed solution technique always attain the global optimum of the problem and demands only the exploration of a fraction of the search space. Preliminary numerical results show that the Smart Enumeration can demand an smaller computational effort than mathematical programming.

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ORAL PRESENTATION 14

DECISION SUPPORTED BY DIGITAL TWIN AND MACHINE LEARNING ALGORITHMS IN THERMAL POWER PLANT WITHCOMBUSTION ENGINES

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Thermoelectric power plants (TPPs) commonly have a strategic and emergency character due to the flexibility of operation and for not depending on weather conditions, so the availability and reliability of TPPs are critical issues. The challenge of ensuring these characteristics is intrinsically associated with maintenance processes. Through the Research and Development Program of the National Electric Energy Agency, Radix Engineering and Software, in partnership with the Federal University of Santa Catarina, developed an anomaly detection system to aid decision-making in predictive maintenance with a Digital Twin approach for the Diesel Generating Units (DGUs) of the Paraíba State Electric Power Plants - Epasa. By associating historical sensor data with maintenance notes, it was possible to train regressive models in the best operating conditions to create digital twins that mimic the main variables of four subsystems that are part of the DGUs: fuel admission system, cooling, lubrication, combustion air admission and exhaustion gases (the latter two were combined, since they are correlated by the turbocharger). For analysis and validation, the data of five DGUs were combined so it could be trained and tested in groups. A health index was created by normalizing the errors and submitting them to a moving average, thus reflecting the performance of each subsystem and being able to evaluate the occurrence of anomalous deviations. By correlating such deviations with the maintenance notes, using time windows, it was possible classify the events based on the regressive models. The models were further optimized using a genetic algorithm, which sought the best inputs, regressive algorithms and respective hyperparameters, while improving regression metrics as well as classification simultaneously. This approach resulted in a final average R^2 of 0.93 and RMSE of 0.072 for the regressions, and for the classification metrics an average accuracy of 0.86 and F1-Score of 0.52 for the anomalies detection were achieved. Finally, the models were implemented in a SCADA supervisory system with customized dashboards for real-time monitoring. This methodology can be replicated in different industries that use a similar data acquisition system.

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ANN ARCHITECTURES FOR THE PREDICTION OF DRYING KINETICS OF RED HUSK RICE

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In the present work, different artificial neural networks were used to predict the drying kinetics of red husk rice. Drying of red husk rice was carried out under 5 temperature experimental conditions of 40, 50, 60, 70, and 80 °C and initial water contents of 20 and 30%. The input variables used for the construction of the ANNs were time (min), temperature (ºC), and water content (%), and the output variable was the final water content. ANNs with a single hidden layer were built by varying the number of neurons in the hidden layer: 2, 5, and 10. The results showed that, for all studied temperatures and all initial conditions of water content, an ANN with 10 neurons in a single hidden layer can accurately predict the experimental data.

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ORAL PRESENTATION 16

EXPERIMENTAL VALIDATION OF A MULTIPHYSICS MODEL FOR THE MICROWAVE-ASSISTED PASTEURIZATION OF APPLE JUICE

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Continuous thermal processing of liquid foods require that a given level of sterility is reached with minimal degradation of quality attributes (sensorial and nutritional characteristics). In order to guarantee safety and optimize quality of the food, the thermal process should be modeled considering flow, heat transfer and flow principles. A microwave cavity designed for continuous flow heating of liquid foods was simulated using the finite element method in COMSOL Multiphysics (v. 6.0, Stockholm, Sweden). The physics for electromagnetic waves, laminar flow and heat transfer were combined iteratively to solve and predict the electric field intensity, velocity profile and temperature distribution through the fluid domain. The COMSOL model was built in five main steps: geometry definition, physics boundary conditions and initial values, meshing, results and post-processing. To validate the model, cloudy apple juice was processed with a flow rate of 0.8 L/min to reach the pasteurization temperature of 80 °C. The experimental test was carried out in a microwave-assisted unit Lab25-UHT/HTST EHVH (MicroThermics, USA) (2450 MHz, 6 kW) and the experimental process temperature was measured and compared with the value predicted by the model. Model simulations showed good temperature prediction. Temperature distribution was useful for determining possible overprocessing zones. The main results show that the proposed model is reliable for predicting time-temperature histories during thermal processing, and can be used for process and product quality improvement.

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AUDIO SIGNALS AND ARTIFICIAL NEURAL NETWORKS FOR CLASSIFICATION OF PLASTIC RESINS FOR RECYCLING

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Given the increasing consumption of packaging and plastic products, which generate a large part of municipal waste, efforts are needed to properly recycle these materials. For the process to be accessible and environmentally sound, the different types of resins must be separated before they enter the recycling chain. The most common resins are PET (polyethylene terephthalate), HDPE (high density polyethylene), PVC (polyvinyl chloride), LDPE (low density polyethylene), PP (polypropylene), PS (polystyrene) and OTHERS. This classification is usually done manually by the officials of the cooperatives. Sometimes it is difficult to identify them because the symbols for the resin in the materials are missing and they end up in the wrong destination instead of recycling. There are some techniques, such as the simplest density and burning tests, and others, more refined, that require specialized equipment, such as Fourier transform infrared spectrometry (FTIR), magnetic resonance imaging (MRI), image and color identification. Conventional methods cannot provide the flexibility needed, and sophisticated methods can be expensive. When the material is kneaded, it is also possible to perform plastic identification using audio signals, and the sound waves obtained differ from one resin to another. Hence, the audio signals of the kneaded plastic samples from each category were recorded and a corresponding database was created. In order to identify them, signal processing techniques such as the Fourier transform and a feature extraction technique such as MFCC (Mel-Frequency Cepstral Coefficients), which is a short-time representation of the sound power spectrum, must be used. The features of the extracted audio data are used as input to the artificial neural networks. Two types of networks were used, the convolutional neural network (CNN), which is a feed-forward type used in digital image processing, and the recurrent neural network of the LSTM (long short-term memory) type, which processes not only single points but also entire data sequences where the order is important. A comparison was made between the two networks. The metric used was accuracy, which reached over 80% for both networks, and they performed well in classifying most resins. Therefore, the model and techniques were found to be efficient for classifying different types of plastic resins, so it does not require large investments and can be adapted to any recycling cooperative.

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ORAL PRESENTATION 18

A SET-POINT TRACKING CONTROL PROBLEM USING A MULTI-AGENTACTOR-CRITIC ALGORITHM

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A multi-agent actor-critic algorithm to a set-point tracking control problem is proposed,which typically features large time horizons and complex action space to address the problems resulting from sparse rewards, challenging exploration of control actions, and complex off-policy learning. The results showed the efficiency of the multi-agent deep deterministic policy gradient (MADDPG) applied in a single-input single-output system (SISO). Specifically, 4 control agents were analyzed in an offline and online control experiment, achieving set-point tracking in both cases and withstanding measurement noise in the online experiment. The 4th agent had the best convergence and learning rate results and made the 1st agent robust even when subjected to the online process

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ORAL PRESENTATION 19

BIOPROCESS ONTOLOGY FOR SOFTWARE DEVELOPMENT

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Data acquisition techniques have improved over the years and consequently, the amount of data from bioprocesses has increased. Often this extensive amount of data can be processed and interpreted only through the development of quantitative methods [1]. Thus, the development of tools that can integrate experiments with computational models becomes fundamental, which gives rise to a multidisciplinary field known as systems biology [1, 2, 3]. In this context, developing computational frameworks for simulation, parameter estimation and optimization of bioprocesses is desirable. Ideally, these frameworks should be easy to use by researchers with different backgrounds, and comprehensive to be employed in a variety of different scenarios [4, 5]. Therefore, the structure of such frameworks must be carefully designed by the programmer. In this work, the design of an ontology to describe bioprocesses is proposed based on ontological software engineering, which emphasizes the theorical concepts that can be represented by logical abstraction, and methods and tools that may be required for implementation and usability of the software. An ontology is an explicit specification of a conceptualization, and typically involves classes, their relationships and axioms to describe the intended semantics [5]. It is important that every party involved, from developers to users, reach a common understanding of the abstractions and semantics, since the software is intended to be distributed across multiple locals and researchers. The knowledge represented by the ontology allows for instantiations of bioprocess components, which allows for information to be easy and readily shared since these components are standardized and organized [6]. One of the tools that helps in the design of ontologies is the Unified Modeling Language (UML), which provides the basis for developing software architecture based on Object-Oriented Programming (OOP). OOP facilitates frequent incorporation of new methodologies into the software, and can increase the numbers of possible model configurations, turning it more comprehensive [7, 8]. The development of a bioprocess ontology, along with the resulting architecture of the software, should serve as a model or an example of best practice to guide efforts related to this field.

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ORAL PRESENTATION 20

XGBOOST MODEL OF STEAM REFORMING OF METHANE IN A MEMBRANE REACTOR

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The steam reforming of methane is a widely study process for being one of the main methods to obtain hydrogen. The aim of this research was to implement an artificial intelligence model to simulate this process. The dataset used was generated by a phenomenological model that used natural gas as conversion reagent in a membrane reactor. The simulated data was divided into train, validation and test sets to be used by XGBoost model. The XGBoost model received as input: initial pressure, initial temperature, initial molar flow of carbon dioxide per methane ratio and initial molar flow of hydrogen to predict Methane molar fraction, molar flow of hydrogen on permeate, molar flow of hydrogen, carbon dioxide molar fraction, molar flow of methane, molar flow of carbon dioxide and final pressure. The model obtained an coefficient of correlation above 0,9 for the predict variables. This modeling approach provides an alternative possibility for intelligent control of the steam reforming of methane.

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ORAL PRESENTATION 21

STABLE NMPC WITH ZONE CONTROL AND OPTIMIZING TARGETS

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Nonlinear model predictive control formulations with terminal equality constraints, terminal inequality constraints, terminal contracting constraints and no stabilizing constraints were extended to work with zone control and control move saturations and their performances were compared, with respect to these metrics. These are used in closed-loop system with a quadruple-tank system, and have had their computational effort equalized in order to compare their performances. Three metrics are proposed in this work: distance-to-zone, control effort and economic target distance.

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ORAL PRESENTATION 22

A RECURRENT NEURAL NETWORKS-BASED APPROACH FOR CONTROLLING THE SOLUTE CONCENTRATION OF A CRYSTALLIZATION PROCESS

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This work aims to model a crystallization process to predict the solute concentration with neural networks used as the internal model in the predictive controller. Three different neural networks paradigms were considered: a classic single Multilayer Perceptron (MLP) network, the Echo State Network (ESN), and the Long Short-Term Memory (LSTM). First, the three network structures were trained to predict the solute concentration one step ahead, using the current temperature and concentration values as feed. Then, the network's predictive performance was studied for larger prediction horizons. Finally, a Nonlinear Model Predictive Controller (NMPC) based on the most efficient neural network's design was successfully applied to the batch crystallization process to maintain the solute concentration on its desired trajectories by manipulating the operating temperature. The performance of the proposed NMPC was compared to a controller based on MLP networks.

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ORAL PRESENTATION 23

ESTIMATIVA DA COMPOSIÇÃO ELEMENTAR DO CARVÃO MINERAL DE CANDIOTA–RS POR REDE NEURONAL ARTIFICIAL

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O carvão mineral é uma fonte de energia presente na região Sul do Brasil, principalmente na cidade de Candiota - RS, onde está localizado 38% da reserva nacional. Para o carvão ser usado com a maior eficácia é necessário conhecer suas propriedades, e para isso são realizadas duas análises, a imediata e a elementar. A imediata consegue medir a porcentagem mássica de cinza, massa volátil e carbono fixo, enquanto a elementar mede sua composição elementar, determinando a porcentagem mássica de carbono, hidrogênio, oxigênio, nitrogênio e enxofre. A análise elementar possui um custo muito maior e exige mais tempo em comparação com a análise imediata. Por isso este trabalho propõe um modelo de rede neuronal artificial para a predição da composição elementar a partir da análise imediata, utilizando um conjunto de dados contendo 145 amostras das análises imediata e elementar do carvão de Candiota. O modelo sugerido apresenta coeficientes de determinação (R^2) igual a 0,7 para o carbono, 0,54 para o hidrogênio e 0,6 para o oxigênio. A precisão da rede neuronal artificial foi comparada com a de uma regressão linear e de uma correlação utilizando um polinômio de 3° grau, o modelo proposto neste trabalho teve seus parâmetros estatísticos melhores para todos os elementos.

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ORAL PRESENTATION 24

ADDRESSING MACHINE LEARNING-BASED FAULT DETECTION AND DIAGNOSIS IN SOUR WATER TREATMENT UNITS UNDER PRE-FAULT AND FOULING SCENARIOS

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This work aims to study pre-fault and fouling scenarios in a sour water treatment unit (SWTU) using artificial intelligence. Fault studies can be useful in SWTU, due to operational difficulties when disturbances occur. Pre-fault here is the initial transient after a disturbance or failure, between the normal operation and the controllable region boundary. The fouling effect was applied reducing the 1st column's closest heater's U-value. The benchmark created by [1] with Aspen Plus Dynamics® V10 presents normal operation and 6 faults. In fouling scenarios, linear Support Vector Machines (SVM) presented the best accuracy, 88.45%. Few studies are dedicated to identify the pre-fault region, despite of its operational relevance. Firstly, the samples were split between normal and abnormal behavior (Random Forest - 94.77%). Then, the classification was made in two distinct scenarios: a single pre-fault region (linear SVM - 98.20%) and a pre-fault region for each fault (Gaussian SVM - 95.59%).

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ORAL PRESENTATION 25

APLICAÇÃO DE ANÁLISE WAVELET PARA DETECÇÃO DE INSTABILIDADES FLUIDODINÂMICAS EM UM PROCESSO DE UMEDECIMENTO DE PARTÍCULAS EM LEITO DE JORRO

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O leito de jorro é uma operação unitária utilizada em processos de secagem e recobrimento de partículas, devido especialmente ao movimento cíclico do material, que promove altas taxas de transferência de calor e massa. O objetivo deste trabalho foi empregar a análise wavelet no processamento de sinais de queda de pressão para identificar instabilidades fluidodinâmicas durante a atomização de água em um leito de jorro. Em síntese, verificou-se a robustez e reprodutibilidade das estruturas macro e mesoescalas do sistema de jorro, oriundos da transformada wavelet. Instabilidades fluidodinâmicas, tais como aglomeração das partículas, podem ser detectadas em valores abaixo do limite inferior de controle, em 59,37% para 1,0 kg e 47,97% para 1,5 kg de esferas de vidro.

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ORAL PRESENTATION 26

FORECASTING FIXED-BED COLUMN SOYBEAN OIL EXTRACTION THROUGH ADAPTIVE NEURO-FUZZY INFERENCE SYSTEM (ANFIS)

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The soybean oil extraction in a fixed-bed column was modeled using an adaptive-neuro fuzzy inference system (ANFIS). The overall results obtained a good correlation to the data with R^2 equal to 0.9492, and low values of *SSE*, *SAE*, *MSE*, and *RMSE*. Besides, the non-normality of the residues when using ANFIS was rejected, in contrast to what was found for the phenomenological model.

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ORAL PRESENTATION 27

A MATHEMATICAL MODEL TO SOLVE THE CAPACITATED VEHICLE ROUTING PROBLEM FOR MUNICIPAL SOLID WASTE COLLECTION AND TRANSPORTATION

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Municipal Solid Waste (MSW) management has been presented as a priority in countries that seek sustainable development. In addition, MSW management must be done in a way that is economically and technically feasible, and must comply with the environmental legislation. The collection and transportation of MSW can be modeled as a vehicle routing problem (VRP). Constraints to the VRP can make the model more realistic. This work aimed to present a mathematical model to solve the capacitated VRP with time windows applied to MSW collection and transportation. A mixed integer linear programming model was derived, and it was applied to 26 benchmark problems and solved in GAMS environment. Results showed that the model was able to generate optimal solutions for the proposed datasets, and validated the model to be used as a tool in the development of a MSW management system.

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ORAL PRESENTATION 28

COMPARATIVE ANALYSIS OF MACROSCOPIC MODELLING AND SIMULATION APPROACHES FOR COAL COMBUSTION IN A FLUIDIZED BED

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A comparative analysis was conducted to evaluate two approaches for the macroscopic modeling and simulation of a fluidized bed combustion process in Aspen Plus. Sotudeh-Gharebaagh et al. (7) published one of the first modeling and simulation studies using Aspen Plus software for a fluidized bed combustor (FBC). In this work, the FBC was modeled as a series of ideal continuous stirred-tank reactors (CSTR) and the hydrodynamic and kinetic parameters were calculated with a FORTRAN subroutine. Since until version 8 of Aspen Plus there was no specific unit block for FBC simulation, over the years other authors have followed this same approach (2; 3; 5; 6; 10-13). Using Aspen Plus version 11, Saparov et al. (1) developed a simpler model involving the steps of coal drying, pyrolysis, combustion, and gas-solid separation. The FBC was modeled only with the unit FLUIDIBED available in the software. This unit block includes a variety of semi-empirical correlations for the incorporation of the hydrodynamic parameters of the reactor. However, some of these correlations differ from those applied in FORTRAN subroutines. Thus, in this work, a simulation model was developed based on Saparov et al. (1), using the same approach for the pre and post combustion stages. However, for the FBC modeling, a series of CSTR reactors was applied and the hydrodynamic and combustion kinetics were defined by a FORTRAN subroutine. In this subroutine, the minimum fluidization velocity was calculated using the equation proposed by Kunii and Levenspiel (4), the bubbles volume fraction and the height of the dense bed was calculated based on Babu et al. (8), the voidage of the bed at minimum fluidization was calculated according to Broadhurst and Becker (9), and the freeboard region modeling followed the works of Nikoo and Mahinpey (6) and Pauls, Mahinpey and Mostafavi (5). Preliminary results indicate that the model tends to over-predict the oxygen and carbon consumption rates in the combustion reaction and the solid volume fractions and under-predict the fluidization velocities and the heights of the dense and freeboard regions, in relation to the modeling applied in Saparov et al. (1). Finally, a sensitivity study was performed, including an assessment of NO_x, SO_2, CO and CO_2 emissions and a comparison with experimental data.

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ORAL PRESENTATION 29

MODELAGEM E SIMULAÇÃO DO PROCESSO QUÍMICO DA TENNESSEE EASTMAN UTILIZANDO REDES NEURAIS ARTFICIAIS COM A LINGUAGUEM DE PROGRAMAÇÃO PYTHON

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Vivemos na era da Indústria 4.0 com uma geração imensa de volume de dados, Big Data, devido principalmente à Internet das Coisas, tendo como desafio principal organizar os dados de uma forma que seja capaz de serem interpretados e utilizados. Os processos químicos apresentam uma forte não-linearidade devido aos fenômenos físico-químicos que estão associados, o que justifica o grande uso das Redes Neurais Artificiais (RNAs), tanto para regressão como para classificação. Este trabalho teve como objetivo aplicar uma RNA do tipo *feedforward* em uma expansão de um conjunto de dados bem conhecido na área de monitoramento e controle de processos: o *Tennesse Eastman Process*. Utilizou-se a linguagem de programação *Python* devido a sua grande quantidade de bibliotecas para a área de aprendizado de máquinas, como *pandas*, *numpy*, *matplotlib*, *sklearn* e *keras*. O modelo proposto não conseguiu obter ajustes favoráveis para uma boa predição do processo, embora fosse possível observar uma tendência de comportamento dos dados. Para trabalhos futuros, sugere-se o uso de modelos mais complexos, como uma rede neural recorrente, que leva em consideração a atuação de séries temporais.

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ORAL PRESENTATION 30

DEVELOPMENT AND IMPLEMENTATION OF A LINKAGE BETWEEN MODEL PREDICTIVE CONTROL AND REINFORCEMENT LEARNING

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Reinforcement learning (RL) is an area of machine learning (ML), in which an agent learns a specific task through direct interaction with its environment with the objective of maximizing the expected cumulative reward. Based on the algorithm, an RL agent learns from the consequences of its actions, rather than being explicitly taught. In the field of chemical engineering, the initial motivation is connected with the limitations associated with model-based predictive control (MPC) techniques, in the case of nonlinear processes. Among these limitations are the fact that rigorous models are complicated and time-consuming to obtain; and even when they are available, the computational cost for computing the control actions is very high. On the other hand, RL-based algorithms constitute an adaptive control technique that can be either "learned" offline through simulations, or online through the direct interaction of the controller with the process. When the policy and the value function are approximated by deep neural networks, they enter the set of deep reinforcement learning (DRL). The main objective of this work is to assess the performance of a DRL based agent for the control of the Van de Vusse Reactor when the reward function is derived from MPC. The results show that the proposed strategy is effective in controlling that environment, considering a previous tuning of the coefficients of the reward function.

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ORAL PRESENTATION 31

COMPARAÇÃO DA PRODUÇÃO DE DIMETIL ÉTER VIA REAÇÃO DIRETA ATRAVÉS DE DOIS SIMULADORES DE PROCESSOS

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Por conta de suas propriedades químicas, o dimetil éter é um composto com alto potencial para ser utilizado como combustível. Sua produção se dá através da desidratação do metanol que pode ser obtido pelo gás de síntese através da sua reforma. Neste estudo, sugere-se a produção do metanol via gás de síntese modelada por dois programas de simulação de processos diferentes: DWSIM e UniSim Design. O resultado foi de acordo com o esperado pela literatura para os dois programas, obtendo-se uma pureza na composição final da corrente de DME superior a 98,5%.

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ORAL PRESENTATION 32

FLOW ASSURANCE IN OFFSHORE PIPELINES: KINETIC AND THERMODYNAMIC ASPECTS OF HYDRATE FORMATION AND DISSOCIATION IN OIL-DOMINATED SYSTEMS.

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Hydrates are the central issue in flow assurance because these solids can be formed and block a pipe in a shorter time frame than wax or asphaltene deposits. Computational simulations combine the expertise of flow modeling and fluid characterization to develop strategies to ensure optimal production rate and surveillance during operations. This work aims to create a tool that performs simulations for flow assurance purposes, including hydrate prediction of multi-component hydrates in oil-dominated systems without inhibitors. The Drift-Flux model set as a differential-algebraic system performs steady-state multiphase flow simulation in consonance with well-known, standard commercial simulator, such as *OLGA*®. In addition, we included an algorithm for simultaneous fluid characterization and prediction of hydrate conditions formation available in the literature. In the partial results, the obtained hydrate formation curve agrees with *Multiflash*®, which allows this research to determine other hydrate properties and include kinetics of hydrate formation simulations.

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ORAL PRESENTATION 33

EMPREGO DE REDES NEURAIS RECORRENTES PARA PREDIÇÃO DA DINÂMICA DE REMOÇÃO DE TURBIDEZ EM UM PROTÓTIPO DE FLOTAÇÃO POR AR DISSOLVIDO

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O tratamento de água para abastecimento público é um processo que envolve várias etapas distintas. Dentre elas, a fase de clarificação objetiva remover a turbidez presente na água bruta e pode ser realizada pelo processo de flotação por ar dissolvido (FAD). Entretanto, representar os fenômenos que ocorrem na FAD por meio de equações matemáticas é complexo, o que dificulta seu estudo e a busca por melhorias. Assim, este trabalho avaliou o emprego da modelagem empírica, utilizando redes neurais recorrentes (RNN), para descrever a dinâmica de remoção de turbidez de um protótipo de FAD. Modelos neurais recorrentes foram treinados a partir de um banco de dados experimentais da dinâmica do processo. A melhor RNN obtida possui uma camada oculta composta por 5 neurônios e 3 entradas atrasadas em intervalos de 25 s, apresentando erro médio quadrático de 0,027 NTU^2 na etapa de teste, indicando o bom ajuste do modelo e validando a eficiência da metodologia empregada.

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ORAL PRESENTATION 34

MODELLING AND PARAMETER ESTIMATION OF METHYL METHACRYLATE DISPERSION POLYMERISATION IN SUPERCRITICAL CARBON DIOXIDE

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This work addresses the modelling and parameter estimation of the dispersion polymerisation of methyl methacrylate in supercritical carbon dioxide ($scCO_2$). A combined correlation for the gel and glass effects, proposed as a single empirical model, had its parameters successfully estimated based on a sequential optimisation numerical procedure with help of a particle swarm optimiser. The proposed two-phase polymerisation model proved to be reliable in describing monomer distribution between $scCO_2$ continuous and polymer-rich phases throughout the reaction, showing a good agreement with the experimental conversion data. Based on the polymerisation model performance, important nonlinear polymerisation behaviour for instance auto-acceleration related to strong mass-transfer limitations can be properly evaluated to give important insight into the polymerisation process.

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ORAL PRESENTATION 35

A NUMERICAL AND EXPERIMENTAL INVESTIGATION OF A FIXED BED CO2 ADSORPTION PROCESS USING PHASE CHANGE MATERIAL

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Carbon Capture and Storage (CCS) has been studied over the past two decades and technologies developed to tackle the challenge of reliably capturing carbon dioxide at industrial scale. In order to reduce the energy required by adsorption and to increase the specific adsorption capacity, measures have been proposed to counteract the undesired exothermic behavior of adsorption processes, such as U-tubes inserted on the adsorption bed and phase change materials (PCM). The latter offers great potential for latent heat storage systems with materials capable of storing substantial amounts of energy. This work is aimed at analyzing the behavior of a fixed bed CO2 adsorption system with PCM and provide a comprehensive interpretation to explain the phenomenon. The bed is filled with activated carbon as adsorbent and paraffin wax as phase change material. The dynamic model of Schumman was modified and combined with fundamental equations of the adsorption phenomenon. The results obtained from the numerical solution were used to analyze the thermal performance of the charging mode of the adsorption process and the model was validated with experimental data. The studies revealed that the use of PCM increases the theoretical CO2 adsorption capacity, due to the reduction of the maximum temperature of the process. To be the most effective, the PCM requires a design in which the heat transfer zone of the phase change material aligns with the adsorption breakthrough curve.

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ORAL PRESENTATION 36

REDE NEURONAL ARTIFICIAL PARA MODELAGEM E OTIMIZAÇÃO DA SÍNTESE DE ACETATO DE ISOPROPILA CATALISADA POR ÓXIDO DE NIÓBIO

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Desenvolveu-se um modelo de rede neuronal artificial (RNA) para prever e otimizar a síntese de acetato de isopropila catalisada por óxido de nióbio, correlacionando a conversão de ácido acético em acetato de isopropila (variável de saída) com temperatura, razão molar de ácido acético para isopropanol, massa de catalisador e tempo de reação (variáveis de entrada). A arquitetura ótima da RNA é [15 10] com retropropagação de regularização Bayesiana como função de treinamento da rede para otimizar os valores de peso e bias. Os resultados mostraram que a rede neuronal artificial pode prever com precisão a conversão de ácido acético em acetato de isopropila, apresentando $R2$ e SSE de 0,9999 e 0,0182, respectivamente.

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ORAL PRESENTATION 37

ANALYSIS OF THE INTERFACIAL FORCE EFFECT ON SIMULATED OXYGEN TRANSFER OF A BUBBLE COLUMN BIOREACTOR USING COMPUTATIONAL FLUID DYNAMICS

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Pneumatic bioreactors are a class of reactors increasingly used in bioprocesses, since they provide adequate heat and mass transfer, rapid mixing and good suspension of solids. In this work, oxygen transfer from a square-cross section bubble column bioreactor was evaluated experimentally and numerically using computational fluid dynamics (CFD), and the results were compared with data obtained experimentally. Different specific air flow rates (1.0, 3.0 and 5.0 vvm) and drag and lift interfacial forces, were considered in the numerical simulations using the two-fluid Eulerian model. The simulations considering the presence of lift force showed results closer to the experimental data, with the highest values of kLa found for the higher specific air flow rate (5 vvm) analyzed in this study.

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ORAL PRESENTATION 38

NLP REFORMULATION OF A SYSTEM OF DIFFERENTIAL ALGEBRAIC EQUATIONS WITH EMBEDDED OPTIMIZATION

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Differential-algebraic equations with embedded optimization (DAEO) are a widely applied class of models. They appear on separation process simulations assuming chemical equilibrium, organic aerosol particle modeling, and dynamic models of cellular metabolism (Ploch et al., 2020). The solution of these models can be tricky, especially on the interaction between optimization and DAE solvers. Furthermore, when DAEO is included on an outer optimization problem (e.g., inside an MPC) the solution can be even harder, particularly for non-smooth models. Here, we propose Nonlinear programming (NLP) reformulation of DAEO models that can be easily integrated into an outer optimization problem. The inner optimization problem was replaced by the first-optimality conditions (i.e., KKT conditions), and the DAE system was discretized using the orthogonal collocation technique. The complementary constraints (CC) originated from the KKT conditions were solved using the penalization method, where the CC is inserted in the objective function as a penalty parameter (Baumrucker et al. 2008). In order to deal with active set constraints changes, constraints on the optimization variables were imposed, and an adaptive mesh scheme was also applied. We implemented the method on Julia language and solved in JuMP using the automatic differentiation package. The method was applied to study cases of Dynamic Flux Balance analysis models (dFBA). We solved problems of parameter estimation, dynamic control of metabolism, and bioreactor dynamic optimization using dFBA models. The method was compared with state-of-the-art software (Gomez et al., 2014) and showed a better performance in solving bi-level optimization problems.

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ORAL PRESENTATION 39

COMPARISON OF MULTISTEP METHANOL PRODUCTION PROCESSES FROM BIOGAS USING ASPEN HYSYS

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Global warming and the growing energy demand have created the necessity of developing alternate fuels and sustainable and clean production routes. Within the approaches to solve this issue, the commonly named methanol economy stands out, since methanol, as fuel, has advantages that go from the facility to storage and transport to its properties as an alternate fuel. However, the traditional process to produce it from natural gas (steam reforming) depends on large energy expenditure and capital cost. It also emits more carbon dioxide, contributing to global warming. In this context, the present work simulated three different routes to produce methanol using Aspen Hysys v.8.8. Moreover, economic evaluation and energy analysis were also done. The results indicate the alternative route to produce methanol, from biogas, using carbon dioxide (dry reforming), is more advantageous both to the environment and to the investor as it demands less energy, produces more methanol and costs less to install and operate.

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ORAL PRESENTATION 40

DYNAMIC FLUX BALANCE ANALYSIS APPROACH FOR THE OPTIMIZATION OF BIOPROCESSES

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The bioprocess industry has been steadily increasing due to concerns with environmental impacts and the search for sustainable processes (IOANNIDOU et al., 2020). However, economic viability can still be a bottleneck (MCADAM et al., 2020). In order to make bioprocesses more competitive with the oil industry, metabolic engineering strategies are often employed (ZHUANG et al., 2013). Metabolic engineering frequently makes use of available metabolic models and mathematical approaches such as Flux Balance Analysis (FBA) to acquire phenotypical insight of microorganisms and to assist with strain design by identifying genetic modifications that would improve the yield of desired metabolites (ZHUANG et al., 2013). But while increasing product yield can be beneficial, other process parameters such as product titer and productivity need to be considered. In the case of growth associated products or intracellular metabolites, a trade-off between product yield and biomass formation can occur, and that in turn can negatively affect parameters like titer and productivity, and ultimately, the profitability of the process (ZHUANG et al., 2013). This work therefore presents a DFBA approach for identification and pre-evaluation of the production potential for products of industrial interest through a biological route. Using the bioplastic polyhydroxyalcanoate (PHB) production by *C. necator* H16 as a case study, the proposed approach estimated the monthly gross profit for each simulation performed and identified the break-even point and the theoretical maximum PHB production potential, together with the set of yield, titer, and productivity in a batch culture that would lead to them.

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ORAL PRESENTATION 41

SYNTHESIS OF HIGHER ALCOHOLS FROM AN ETHANOL SOURCE ON A PFR

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Chemical processes may be sometimes harmful to the environment, leading to alternative methods to reduce environmental damage but keeping the availability of the chemical products. Higher alcohols have important uses in the industry, such as solvent, paintings, plasticizer and fuel. As an example, n-butanol is a higher alcohol produced usually by the Oxo Process, which is harmful to the environment once it requires large amounts of energy. This work investigates a route to produce n-butanol, n-hexanol and n-octanol, using na environmentally-friendly process. The process consists of an input of ethanol mixed with an inert in a Plug Flow Reactor - PFR and an output of higher alcohols and other subproducts. Initially the process was simulated on a PFR to validate the model using data from the literature. Then a recycle was implemented in order to increase ethanol's conversion and evaluate n-butanol, n-hexanol and n-octanol's yields.

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ORAL PRESENTATION 42

APPLICATION OF A PREDICTIVE Q-LEARNING ALGORITHM IN A SUGARCANE ETHANOL BIOREFINERY MULTIPLE-EFFECT EVAPORATOR

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With the recent development of machine learning, reinforced learning is an interesting alternative to PID controllers. In this context, a discrete predictive Q-learning approach is applied in the control of a sugarcane biorefinery multiple-effect evaporation system. The algorithm is built using Scilab and learns to control the multiple-effect evaporator outlet concentration by manipulating its feed steam flow rate. Based on multiple episodes, the state-actions that consist of discrete changes on steam flowrate are chosen with a greedy algorithm. The control policy was built and tested through simulations on a phenomenological model. The controller performance was evaluated in set-point tracking and disturbance rejection tests and compared with PID responses. The research showed that the Q-learning controller exhibited better performance than the PID controller.

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RESUMOS
ABSTRACTS

POSTER PRESENTATIONS
APRESENTAÇÕES EM FORMATO POSTER

POSTER 1

SIMULAÇÃO DO EQUÍLIBRIO DE FASES E CINÉTICA NA TRANSESTERIFICAÇÃO DE ÓLEO DE SOJA E METANOL

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O biodiesel é um combustível oriundo de fontes renováveis, com caráter menos poluente do que o diesel. Em escala comercial esse biocombustível é obtido a partir da reação de transesterificação entre um óleo ou gordura e um álcool de cadeia curta. Contudo, a baixa miscibilidade que se tem entre a matéria-prima graxa e os alcóois é uma limitação na reação de transesterificação. Assim, o objetivo principal desse trabalho é o de estudar o equilíbrio de fases durante a reação de transesterificação de metanol e óleo de soja. Para isso, o equilíbrio de fases nesse sistema foi avaliado em Aspen Plus, utilizando interface criada com o Matlab. Para o estudo da cinética da reação, tomou-se um modelo da literatura, no qual se levou em conta a presença de mono e diglicerídeos, em reações elementares e de segunda ordem, supondo-se operação num reator batelada e de mistura perfeita. O sistema de equações diferenciais ordinárias que descreve o sistema foi resolvido em Matlab, usando-se o método explícito de Euler. Os resultados mostraram que a conversão da reação de transesterificação é positivamente impactada pelo excesso de metanol, que acaba aumentando a velocidade de reação. Para 5 minutos de reação e com uma proporção molar de metanol e óleo de soja de 6:1, chegou-se num grau de conversão de 42%. A análise do equilíbrio de fases mostrou que há a formação de duas fases, sendo uma leve e outra pesada. O metanol se distribuiu nessas duas fases, mas o óleo de soja se mostrou praticamente insolúvel na pesada e os ésteres metílicos formados se concentraram na fase leve.

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POSTER 2

MODELING THE OXIDATIVE COUPLING OF METHANE PROCESS VIA MACHINE LEARNING

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The application of machine learning (ML) models in the oxidative coupling of methane (OCM) process is presented in the current research. In this research, the database was generated by a deterministic model. The random forest models receive as input CH4 feed molar fraction, CH4/O2 feed molar ratio, temperature, pressure, and STP gas volume flow rate to predict the yield, conversion and selectivities of the reaction. The best regression ML model showed a response of 0.999 for coefficient of determination (R2). The random forest model proved to be efficient and powerful and due to the low required computation times and its simplicity, it can be a competitive advantage tool for control and monitoring at industrial facilities.

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POSTER 3

OPTIMIZATION OF REACTIVE DISTILLATION FOR PRODUCING ETHYL LACTATE AND ITS OLIGOMERS USING MATLAB LINKED WITH ASPEN PLUS

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Reactive distillation is an example of process intensification, combining reaction and separation systems and which can be applied to different chemical processes, such as solvent production. Ethyl lactate is a biodegradable and non-toxic solvent, appealing to replace petroleum-based solvents. However, most of the studies with ethyl lactate did not tackle the formation of oligomers in the reaction kinetics. With this in mind, this work carried out an optimization study in a black-box framework, having as a constraint the purity of ethyl lactate in the bottom product and as decision variables the number of stages, the number of reactive stages, the reflux ratio, and the feed stages of lactic acid and ethanol in order to minimize reboiler duty. The process was simulated using Aspen Plus and MATLAB was used via ActiveX link for optimizing reboiler duty and ensuring high purity ethyl lactate is obtained. A bottom product with 99.1% molar of ethyl lactate was obtained.

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POSTER 4

MODELAGEM HÍBRIDA BASEADA EM REDES NEURAIS FISICAMENTE INFORMADAS (PINN) APLICADA A SISTEMAS DE ELEVAÇÃO ARTIFICIAL DE PETR´OLEO POR BOMBEAMENTO ELÉTRICO SUBMERSÍVEL (BCS)

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Electric Submersible Pump (ESP) is installed in many oil wells around the world to perform artificial lift. The literature has many methods to develop mathematical models for process monitoring, control, diagnosis, optimization, and design. The power of computational resources available by recent digitization makes possible collect and process large volume of data for knowledge extraction using machine learning frameworks. Since fenomenological-based solutions can not be discarded, this paper proposes a hybrid modeling of ESP-lifted well system through machine learning strategy called physically informed neural networks (PINN). Unlike conventional PINN, this proposal implements na architecture with arbitrary exogenous inputs using a LSTM-based recurrent neural network. This model does not use independent variables time or space as inputs, so residues are computed using numeric differentiation. After model training, it computes predictions as good as traditional approachs and estimates model parameters accurately. A case study is used to illustrate the benefits of the proposed strategy.

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POSTER 5

SIMULAÇÃO DE CONVECÇÃO NATURAL EM CAVIDADE CÚBICA CONTENDO MEIO POROSO HETEROGÊNEO: EFEITO DA RAZÃO DE CONDUTIVIDADE K*

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Neste estudo um modelo tridimensional foi empregado para investigar numericamente a convecção natural em uma cavidade cúbica contendo meio poroso heterogêneo formado pela deposição de partículas esféricas aleatoriamente distribuídas em seu interior. As condições e contorno são definidas de modo que duas paredes verticais opostas são mantidas a diferentes temperaturas constantes, enquanto todas as outas são consideradas adiabáticas. Foram avaliados diferentes valores para a razão de condutividade térmica K^* para Rayleigh variando de 10^3 a 10^5. Os resultados mostram uma influência significativa de K^* no número de Nusselt médio e no fluxo de escoamento do fluido nas regiões centrais da cavidade.

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POSTER 6

PREDICTING ASPECT RATIO OF MICRO/NANOCELLULOSE FIBERS USING MACHINE LEARNING TECHNIQUES

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Biopolymers are the key materials for a sustainable future and cellulose derivatives play an important role in this scenario. Cellulose nanocrystals (CNC) and cellulose nanofibers (CNF) have received special attention due to their biodegradability, biocompatibility and good mechanical and barrier properties, which give rise to a wide range of applications [1]. Regarding CNFs, a pre-treatment step followed by a fibrillation process, usually by mechanical means, are required for their production. The operational conditions used in both processes and the characteristics of the pulp used as raw material have great influence on the properties of the resulting CNFs. However, the complexity of the relationships between these features makes the mathematical modeling of the fibrillation process/product a quite difficult task. Therefore, the use of Machine Learning (ML) modeling techniques represents an interesting alternative which is still little explored in the nanocellulose field. ML techniques applied to the prediction of CNFs properties might indeed expand the range of applications of this class of material worldwide. In the current work, spruce and pine softwood pulps subjected to different fiber treatment processes and fibrillation intensities in a highpressure homogenizer generated 20 different samples of cellulose micro/nanofibers (CMNFs), according to [2]. These samples were used for training and testing different ML algorithms, such as Linear Regression (LR) and Random Forests (RF), for prediction of the CMNFs' aspect ratio, an important morphological property. The performance of the models was evaluated by Mean Absolute Percentage Error (MAPE) and R^2. Although one of the problems regarding the application of ML techniques in material science is the lack of extensive data sets to produce robust models [3], the model provided here was able to achieve very good results with 20 datapoints. RF model achieved a MAPE of 8.18% and an R^2 of 0.9313, with a 17-estimator forest and employing only four easily obtainable inputs regarding the chemical composition of the pretreated fibers: Total lignin (wt.%), Cellulose (wt.%), Hemicellulose (wt.%) and Extractives (wt.%). LR model consisted in a linear function using as input features all the mentioned above plus the energy in kWh/kg required for the fibrillation step. The performance achieved with it was a MAPE of 9.07% and an R^2 of 0.9508. It's possible to observe that both algorithms delivered very good predictions. While LR model ensued better correlation between experimental versus predicted values, RF provided lower percentual error and was able to indicate aspect ratio trends better than LR. Nevertheless, one can conclude that both RF and LR show great potential as ML models for prediction of aspect ratio, using low-cost operation variables as inputs. Further ML studies will be conducted considering the continuous insertion of new data combined with exploring other models, in order to improve the prediction performance and generalization capacity.

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POSTER 7

ANALYSIS OF BIOGAS REFORMING PROCESS TO SYNGAS VIA DRY REFORMING AND BI REFORMING

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Considering the liquid bio-fuels production, it is well known that biogas is one of the most requested feedstocks. Not only due to its high heat capacity, but because it shows flexibility, in its ability to produce clean energy, biomethane, biofertilizer, and liquid hydrocarbons. For the latter process, biogas needs to be converted into syngas before going through multiple reactions to reach the desired product. This initial process is Catalytic Reforming, and it can follow six different routes. In the present work, all the possible methods to convert biogas into syngas were theoretically analyzed: Dry Reforming, Steam Reforming, Partial Oxidation, Bi Reforming, Tri Reforming, and Autothermal Reforming. For the next step of the process, Dry Reforming (DR) and Bi Reforming (BR) were selected for the Fischer-Tropsch synthesis and simulated in Aspen Plus V12.1® while varying different reaction parameters. Aspen Plus® requires a thermodynamic analysis, and therefore, for this system, the Peng-Robinson equation of state was chosen. The chemical reactions for both reforming processes were modeled using RGibbs reactor block. Its objective is to minimize the Gibbs free energy of the system. Also, three properties were selected to perform the entire evaluation of the system: CH4 conversion, CO2 conversion and H2/CO ratio. The first analysis executed was the pressure effect in both reforming processes. The feedstock composition of the DR was set to 3:2, methane and CO2 respectively, and flow rates of 600 kmol/h of CH4 and 400 kmol/h of CO2. For BR, the composition was set 3:2:2 for methane, CO2 and water respectively. In addition, to analyze the effect of pressure, the values were varied over a range of temperatures using the Sensitivity Tool. Data was obtained on conversion and H2/CO ratio. Then, the composition of CH4 and CO2 was varied while the pressure was kept constant at 0,1 MPa. For Bi Reforming, the H2O composition was also varied. For all cases, an increase in both CH4 and CO2 conversion was observed when temperature was increased regardless of the variable. It was observed that an increase in pressure resulted in a shift in equilibrium to favor the reactant side which in turn lead to a decrease in the conversions. However, a change in feedstock composition showed no significant impact on conversion. This was most apparent for the Dry Reforming. Furthermore, a decrease in the molar fraction of water contributed to a higher CO2 conversion while no significant change was observed for CH4. Analyzing the H2/CO ratio, it was noticed that an increase in temperature resulted in a reduction of the ratio for both reforming processes. However, due the presence of water in the system, the ratio is higher in Bi Reforming. All simulations performed for both processes showed promising results for conversion of biogas into syngas. The Bi Reforming process with a molar ratio of CH4, CO2, and H2O to 3:2:1 respectively, temperature of 850 °C, and pressure of 0,1 MPa showed the most promising combination of results for the Fischer-Tropsch synthesis. The CH4 conversion, CO2 conversion and H2/CO ratio obtained were, respectively, 94,11%, 96,45%, and 1,376.

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POSTER 8

OPTIMIZING CO_2 EMISSIONS FOR A BIOGAS-TO-METHANOL PROCESS PLANT

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Methanol is an important product in chemical industries, having many applications: solvent, fuel and mainly being a feedstock for a large number of industrial processes. In this work a design of a methanol synthesis plant using biogas as feedstock, considering different plant configurations, was proposed. In order to account for the overall CO2 emissions, the main process plant and the utility plant were modeled and simulated. A multi-objective optimization was performed to obtain the optimal trade-off between the economic performance and the overall CO2 emissions. The results show that the optimized design can be economic profitable and also reduce up to 9% of the CO2 emission of the process.

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POSTER 9

LEARNING FROM SUB-OPTIMAL DEMONSTRATIONS WITH DDPG ALGORITHM AND OFF-POLICY DISCRIMINATOR: AN OPTIMAL CONTROL PROBLEM

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A new reinforcement learning algorithm augmented by an off-policy discriminator was proposed. It allows learning from sub-optimal demonstrations. Considering the problem of optimal process control, an approach that uses information from policies already established in the process line or from operators could be essential to obtain new control policies with implicit information about process constraints and control objectives. For a simplified example of a batch process, the obtained results proved viable since they met the optimization objective through sub-optimal demonstrations originated from an expert.

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POSTER 10

MULTI-LAYER HEALTH-AWARE OPERATION AND CONTROL OF SUBSEA OIL LIFT SYSTEMS SYSTEMS

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One of the major priorities concerning subsea operations for oil processing is the reliability of the process. Since subsea equipment is hardly accessible and operations occur in hard conditions, it is necessary to predict breakdowns and failures in order to ensure that equipment health will be preserved until the next planned maintenance. Health-aware control (HAC) frameworks are strategies designed to include both health and operational constraints in the control objectives, adding the concern with unpredicted failures to the typical operational economic and environmental losses. The hardly reachable subsea environment leads to the need for developing optimization strategies under parameter uncertainty. Electric Submersible Pumps (ESPs) are widely employed in deep water wells due to their high efficiency and reliability. However, high consumption power and expensive maintenance costs can be a disadvantage, which justifies the need for developing efficient prognostics frameworks. In this context, the present works aims to develop a two-level control and optimization approach for dealing with uncertainties in a subsea artificial lift system equipped with ESPs. The main purpose of developing a two-level approach based is to reduce computational effort and reach a less conservative yet robust solution. The lower layer for a single oil lift was developed and results showed that power consumption and ESP inlet pressure are critical variables for health management. The remaining useful life (RUL) for the equipment will be estimated in the upper layer, and the developed framework will be applied to a multiple wells system. It is expected that it will be able to distribute the control effort between the system actuators, optimizing production and avoiding the system breakdown before a specified maintenance time.

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POSTER 11

OPTIMIZATION OF A MICRO-PHOTOCATALYTIC REATOR USING A CFD-ANN-GA HYBRID METHOD

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To accurately predict the complex nonlinear relationship between operational parameters in a micro-photoreactor, a hybrid method based on the combination of CFD simulation, artificial neural networks (ANN), and genetic algorithm (GA) was proposed. This approach was applied to a model reaction of photocatalytic NOx abatement, which was previously studied by our research group. Process parameters such as residence time (τ), light intensity (E), relative humidity (RH), and initial NO concentration (C^{in}_{NO}) were used as inputs for the ANN, and they were also applied to find the optimal process conditions. The artificial neural network was trained and tested by the CFD dataset. Two distinct ANN architectures were presented considering multiple inputs and a single output (MISO) and for multiple inputs and multiple outputs (MIMO). The MISO system objective was to maximize the NO conversion. However, additional studies were carried out with the MIMO system to maximize the NO consumption rate and minimize the pressure drop, characterizing a multi-objective problem. The best structure was chosen based on the MSE, RMSE, and R2 performance factors. The results showed that the CFD-ANN-GA hybrid method offers a powerful approach to model and predict the micro-photoreactor performance from the operational parameters. The MATLAB 2013a software (Math-Works Inc, USA) was used for the development of the neural network architecture and the optimization of the operational parameters by a genetic algorithm. The ideal ANN model consisted of a feed-forward backpropagation structure with three layers and 11 neurons in the hidden layer (4:11:1), logsig-logsig transfer function, and Levenberg-Marquardt (LM) as a training algorithm. The model showed high predictability, considering the value of the correlation coeficient obtained (R2 = 0.9997, MSE = 4.75 ´ 10-5, RMSE = 6.90 ´ 10-3), and was used for the optimization by GA to determine the optimal process conditions. Furthermore, the relative importance (RI) of the operational variables in the process was investigated. The residence time had a greater effect on the prediction of NO conversion with RI = 48.97%, followed by light intensity (RI = 28.17%), relative humidity (RI = 19.34%), and initial NO concentration (RI = 3.52%). Finally, the MIMO system was applied, and the ANN was modified, considering the NO consumption rate and the pressure drop as output variables. All ANN settings were kept constant, except the number of neurons in the hidden layer, which in the MIMO system was equal to 17. ANN's ideal model with the MIMO system was used as a multi-purpose function for GA. The result can be observed by the Pareto front plot, where the trade-offs of the objectives were captured, identifying promising solutions from the population. Four points were highlighted in the Pareto front plot: (1) minimal pressure drop, (4) maximum NO consumption rate, and (2 and 3) transition points. Thus, a set of operating conditions was identified as optimal in this new scenario, characterized by point (3) (τ = 0.47 s, E = 3.36 W.m^{-2}, RH = 67.8% and C^{in}_{NO} = 2.19 ´ 10-8 kmol.m^{-3}). This point was chosen because path (2) $\rightarrow$ (3) presented the highest increase in NO consumption and the smallest increase in pressure drop, considering an optimal condition of the process. Therefore, the hybrid CFD-ANN-GA method proved to be a suitable technique to model reactive systems and could be applied in the future to predict and optimize microreactors with different geometric configurations and operating conditions

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POSTER 12

KINETIC MODELLING CONSIDERING PHASE EQUILIBRIA THE NON-ISOTHERMAL ESTERIFICATION REACTION FOR THE DI(2-ETHYLHEXYL) TEREPHTHALATE PRODUCTION

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The di(2-ethylhexyl) terephthalate (DEHT) is an important plasticizer. DEHT can be produced by the esterification of terephthalic acid (TA) with 2-ethyl-1-hexanol (2EH), where solid TA particles react with the liquid 2EH in a heterogeneous medium. In this work, the esterification to produce DEHT catalyzed by the titanium tetraisopropoxide (TTIP) was studied in a batch reactor at non-isothermal reflux temperature and atmospheric pressure. Finally, a kinetic model was proposed considering theses physical and chemical phenomena: the catalyst deactivation influence by TTIP hydrolysis, the non-isothermal temperature due bubble point of the reactional mixture, the reaction solid-liquid equilibrium and the mass transfer rate. The model presented a good agreement with the experimental data.

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POSTER 13

MODELLING CONSIDERING COMPOUNDS' VOLATILIZATION INFLUENCE FOR TRANSESTERIFICATION REACTIONS FROM FFA AND METHYL ACETATE AT HIGH TEMPERATURE AND PRESSURE

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It has been proposed a model considering the compounds' volatilization influence in simultaneous non-ideal phase equilibrium, reaction kinetics, and chemical equilibrium for batch transesterification reactions from free fatty acids at high pressure and temperature. The kinetic and thermodynamic parameters were estimated from reaction data of oleic acid with methyl acetate catalyzed by niobium phosphate. Kinetic data at conditions of the liquid-vapor system were measured/obtained by varying temperature, molar ratio, and initial reaction volume. The hypothesis of volatilization influence was evaluated and proved to be very relevant to ensure the model fitting, which its use proved necessary mainly for experiments with different initial ratios of reaction volume/headspace or scale-up process. For the applied transesterification system, the proposed model with volatilization influence proved to fit pressure and concentration data very well.

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POSTER 14

AVALIAÇÃO DA SELETIVIDADE DE MECANISMOS DE HIDROTRATAMENTO PARA OBTENÇÃO DE HVO POR MEIO DE SIMULAÇÃO DE MODELOS CINÉTICOS

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O HVO, biocombustível avançado, possui um papel essencial na transição energética sustentável para a expansão dessa tendência para o setor de transportes no mundo, o qual é responsável por grandes impactos do aquecimento global. Nesse contexto, utilizou-se da simulação de dois modelos cinéticos, com propostas diferentes de estudo, para a avaliação dos efeitos na seletividade dos mecanismos de conversão de hidrocarbonetos parafínicos. Observou-se que o mecanismo de desoxigenação, desejado nos processos industriais de obtenção do biocombustível, é diretamente favorecido pelo aumento de temperatura do meio reacional e pela pressão do meio, atrelado à carga de hidrogênio. Dessa forma, observa-se uma região de interesse de operação onde se obtém elevada conversão do composto desejado com o balanceamento dos custos envolvidos aos parâmetros avaliados.

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POSTER 15

SIMULAÇÃO DA GASEIFICAÇÃO DE BIOMASSA POR MODELO DE EQUILÍBRIO

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O estudo teve como objetivo aplicar um modelo de equilíbrio para estimar a composição do syngas obtido com a gaseificação de biomassas. Utilizou-se dados da literatura para a entrada no modelo, e os resultados foram comparados com os resultados experimentais. Os casos estudados partiram de temperaturas de gaseificação baixas (700-900°C) para a palha de milho, até temperaturas mais altas (1000-1400°C) para a casca de arroz e serragem de madeira. Os resultados mais significativos foram obtidos em temperaturas acima de 1000 °C, pois o modelo melhor adequou-se em valores de composição gasosa com relação aos resultados experimentais relacionados. Percebeu-se que a melhor estimativa foi para a espécie CO da casca de arroz, com uma ótima aproximação. Observou-se que o modelo de equilíbrio superestimou valores de CO e H2, e subestimou os valores de CO2 e CH4, justificando as discrepâncias observadas por meio de possíveis reações gás-água e de reforma envolvidas no equilíbrio químico. É possível concluir que o modelo de equilíbrio é mais adequado a temperaturas acima de 1000 °C, por considerar condições que favorecem o estado de equilíbrio químico nessa conjuntura.

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POSTER 16

DEVELOPMENT OF VAPOR COMPRESSION SYSTEM DYNAMIC MODELS FOR CONTROL AND SIMULATION PURPOSES USING MOVING BOUNDARY APPROACH

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The development of nonlinear dynamic models for Vapor Compression System (VCS) is important for analysis and optimization purposes and to obtain linear models from linearization or identification that can be used for control purposes. However, the nonlinear nature of VCS process poses a challenge in the control since most controllers are based on linear models. Therefore, this work had two main purposes. Fist, nonlinear transient models of VCS were developed using the moving boundary (MB). Second, transfer function models were obtained from a step test in the manipulated variables in two different operating points: low charge (2 °C of cooling) and high charge (10 °C of cooling). The results showed that the transient behavior and the steady state gains change significantly when the system is operated in different regions indicating that a conventional control technique may not work well in the entire operating range.

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POSTER 17

ASSESSMENT OF CO_2 HYDROGENATION TO FORMIC ACID USING TERNARY AMINE AND DIOL SOLVENTS

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The CO_2 hydrogenation to higher added-value products, such as formic acid (FA), is a promising approach to reduce CO_2 emissions by a profitable path. This reaction can be performed through ternary amines and diol solvents. Despite promising, this process requires a complex thermodynamic representation due to a triphasic reacting system containing an ionic species. Suitable property predictive methods were assessed, and different sized amines were evaluated. High temperatures and low pressures increase the first reaction conversion but decrease the second reaction one. Ternary sized from tri-ethylamine to tri-hexylamine presented the most equilibrated conversions; the first was the most promising one.

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POSTER 18

TREE-BASED MACHINE LEARNING MODELS FOR OCM PROCESS: A CORRELATION STUDY OF HARD-TO-PREDICT PROCESS VARIABLES

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Oxidative coupling of methane (OCM) is a promising route to directly convert methane from natural gas resources to C2 compounds (C2H4 and C2H6) via heterogeneous reaction between methane and oxygen under steady-state catalysis conditions [1,2]. It is an economical and more sustainable route than the thermal cracking of the naphtha process, the most common chemical route to produce these C2 compounds [3]. However, the OCM process still exhibits selectivity and yield of ethylene and ethane lower than expected for commercial purposes (< 30 %) [2]. In that sense, it is useful to analyze and identify the process operating conditions regarding efficiency and control purposes. Still, low correlated variables are usually harder to be studied and predicted. In this paper, the tree-based machine learning supervised regression algorithms Random Forest, XGBoost, CatBoost, and LightGBM have been developed to recognize the relationship of the input-output variables, in particular the low-correlated and hard-to-predict variables. Performance assessment considered distance-based error and correlation metrics. The methodology was implemented in Python language. The kinetic model of the OCM on La2CO3/CaO catalyst proposed by Stansch et al. [4] was used to build a phenomenological model for data generation. In this case, it was implemented an inverse-design machine learning modeling approach, wherein the required process experimental conditions were deduced from a set of reaction properties data based on the industrial plant parameters. It was found the variables pressure and methane molar fraction are low correlated to the other monitored process variables, making the machine learning regression task challenging and prone to over-fitting. To overcome that, the model's hyperparameters have been fine-tuned by a sequential Bayesian optimization strategy using the Optuna library.

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POSTER 19

IMPLEMENTAÇÃO EM *ASPEN CUSTOM MODELER* DE UM MODELO CINÉTICO DE POLPAÇÃO KRAFT

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Predominante na indústria de Papel e Celulose, o processo Kraft é utilizado em mais de 90% das fábricas em todo o mundo para a produção de polpa celulósica. No Brasil, a principal matéria-prima das plantas existentes é a madeira de eucalipto. Entre seus componentes, a lignina, uma macromolécula heterogênea tridimensional de natureza aromática, é considerada o mais complexo. Devido à tamanha complexidade e por se tratar essencialmente da unidade monomérica que mais necessita de estudos de suas reações no digestor Kraft, este trabalho possui como foco propor rotas reacionais de lignina e suas cinéticas de reação a partir de buscas em artigos científicos e conhecimentos técnicos específicos. O artigo de Fearon et al. (2020), que apresenta uma série de rotas reacionais propostas para a deslignificação da madeira de *pinus*, foi utilizado como referência base, tendo sido feitas modificações para adequar os modelos cinéticos apresentados para a madeira de *eucalyptus*. Ao total, foram consideradas 6 reações de deslignificação e 13 componentes químicos na modelagem cinética. O digestor de polpação Kraft, por sua vez, foi modelado como sendo um reator tubular com dispersão axial, fase pseudo-homogênea, contendo apenas uma zona reacional e sem considerar o termo difusivo, resultando em uma equação diferencial parcial de 1ª ordem para o balanço de massa por componente. Os modelos propostos foram implementados em Aspen Custom Modeler, um *software* de modelagem matemática orientada a equações da Aspen Tech®, capaz de resolver sistemas de equações algébricas e diferenciais e de realizar simulações dinâmicas e em estado estacionário, estimação de parâmetros e otimização de processos. A grande vantagem de sua utilização é a possibilidade de exportação do modelo criado para o ambiente de simulação do Aspen Plus ou Aspen Hysys, objetivando sua integração com outros módulos e operações unitárias do processo. O modelo desenvolvido foi rodado, inicialmente, em estado estacionário com um número de pontos de discretização igual a 10, de forma a possibilitar a observação das concentrações dos treze componentes envolvidos nas reações ao longo do digestor. Em um segundo momento, foi rodada uma simulação dinâmica com número de pontos de discretização igual a 50 e observadas, para pontos específicos do digestor, as concentrações da lignina e dos reagentes da polpação ao longo do tempo de reação. As reações de cozimento da madeira no digestor ocorrem, usualmente, a temperaturas entre 145 e 155 °C. Através da simulação dinâmica foi possível observar, ainda, o perfil de concentração da lignina ao longo do tempo de reação e em cada ponto do digestor. Os resultados da simulação indicam de forma perceptível a redução da velocidade de reação a temperaturas mais baixas, com valores tendendo a zero quando a temperatura do sistema se encontra próxima a 25 °C.

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POSTER 20

APLICAÇÃO DA METODOLOGIA DE BOUND CONTRACTION EM SÍNTESE DE REDE DE TROCADORES DE CALOR

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Neste trabalho é apresentado um algoritmo de otimização global para solução de problemas com formulação não-linear inteira mista (MINLP). Para isso, o algoritmo realiza a linearização (relaxação) dos termos não-lineares do problema original, transformando o modelo MINLP em um modelo linear inteiro misto (MILP), este com sua resposta utilizada como estimativa inicial para a resolução do problema original. Em seguida, realiza-se a contração dos limites de uma variável por vez de cada termo linearizado, com o objetivo de reduzir o espaço de factibilidade na busca do ótimo global do problema original. O problema estará resolvido quando o *gap* de otimalidade entre o problema relaxado (*lower bound*) e o problema original (*upper bound*) atingir um valor menor que uma tolerância predefinida. A metodologia de *Bound Contraction* foi aplicada na resolução de um problema de síntese de redes de trocadores de calor utilizando o modelo simultâneo de Yee e Grossmann com a simplificação de Barbaro e Bagajewicz. O modelo matemático foi implementado e resolvido no ambiente de programação GAMS.

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POSTER 21

INFLUÊNCIA DO COPROCESSAMENTO NA INDÚSTRIA CIMENTERIA EM RELAÇÃO AO ABATIMENTO DAS EMISSÕES DE NO_X

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A indústria cimenteira apresenta um elevado potencial poluente, assim como uma elevada necessidade de energia térmica e elétrica. Devido isso buscam-se constantemente alternativas sustentável e mais econômicas para a utilização de combustíveis. O coprocessamento de resíduos vem ganhando destaque na indústria e representa uma ótima alternativa de combustível alternativo para substituição parcial da injeção de combustíveis mais nobres no setor cimenteiro, como por exemplo o coque. Além disso, está técnica é um caminho sustentável de destinação de diversos resíduos poluentes, em virtude de ser uma forma de descarte mais adequada do ponto de vista ambiental. Desse modo, o objetivo da presente pesquisa é avaliar a influência do coprocessamento dos resíduos com foco na utilização de pneus inservíveis em relação às emissões de NOx (óxidos de nitrogênio). Foram avaliados os gases após a combustão na chaminé do forno utilizando o sistema de monitoramento e análise contínuo de gases da combustão para a determinação das emissões de NOx. Com os resultados obtidos é possível afirmar que o coprocessamento influenciou de forma positiva o conteúdo de emissões na saída da chaminé, dado que teve redução nas emissões atmosféricas de NOx.

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POSTER 22

SYNTHESIS OF PROPYL ETHANOATE BY SULFATED ZIRCONIA: KINETICS AND MECHANISM MODELING

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This work reports experimental kinetic data and mathematical modeling on the esterification of acetic acid with n-propanol using sulfated zirconia as catalyst. Reactions were carried out in an isothermal well-mixed batch reactor at different temperatures (between 60 and 80 °C), n-propanol to acetic acid molar ratio (between 1:1 and 3:1), and the sulfated zirconia loading (between 5 % and 10 wt %) to acetic acid amount. The heterogeneous catalyzed reaction mechanisms were evaluated by the Pseudo-homogeneous, Eley-Rideal and Langmuir-Hinshelwood models. The results obtained indicated that increase of temperature and catalyst amount were favorable to the propyl acetate formation, while the molar ratio showed no significant effect. The estimated enthalpy of reaction was 6.61 kJ mol^{-1} and suggests a slightly endothermic reaction. Eley Rideal model, with acetic acid adsorbed on to actives sites and reaction surface, as limit step, showed most significant mechanism reaction.

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POSTER 23

A NEW FRACTIONAL MODEL APPLIED TO DESCRIPTION OF THE VISCOELASTIC CREEP BEHAVIOR OF TWO BRAZILIAN OILS AND THEIR W/O EMULSIONS

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The objective of this work was to investigate and model the viscoelastic creep behavior of two Brazilian crude oils: A (API 16.8) and B (API 24.6), with different contents of aromatics, resins and asphaltenes and their W/O emulsions with water contents between 0 to 55%. Stable emulsions were prepared using an Ultra-Turrax homogenizer and the viscoelastic flow data were obtained from an Anton Paar controlled voltage Rheometer with plate-plate geometry. For modeling purposes, the fractional model was able to describe the experimental data very well obtaining a mean correlation coefficient R^2 equal to 0.9956. Finally, correlations were determined between the model parameters and the water content present in the emulsions.

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POSTER 24

PERFORMANCE MONITORING AND DIAGNOSIS OF FILTERED SMITH PREDICTOR FOR SISO SYSTEMS WITH DOMINANT TIME DELAY

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The model quality for the dead-time compensators (DTC) is critical for the control loop performance in systems with dominant time delay. Thus, assessing the effect of model−plant mismatch (MPM) and the unmeasured disturbance (UD) is fundamental for performance assessment and monitoring the DTC. In this work, a method for evaluating model quality and the unmeasured disturbances in a DTC structure known as Filtered Smith Predictor (FSP) is proposed for single-input-single-output systems (SISO). The method is based on closed-loop data and nominal output sensitivity function. The approach can identify the presence of MPM or UD to evaluate the actual closed-loop performance through optimization methods.

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POSTER 25

FAULT DETECTION AND DIAGNOSIS BASED ON NEURAL NETWORKS IN THE TENNESSE EASTMAN PROCESS

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Engineers are always worried about keeping the process the safest as possible, and fault diagnosis and analysis using deep learning techniques are of enormous importance to provide this. In this study, artificial neural networks are applied to detect faults and classify them in the Tennesse Eastman process, contributing to innovative results for this analysis. First, the Multilayer Perceptron Networks (MLP) are trained, testing many parameters, such as different kinds of activation functions. After that, Convolutional Neural Networks (CNN) are trained, testing many parameters to achieve the best results of these neural networks. Finally, the results of all neural networks studied are compared, and it is demonstrated that the multilayer perceptron neural networks had an outstanding performance, better than the convolutional neural networks.

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POSTER 26

MODELAGEM DINÂMICA BASEADA EM APRENDIZADO DE MÁQUINA: APLICAÇÃO À INDÚSTRIA DO ÓLEO E GÁS

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Comportamentos complexos e não lineares são comuns dentro da indústria química, sendo assim, a obtenção de modelos fidedignos pode muitas vezes ser impossibilitada ao se empregarem abordagens tradicionais de modelagem. Em função da ampla disponibilidade de dados cada vez mais presente nas operações industriais, estratégias utilizando redes neuronais são justificadas pois possuem boa capacidade de predição. Poços de petróleo com elevação artificial por injeção de gás configuram-se como um problema interessante pois apresentam características que dificultam sua identificação, são estas: inversão do sinal de ganho estático, comportamento de fase não mínima, resposta transitória lenta e instabilidades da malha. Esse trabalho empregou redes neuronais com atrasos temporais na identificação do comportamento do poço. Objetivou-se predizer a vazão de final de óleo a partir de diferentes conjuntos de dados como entrada. Posteriormente, as redes foram utilizadas como modelo interno de controladores preditivos. O comportamento do poço foi satisfatoriamente replicado pelas redes treinadas e os testes aos quais os controladores foram submetidos apresentaram boa capacidade de adequação a curva de referência.

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POSTER 27

CUSTO DO RSU COMO MATÉRIA-PRIMA PARA PLANTA DE WTE

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A crescente geração de resíduos sólidos urbanos (RSUs) acarreta desafios para sua gestão. A Política Nacional de Resíduos Sólidos, instituída em 2010, ainda tem diretrizes não implementadas, como a hierarquia de gerenciamento. Apesar da recuperação energética ser preferencial a aterros, menos de 1% dos resíduos gerados no Brasil são utilizados para esse fim. O país tem grandes desafios para romper o regime de aterramento sendo o elevado custo um deles. O presente trabalho visa encontrar a melhor localização para uma planta de WtE no Rio de Janeiro, considerando aspectos logísticos e mitigação de gases de efeito estufa. A melhor localização para a planta é a região de Campo Grande com capacidade de 50.000 t/ano de RSU advindo da estação de tratamento de resíduos de Bangu. Mas o projeto não apresenta viabilidade econômica, ratificando o desafio atrelado e a necessidade de políticas públicas voltadas para o setor, como aumento da taxa de tratamento (TXRSU), chega-se ao *breakeven* se ela assumir valor de 343,17 reais/t de RSU com Cbio a 56,65 reais/tCO2eq.

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POSTER 28

CODEQ: ENSINO DE PROGRAMAÇÃO NA ENGENHARIA QUÍMICA VIA PLATAFORMA INTERATIVA

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Habilidades técnicas em programação e pensamento lógico são amplamente requisitadas no mercado de trabalho atual. No entanto, cursos de graduação em engenharia apresentam tendem a não acompanhar o rápido progesso feito na área. Visando resolver esse problema, a plataforma online CodeQ apresenta aulas interativas, que auxiliam o usuário a resolver e visualizar problemas com programação em Python. Atualmente, a trilha de aprendizado de Engenharia Química apresenta aulas sobre os tópicos de Termodinâmica e Balanço de Massa e Energia, Fenômenos de Transporte e Cinética e Cálculo de Reatores. Além disso, o CodeQ como projeto de ensino realizou duas integrações com disciplinas do curso de graduação da Universidade Federal de Santa Maria, as quais obtiveram resultados satisfatórios, com grande participação dos alunos das disciplinas.

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POSTER 29

USO DO SIMULADOR EMSO EM AULAS DE OPERAÇÕES UNITÁRIAS PARA PROJETO DE TROCADORES DE CALOR E EVAPORADORES

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Os simuladores de processos são ferramentas computacionais importantes para projeto de equipamentos e processos. Por isso mesmo, o uso dessas ferramentas no ensino de Operações Unitárias se torna importante. Este trabalho avalia a experiência de uso do simulador EMSO em aulas de Operações Unitárias no curso de Engenharia Química da UFSM durante o segundo semestre letivo de 2021. Duas atividades foram propostas envolvendo o pro-jeto de trocadores de calor de geometrias diversas e de evaporadores de efeitos simples e múltiplos. A partir da linguagem de modelagem do EMSO, os grupos implementaram o cálculo da área de troca térmica desses equipa-mentos. Os modelos foram simulados e comparados satisfatoriamente com a literatura. Nenhum dos estudantes teve contato com o EMSO anteriormente e, mesmo com um pequeno tempo de treinamento, conseguiram desen-volver as atividades de modo bastante satisfatório. Os estudantes também consideraram que as atividades propostas no EMSO foram um bom modo de abordar os conteúdos usando *softwares* além da maioria considerar que as atividades conseguiram promover um melhor entendimento dos temas desenvolvidos em aula.

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POSTER 30

STATISTICAL COMPARISON BETWEEN ARTIFICIAL NEURAL NETWORKS AND ADAPTIVE NEURO-FUZZY INFERENCE SYSTEMS TO PREDICT BREAKTHROUGH CURVES IN ADSORPTION SYSTEMS

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In this work, a statistical comparison between artificial neural networks (ANN) and adaptive neuro-fuzzy inference systems (ANFIS) for the prediction of breakthrough curves in adsorption is performed. The case studies chosen were the adsorption of phenol and of 2,4-dichlorophenoxyacetic acid (2,4-D) onto activated carbon-based materials. The ANN architecture of a single-layer with 5 neurons had the best statistical performance for both of the cases. Besides, the use of the ANN makes it possible to obtain the relative importance of each variable, whereas all the input had similar relative importance for phenol, in contrast to what was found for 2,4-D, in which time and flow rate are the most important variables

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POSTER 31

PREDICTING EXTRACTION EFFICIENCY OF METHYL ACETATE IN PRESSURIZED LIQUID EXTRACTION OF CRAMBE SEED OIL USING DECISION TREES REGRESSION

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In the current work, decision trees regression was used to predict the efficiency of methyl acetate as a solvent in pressurized liquid extraction (PLE) of crambe seed oil. The extraction was performed in semi-continuous mode, and the process variables evaluated were the experimental conditions of temperature and solvent flow. The temperatures were 140, 160, and 180 °C at a fixed flow rate of 3 mL min^{-1} as well as solvent flows of 1 and 2 mL min^{-1} at a fixed temperature of 140 °C. The input variables used to construct the decision trees regression were time (min), temperature (ºC), and solvent flow (mL min^{-1}), and the output variable was yield (%). Different decision trees regressions were compared using data without normalization and data with three different data normalization norms: Standard, Robust, and MinMax. The results showed that for all temperatures and solvent flows studied, a decision tree regression with data without normalization can accurately predict the experimental data.

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POSTER 32

TREATMENT OF EVAPORATED WATER FROM CONDENSED MILK PRODUCTION

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Water uses are increasing, and new sources need to be studied. In this sense, the reuse of water derived from industrial processes is an alternative. The cow water comes from the evaporation of milk and its quality must be standardized to enable its use. Electroflotation was the treatment performed and evaluated in this work. Three variables were studied: current, hydraulic retention time (HRT), and the distance between the electrodes in the electroflotation reactor. The chemical oxygen demand removal (COD) was assessed on essays that showed different efficiencies. The highest COD removal was 58,82%, 10 mA, 60 min HRT, and 1,5 cm between electrodes. Our results indicated that electroflotation was a usefull technic to remove organic matter from this wastewater.

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POSTER 33

FROM MISCONCEPTIONS TO ADVANCES ON THE THERMO-KINETIC STUDY OF BIOMASS PSEUDO-COMPONENTS DECOMPOSITION USING MODEL-FREE METHODS: IMPACT ON THE PRETREATMENT PROCESSES BY A MULTI-STAGE MODELING

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A deeper understanding of the kinetics parameters of sugarcane bagasse (SCB) thermal degradation could define appropriate conditions of the primary biorefining in the production of renewable fuels. In this work, the kinetic of thermal degradation of SCB high polymers are investigated through thermogravimetric data. Model-free and model fitting methods are used to calculate apparent activation energies (E_a) and other related kinetic parameters. DTG curves show three major peaks associated with pseudo-components (PSEs): PSE-1 (hemicelluloses+extractives and lignin), PSE-2 (cellulose+extractives and lignin) and PSE-3 (lignin+extractives and residual holocelluloses). An essential advance is related to the degradation process by multi-stage modeling governed by diffusion-controlled reactions and order-based models. The Kissinger-Akahira-Sunose method provided E_a ranges of 124–154 kJ·mol^{-1}, 153–147 kJ·mol^{-1} and 230–530 kJ·mol^{-1}, respectively, while the ranges obtained by the Flynn-Wall-Ozawa method were 120–152 kJ·mol^{-1}, 150–144 kJ·mol^{-1} and 232–545 kJ·mol^{-1}, respectively. SCB biorefining could lead to a degradation of up to 10%, 0.5% and 11% for PSE 1, PSE 2, and PSE 3, respectively at 473.15 K and 200 min.

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POSTER 34

THERMODYNAMIC STABILITY OF FORMIC ACID UNDER AQUEOUS SOLVENTS: A PERSPECTIVE OF DFT CALCULATIONS AND MOLECULAR DYNAMICS SIMULATIONS

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For the CO2 conversion into formic acid (FA), the maximum productivity that can be achieved with the catalyst system is limited by the thermodynamics in the reaction medium. To obtain a better understanding of thermodynamics conditions present in the interactions between FA and solvent, in this work we performed the combination of Density-Functional Theory (DFT) and molecular dynamics (MD) calculations to compare the formation stability of FA from of the reaction of CO2 hydrogenation under different solvents of green-energy interest. Robust simulation models of FA solvation under specific aqueous media from different implicit and explicit solvations and ionic compositions/concentrations were obtained. The results of this work show that the main Chemical environment to the FA stability may be formed by a solution of water and ionic composition with dielectric permittivity values closer to water, such as aqueous solvents of low salinity. Compared to some usual solvents, such as dimethyl sulfoxide (DMSO) and amine, aqueous solvents were mainly found to form the less stable hydrogen bond, which makes this type of solvent less harmful in an H2 recovery. Indeed, the calculations for the Gibbs energy variation using aqueous solventes are identified as preferential thermodynamic conditions to H2 catalytic storage in low temperature. These results are comparable to other works with different theory levels. Therefore, a mixture of specific composition and concentration of salt ions could be used to lead the thermodynamic stability of H2 storage in catalytic processes.

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