FBT 5776 – Tópicos Especiais em Tecnologia Bioquímico-Farmacêutica II

Tema: Desenvolvimento de Microrreatores

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https://www.blogs.unicamp.br/microfluidicaeengenhariaquimica/

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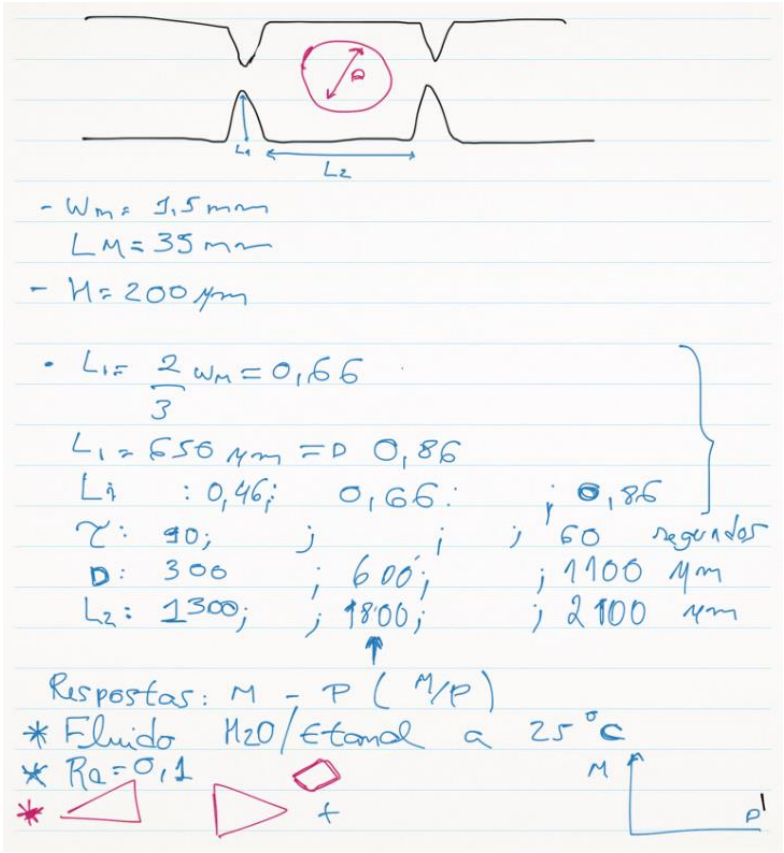
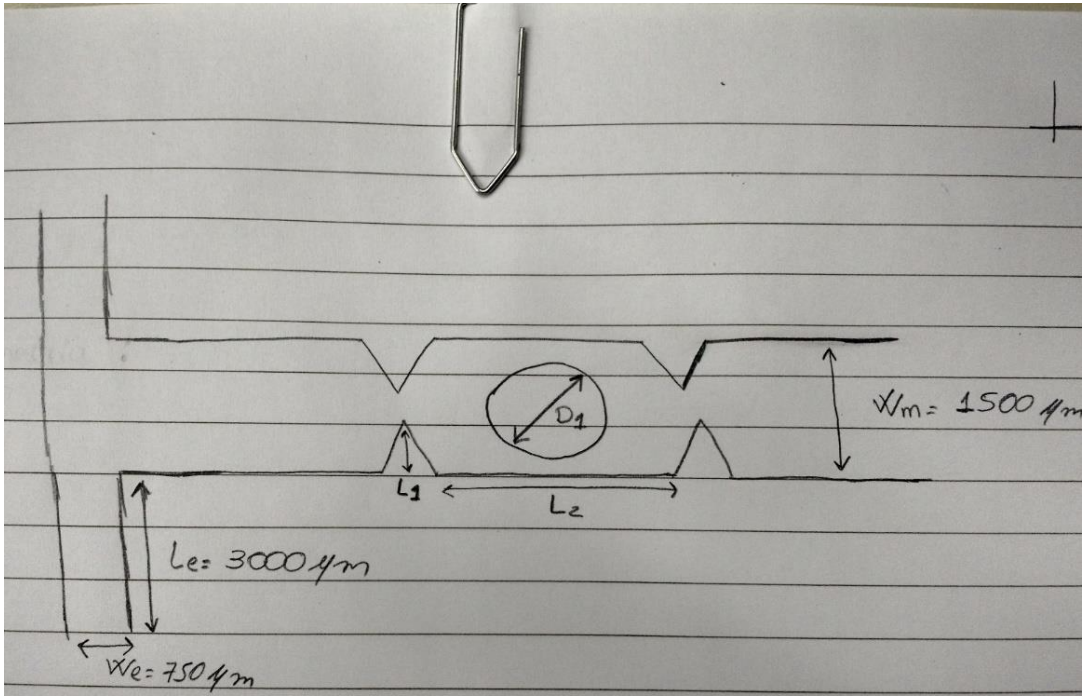
❖Desenvolvimento de processos químicos em microescala – Ideias iniciais





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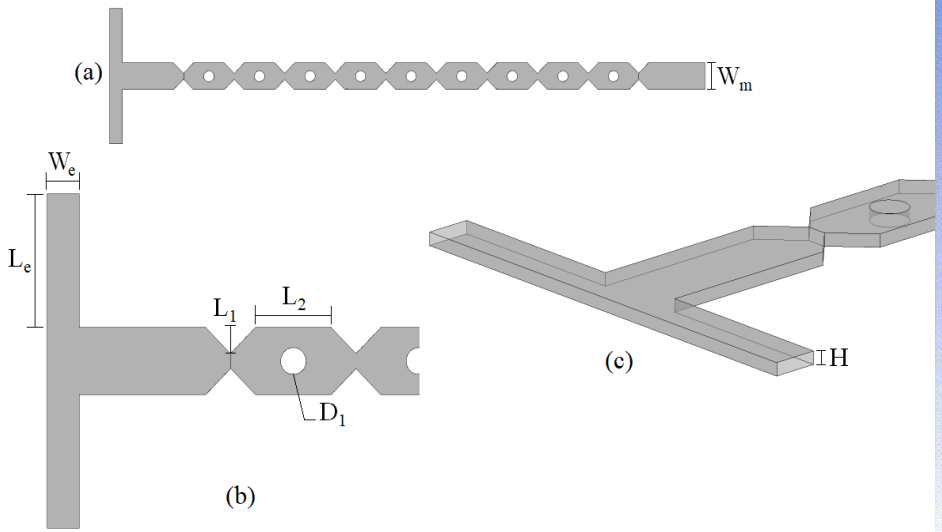
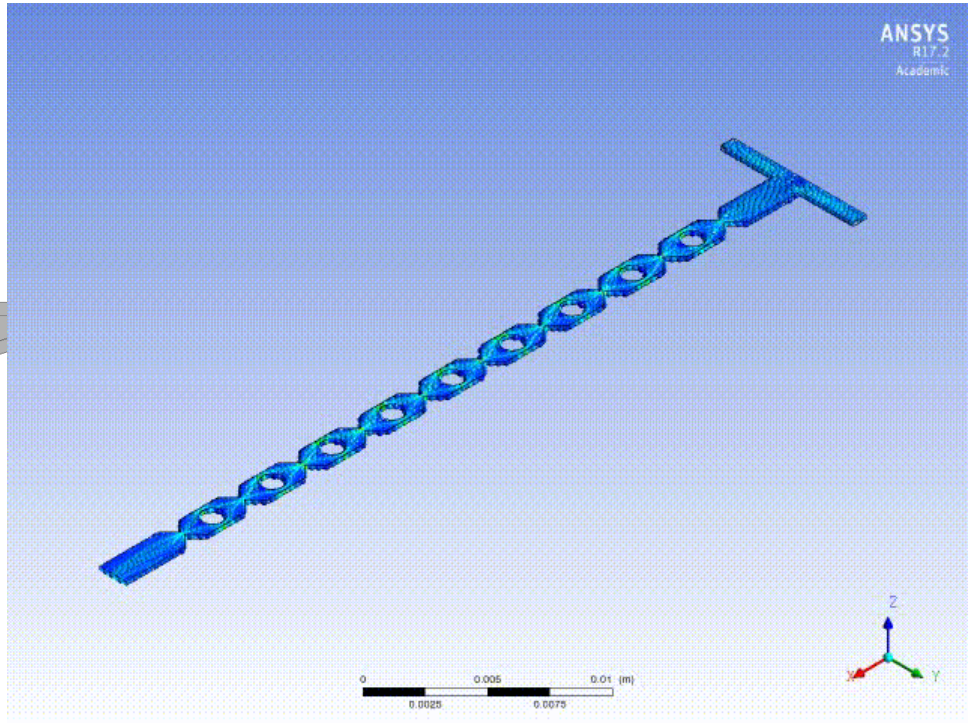
❖ Desenvolvimento de processos químicos em microescala

❖ Modelo do dispositivo em softwares computacionais





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❖ Desenvolvimento de processos químicos em microescala

– Publicação dos resultados computacionais

Sensors & Actuators: B. Chemical 281 (2019) 191–203

Contents lists available at ScienceDirect

Sensors and Actuators B: Chemical

journal homepage: www.elsevier.com/locate/snb

Optimization of micromixer with triangular baffles for chemical process in millidevices

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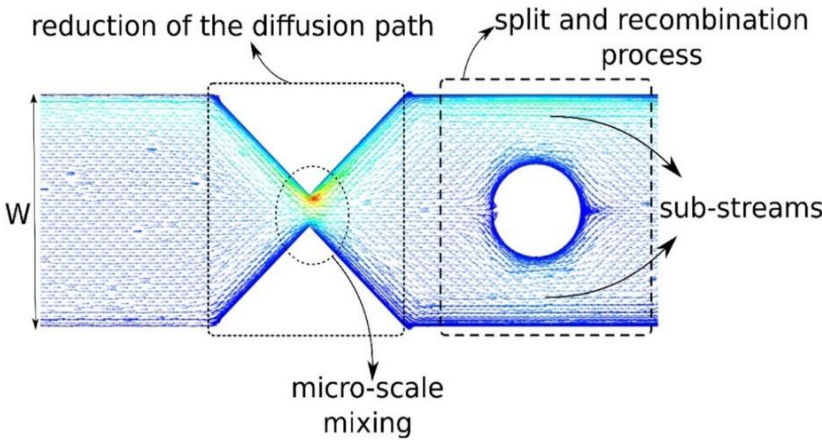
ARTICLE INFO

Keywords:
Micromixers
Baffles
Circular obstructions
Millidevices
Numerical simulation
Process intensification

ABSTRACT

A new micromixer design (MTB – micromixer with triangular baffles and circular obstructions) was proposed aiming the combination of three mass transfer enhancements mechanisms: reduction of molecular diffusion path, split and recombination of streams and vortex generation. The geometric variables were also optimized considering the mixing performance and the required pressure drop. The optimal design was used for the mixing of different binary mixtures (vegetable oil/ethanol and water/ethanol) under the Reynolds number range from 0.01 to 200 and the chemical reaction process of vegetable oil transesterification with ethanolic solution of sodium hydroxide (biodiesel synthesis). High mixing index ($M = 0.99$) was observed for the oil/ethanol mixing for several channel heights (200 μm – 2000 μm) and widths (1500 μm – 3000 μm). The geometry W3000H400 (i.e., MTB with channel width of 3000 μm and height of 400 μm) was employed as the millireactor, providing a maximum oil conversion of 92.67% for a residence time of 30 s. For the water/ethanol mixing, the geometry W1500H200 was used. High mixing index ($M = 0.99$) was observed at very low Reynolds number ($Re = 0.1$) and also in higher Reynolds numbers of 50 and 100. Moreover, at $Re = 0.1$, high mixing index ($M \approx 0.90$) was obtained already at 3.5 mm of channel length. However, for higher Reynolds number the fluids required longer distances to achieve superior mixing, about 10.5 mm at $Re = 100$. The MTB, unlike the ones found in the literature, can be used in microdevices (e.g., sensors) with low flow rates and in microdevices with large dimensions (eg, millidevices and millireactors) with high flow rates, allowing an easier application in chemical process aiming the commercial production.

Graphical abstract



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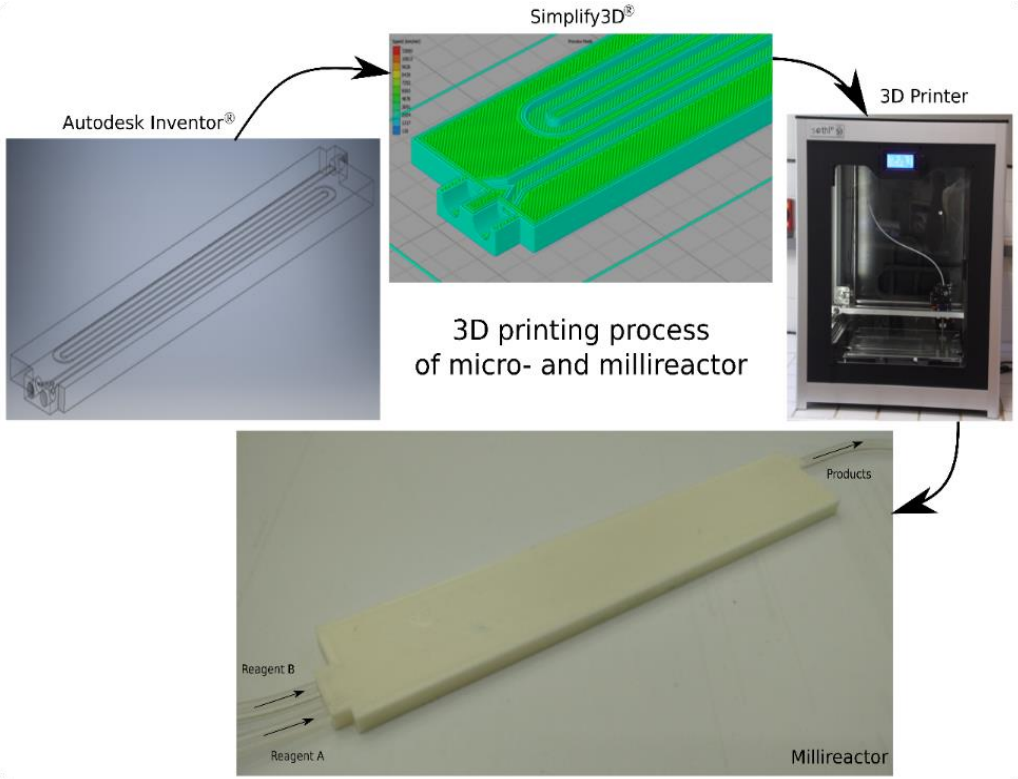
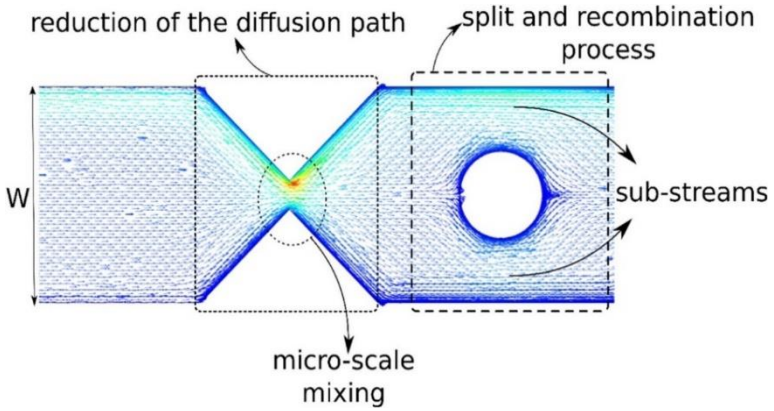
❖ Desenvolvimento de processos químicos em microescala

– Fabricação dos microdispositivos





Processo de impressão 3D de micro- milirreatores para reações químicas.
Santana et al., *Chinese Journal of Chemical Engineering*, 2019.

Objetivos da disciplina

Objetiva-se que ao final da disciplina, os alunos possam projetar e construir seus próprios microrreatores, através da compreensão dos fenômenos de transporte e reação química em microescala e aplicação de ferramentas computacionais no desenvolvimento de microrreatores.

Objetivos da disciplina

Além dos conhecimentos adquiridos, os alunos serão capazes de desenvolver projetos de microrreatores em 3D utilizando o *software Autodesk Inventor*, simular a fluidodinâmica e reação química com o *software ANSYS CFD* (*ANSYS CFX*).

Programa da disciplina

- **O programa da disciplina está dividido em:**
  - ✓ Introdução ao conceito de Microfluídica
  - ✓ Introdução ao conceito de Microrreatores & de Engenharia das reações químicas
  - ✓ Fenômenos de transporte & Micromisturadores
  - ✓ Escalonamento (*numbering-up*) de microrreatores
  - ✓ Impressão 3D de microrreatores
  - ✓ Dinâmica dos fluidos computacional (CFD) no desenvolvimento de microrreatores

Formato do curso & Avaliação

A. Aulas teóricas e práticas

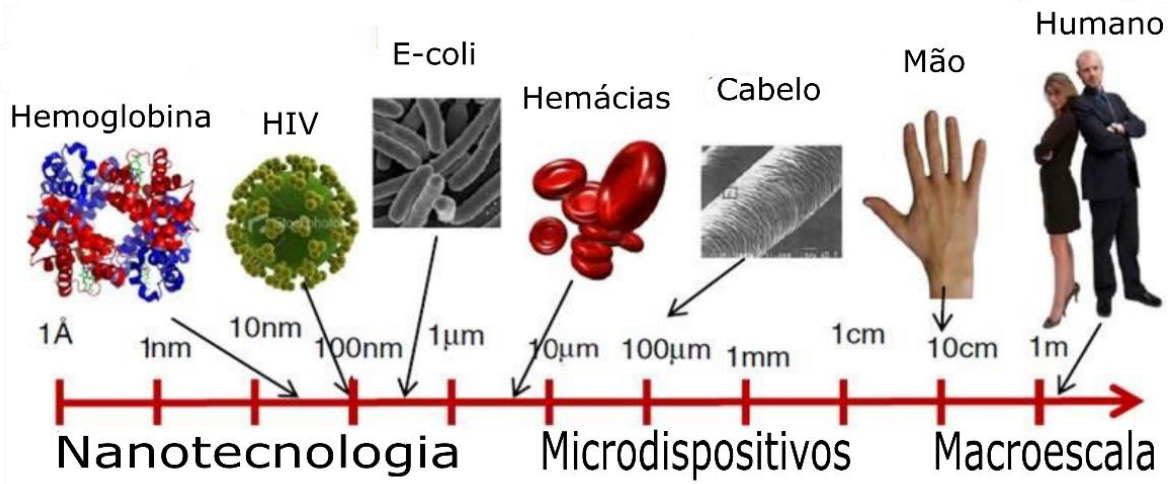
B. Atividades:

I. Apresentação do caso escolhido

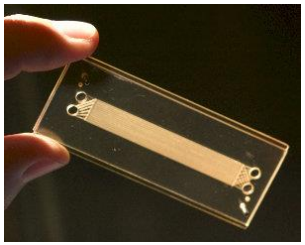
II. Apresentação dos resultados

Definição de Microfluídica

- Microfluídica - ciência e tecnologia de sistemas as quais manipulam e estudam pequenas quantidades de fluidos, utilizando estruturas com dimensões micrométricas. (Whitesides, G. M. *Nature*, v. 442, p. 368-373, 2006)



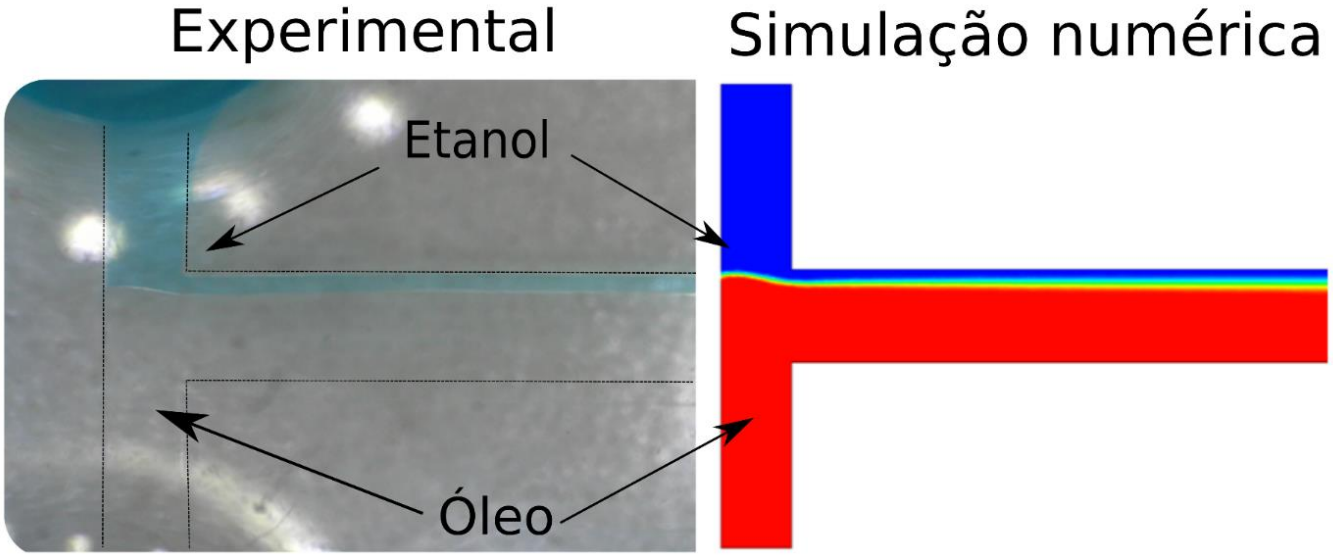
(Adaptado de Nguyen et al. *Advance Drug Delivery Reviews*, v. 65, p. 1403-1419, 2013)



- Menor quantidades de reagentes e amostras;
- Baixo custo de fabricação;
- Área superficial elevada;
- Elevada transferência de calor e massa;
- Escoamento laminar;
- Tempo de reações menores;
- Facilidade de escalonamento

Definição de Microfluídica

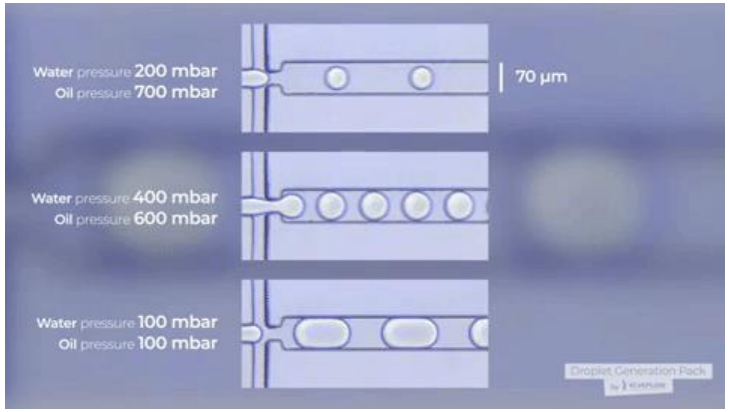
- Microfluídica - ciência e engenharia de sistemas nos quais o comportamento dos fluidos diferem da teoria convencional de escoamento de fluidos, principalmente devido ao reduzido comprimento de escala do sistema. (Nguyen, N-T., Wereley. S. T. *Fundamentals and applications of microfluidics*., 2006)



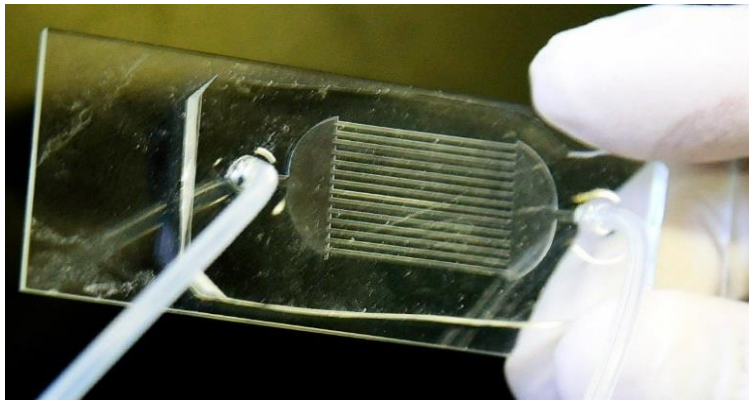
Santana *et al*. *Chemical Engineering and Processing*, v. 98, p. 137-146, 2015.

Definição de Microfluídica

- Microfluídica - ciência e tecnologia que envolve o estudo do comportamento dos fluidos, manipulação controlada de fluidos e o design de dispositivos ou sistemas que possa executar de forma confiável tarefas em microcanais com dimensões típicas de dezenas a centenas de micrômetros. (Lo, R. C. *Chemical Engineering & Process Techniques*, 1:1002, 2013)



Microfluídica de gotas (*Droplet Microfluidics*). Créditos: Elveflow.



Microdispositivo para purificação de biodiesel. Santana et al. *Chemical Engineering Research & Design*, v. 124, p. 20-28, 2017.

Definição de Microfluídica

Aplicações e Mercado da Microfluídica

- ✓ Diagnóstico Clínico e Veterinário (*Clinical and Veterinary Diagnostics*)
- ✓ Diagnóstico do ponto de atendimento *(Point-of-Care Diagnostics)*
- ✓ Pesquisa Farmacêutica e Ciências da Vida *(Pharmaceutical and Life Science Research)*
- ✓ Dispositivos analíticos *(Analytical Devices)*
- ✓ Testes Industriais, Ambientais e Agro-Alimentares *(Industrial, Environmental and Agro-Food Testing)*
- ✓ Entrega de medicamentos *(Drug delivery)*
- ✓ Micro Reação - Química de Fluxo *(Micro Reaction – Flow Chemistry)*

Fonte: *Yole Développement*, Maio 2017.

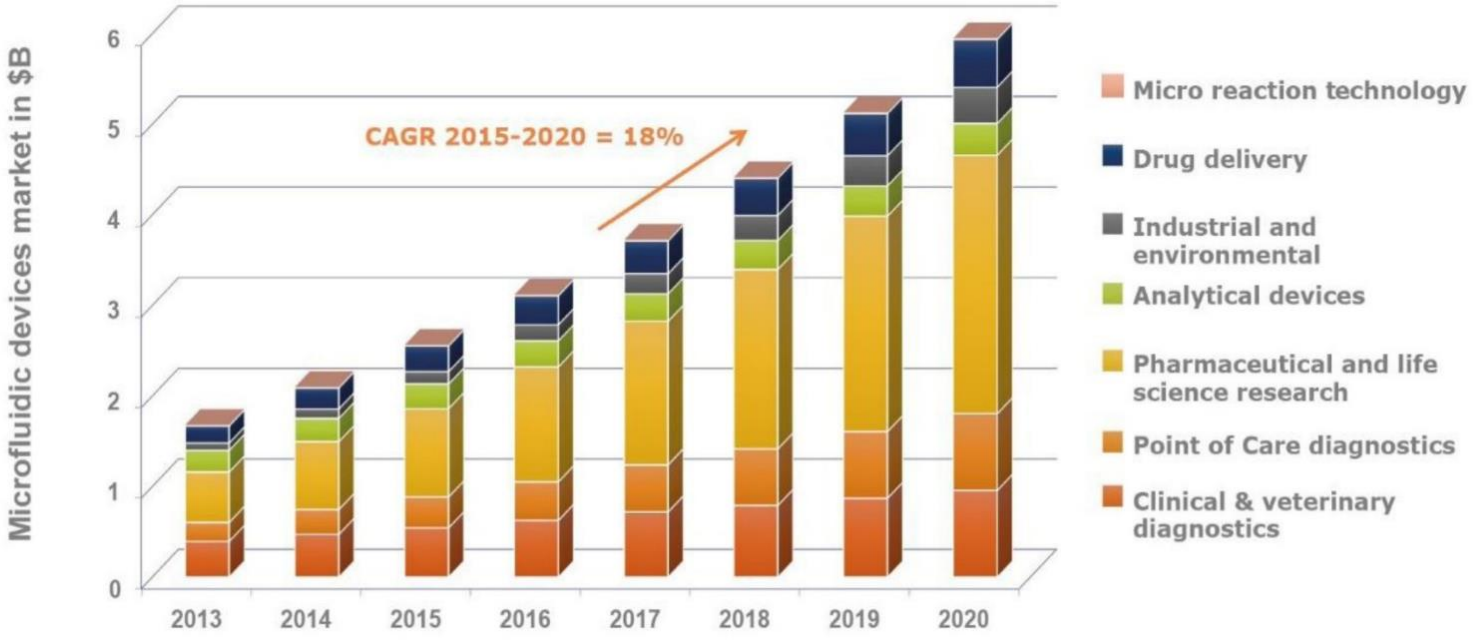
Aplicações e Mercado da Microfluídica

MICROFLUIDIC DEVICES MARKET IN $B

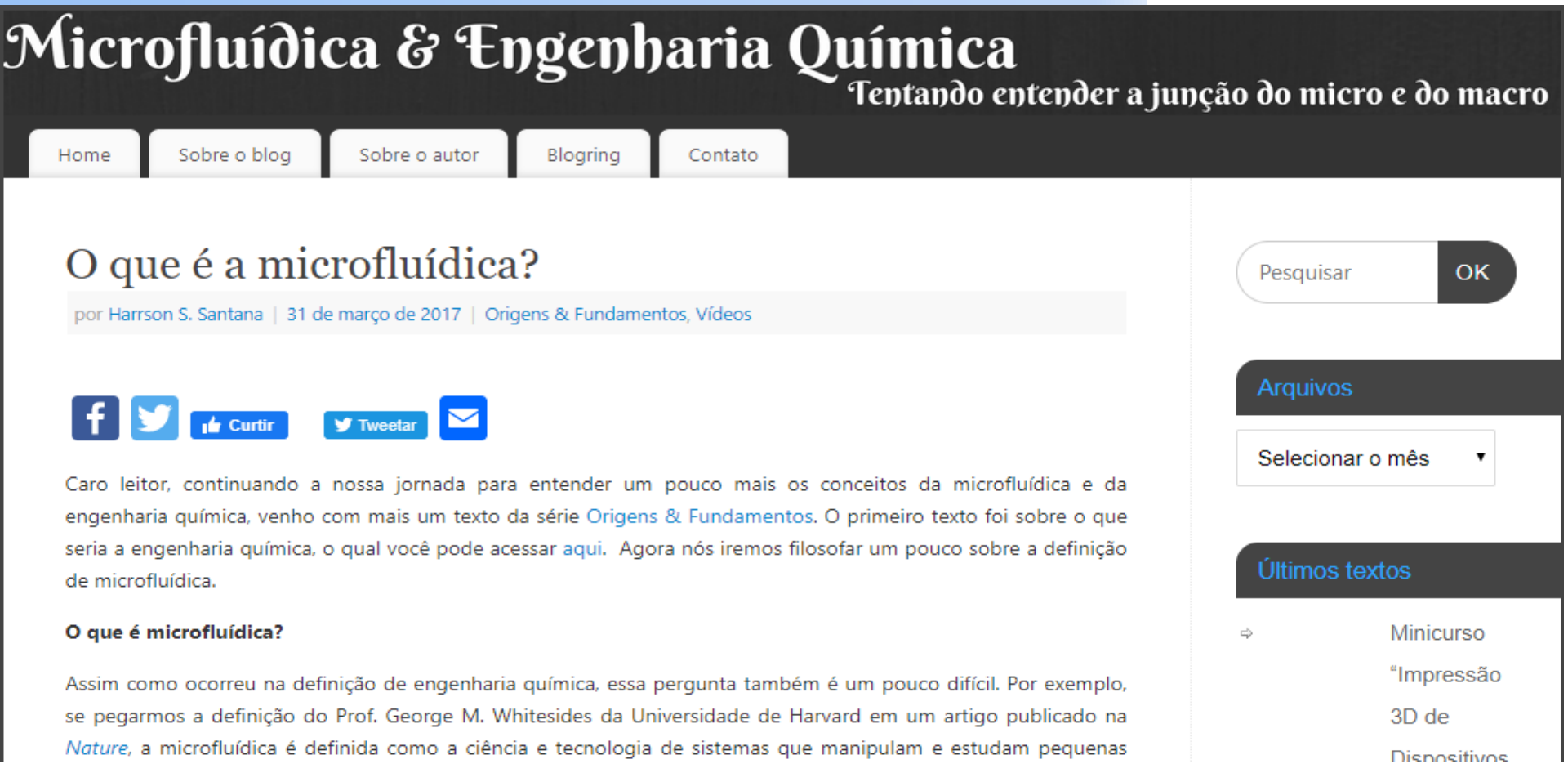
(Source: Microfluidic Applications in the Pharmaceutical, Life Sciences, In-Vitro Diagnostic, and Medical Device Markets report, Yole Développement, June 2015)

The microfluidic industry is now well structured for further growth.

(Source: Yole Développement)



Mais informações



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https://www.blogs.unicamp.br/microfluidicaeengenhariaquimica/

Missão do nosso grupo

Desenvolver microssistemas para processos químicos, físicos e biológicos e compartilhar nossa engenharia com a sociedade.

- Reação de síntese de biodiesel em microrreatores (tempo de residência = 60 s) e em reator de batelada (180 min)

Chemical Engineering Journal 302 (2016) 752–762

Contents lists available at ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Transesterification reaction of sunflower oil and ethanol for biodiesel synthesis in microchannel reactor: Experimental and simulation studies

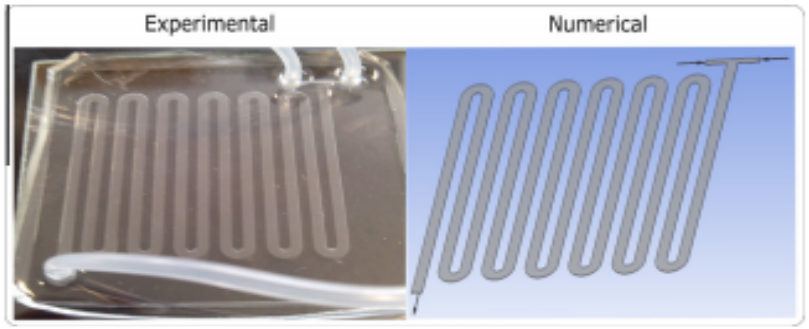
Harrson S. Santana [a,*], Deborah S. Tortola [a], Érika M. Reis [a], João L. Silva Jr. [b], Osvaldir P. Taranto [a]

[a] University of Campinas, School of Chemical Engineering, 13083-852 Campinas, SP, Brazil
[b] Federal Institute of Education, Science and Technology of South of Minas Gerais – IFSULDEMINAS, 37550-000 Pouso Alegre, MG, Brazil

HIGHLIGHTS

- Experimental and numerical study of biodiesel synthesis in microdevices.
- The influence of temperature, ethanol/oil ratio and catalyst concentration.
- Microreactors are a viable option to produce biodiesel.
- Yield parameters and selectivity better capture the experimental process.

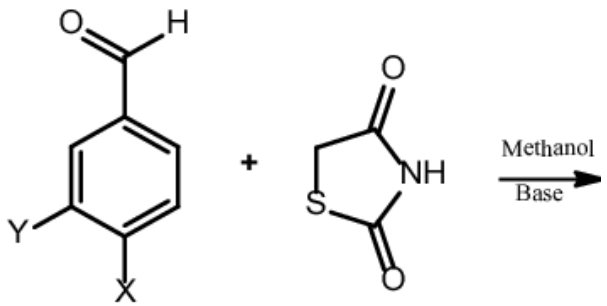
GRAPHICAL ABSTRACT

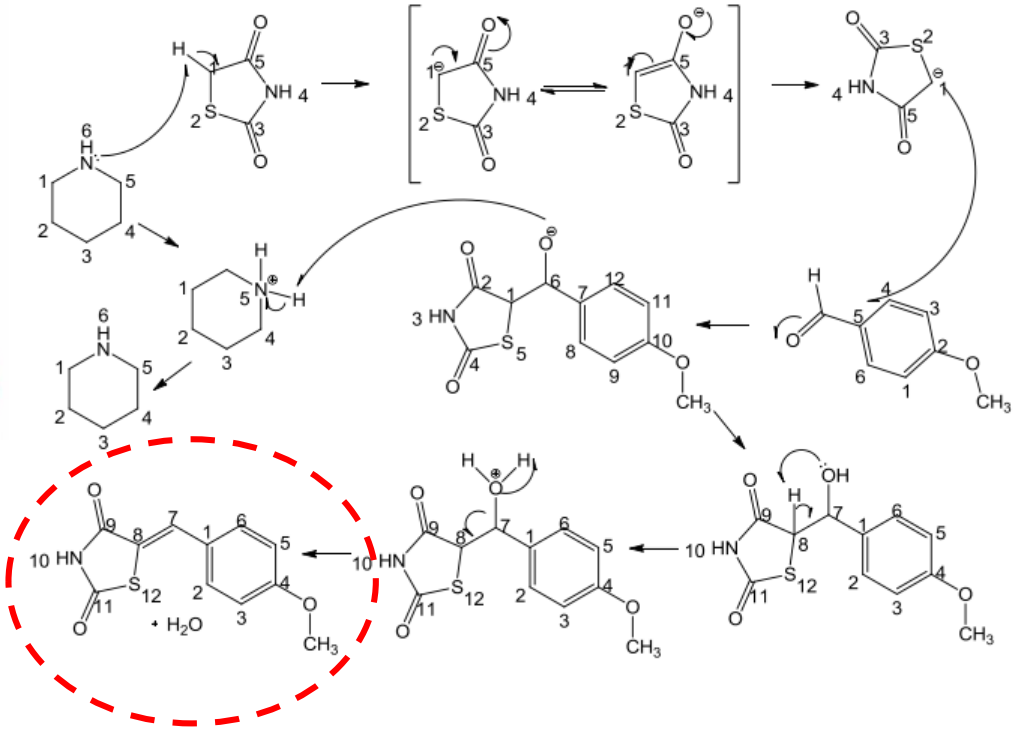


Síntese de medicamentos

❖ Produto intermediário para obtenção de um fármaco com eficácia contra Diabetes Mellitus Tipo II. Vieira *et al*. 2019 (*Em preparação*)

Fonte da imagem: https://bit.ly/2OOVo0P





5-(4-metoxibenzilideno)-2,4-tiazolidinadiona (MBT)

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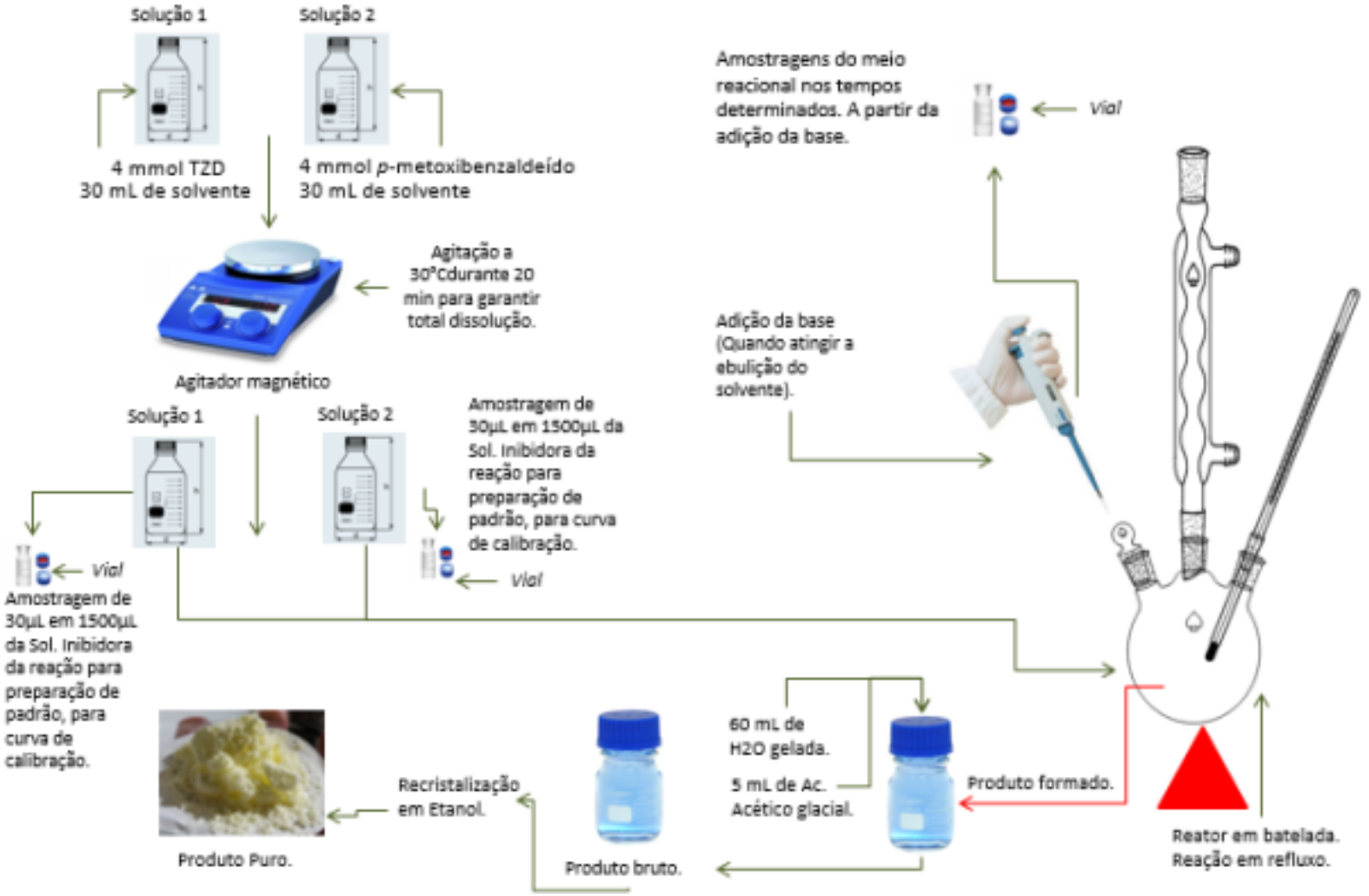
Síntese de medicamentos

❖ Tratamento contra Diabetes Mellitus Tipo II – Vieira *et al*. 2019 (*Em preparação*)



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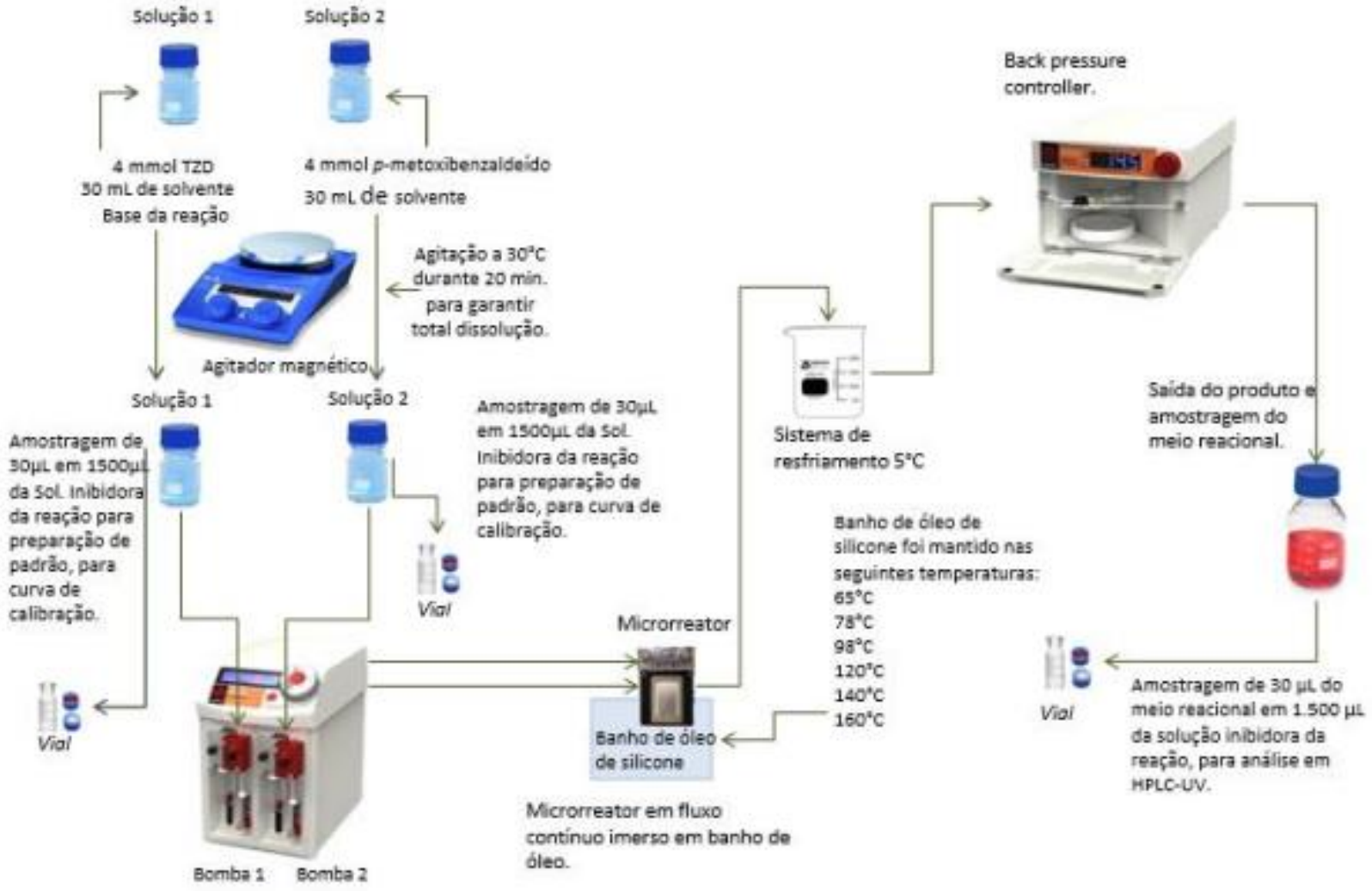

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Síntese de medicamentos

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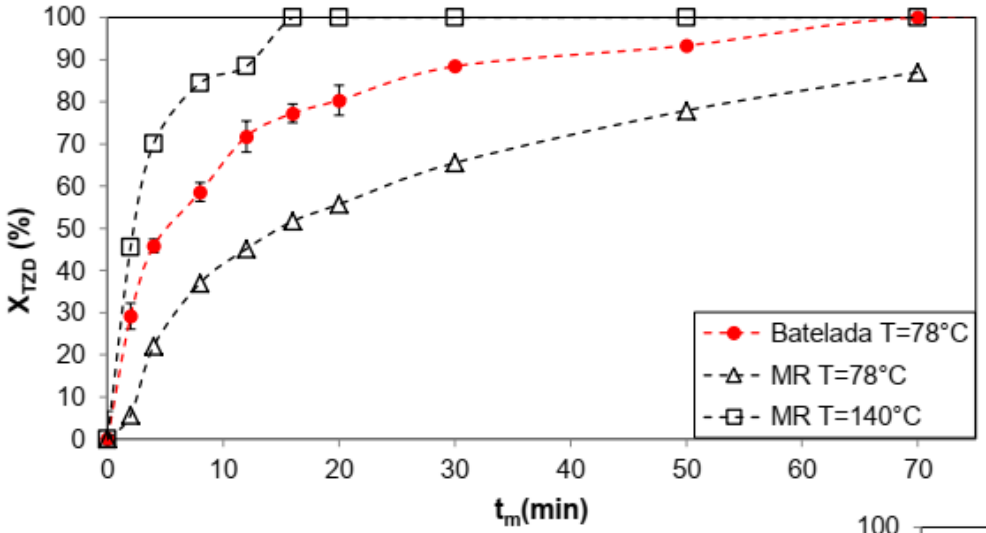
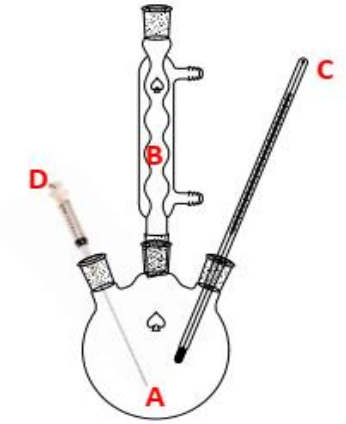
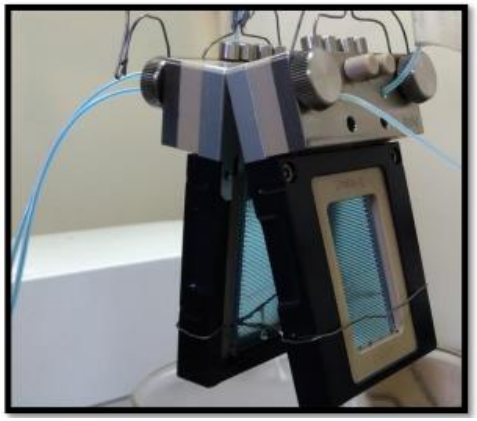
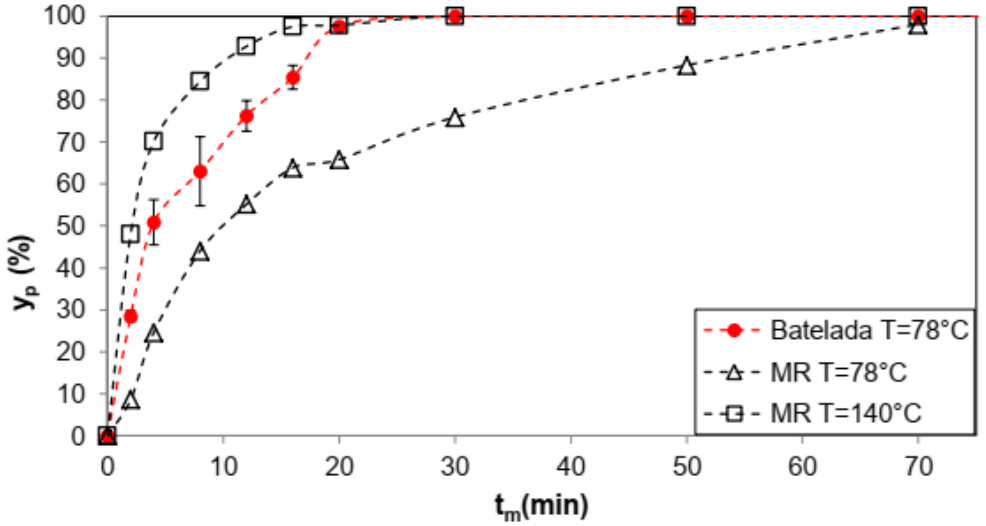






Volume interno de 1000 µL.



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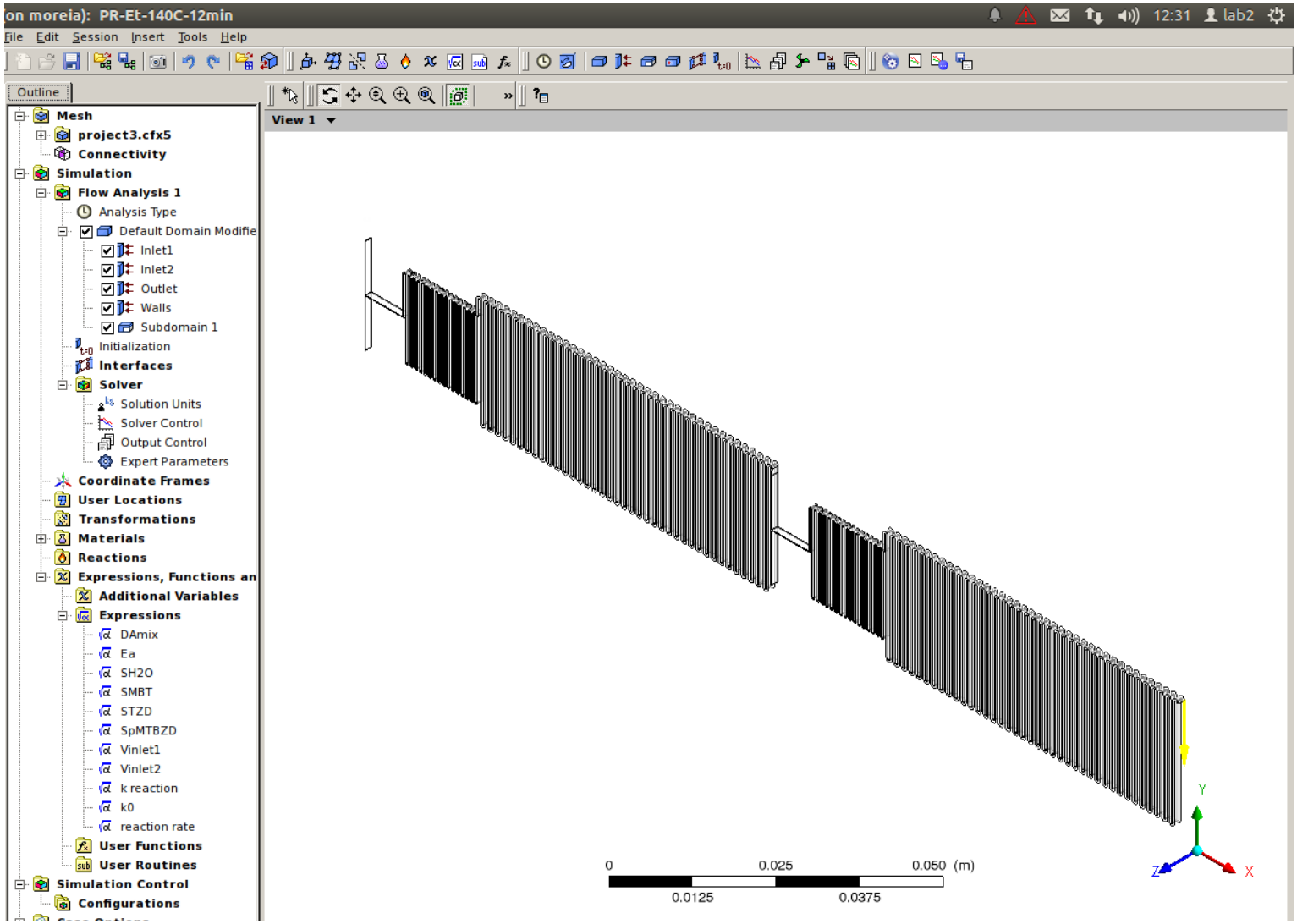
Síntese de medicamentos

❖ Tratamento contra Diabetes Mellitus Tipo II – Modelagem computacional



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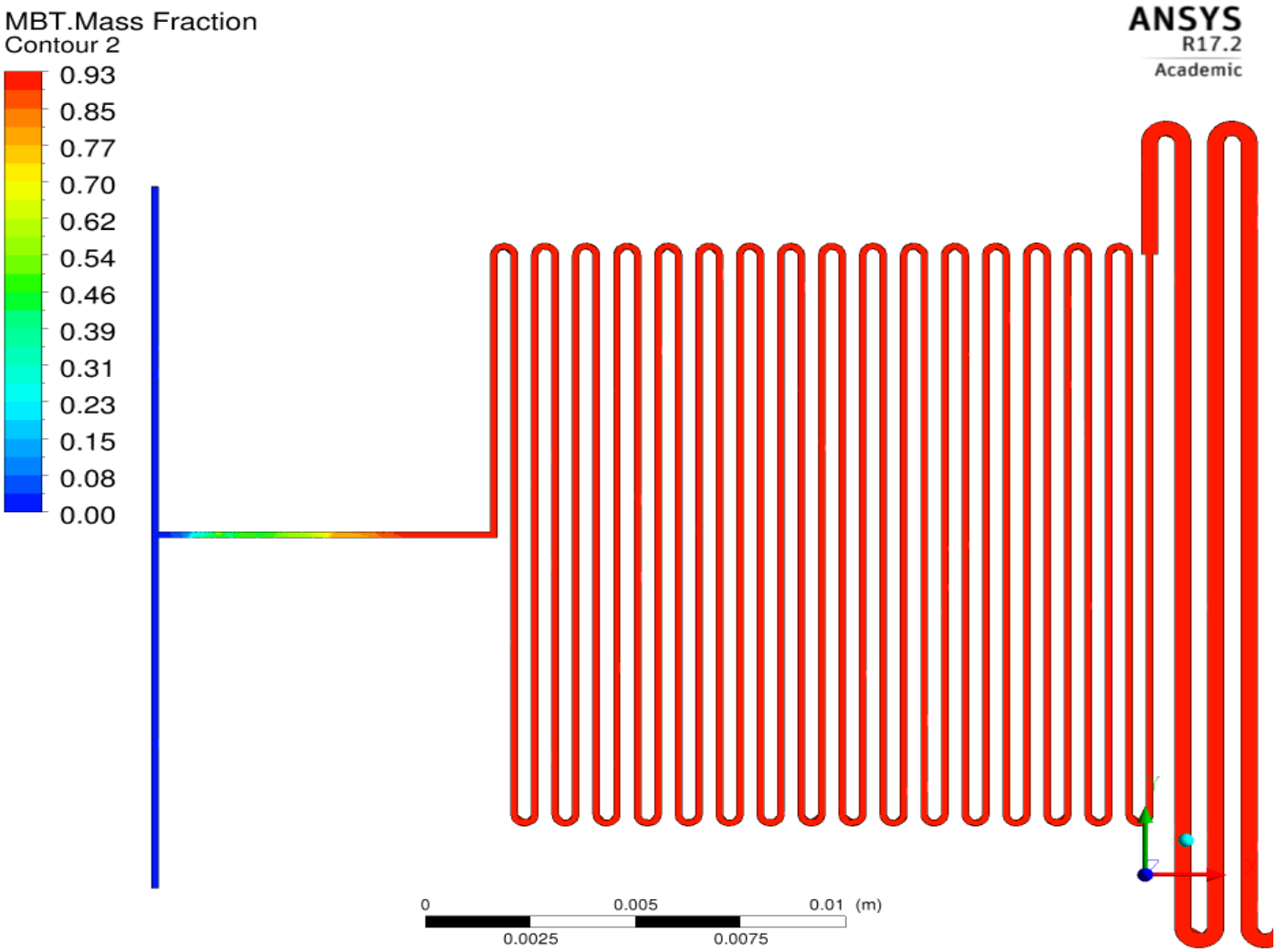
Síntese de medicamentos

❖ Tratamento contra Diabetes Mellitus Tipo II – Modelagem computacional



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Síntese de medicamentos

❖ Tratamento contra Diabetes Mellitus Tipo II – Modelagem computacional

➢ Erro obtido entre as abordagens experimental e computacional na conversão de TZD (T = 140 °C)

τ (min)	Conversão experimental	Conversão computacional	Erro (%)
2	45.45	100	120.02
4	70.07	97.62	39.33
8	84.42	92.12	9.13
12	**88.42**	**91.16**	**3.11**
20	100	90.24	-9.76
50	100	93.34	-6.66

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Fenômenos de Transporte e reações químicas

- A modelagem de microrreatores pode se basear nas seguintes equações:

✓ *Conservação de massa:* $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$

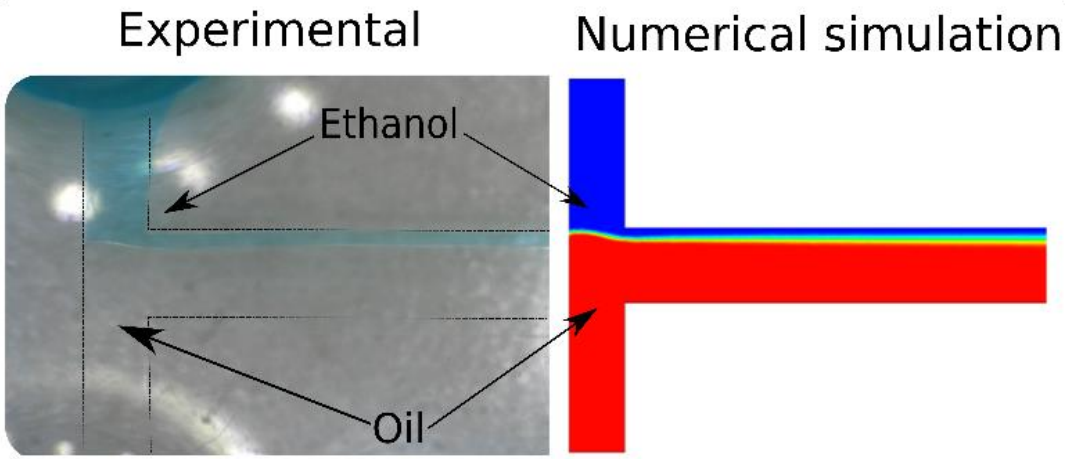
✓ *Conservação do momento:* $\rho \frac{D\vec{v}}{Dt} = \nabla \tilde{T} + \rho \vec{f}$

✓ *Conservação de energia:* $\nabla \cdot k \nabla T + \dot{q} + \Phi = \rho c_v \frac{DT}{Dt}$

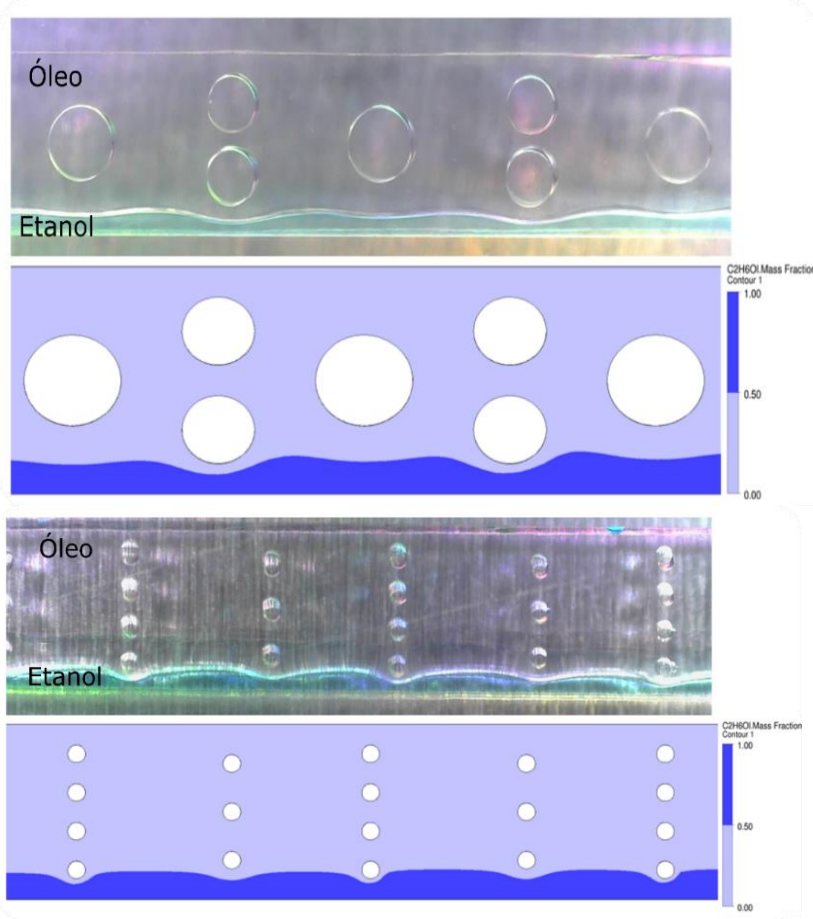
✓ *Conservação das espécies:* $\mathrm{v} \cdot \nabla c_A + \frac{\partial c_A}{\partial t} = D_{AB} \nabla^2 c_A + R_A$

✓ *Leis das reações químicas:* $r_A = k C_A^a C_B^b \cdots C_D^d$

❑ Simulações numérica de processos químicos e físicos em microdispositivos



Santana *et al*. *Chemical Engineering and Processing*, v. 98, p. 137-146, 2015.



Santana *et al*. *Chinese Journal of Chemical Engineering*, v. 26, p.852-863, 2018.

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❖Desenvolvimento de microdispositivos para operações unitárias!

CHEMICAL ENGINEERING RESEARCH AND DESIGN 124 (2017) 20–28

Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Evaporation of excess alcohol in biodiesel in a microchannel heat exchanger with Peltier module

Harrson S. Santana, Geovanni B. Sanchez, Osvaldir P. Taranto*

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ARTICLE INFO

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Keywords:
Microchannel heat sinks
Biodiesel/ethanol
Peltier modules
Evaporation

ABSTRACT

Transesterification is the most common method for biodiesel production, typically occurring with excess alcohol to shift the reaction balance towards the products. After the reaction, this alcohol can be removed and recovered. On both macro and micro scale, such process occurs in evaporators or even in distillation columns. In view of the above, this article intends to apply a microchannel heat exchanger based on a Peltier module on the separation of excess alcohol from the biodiesel in microscale. Three variables were assessed in the process: temperature, fluid flow rate in the micro-exchanger and alcohol/biodiesel molar ratio. The results revealed that temperature has a positive effect on the evaporation efficiency, whereas the variables of flow rate and molar ratio showed a negative effect on the process. Accordingly, we have thus shown the possibility of using heat micro-exchangers on the separation of excess alcohol from biodiesel.

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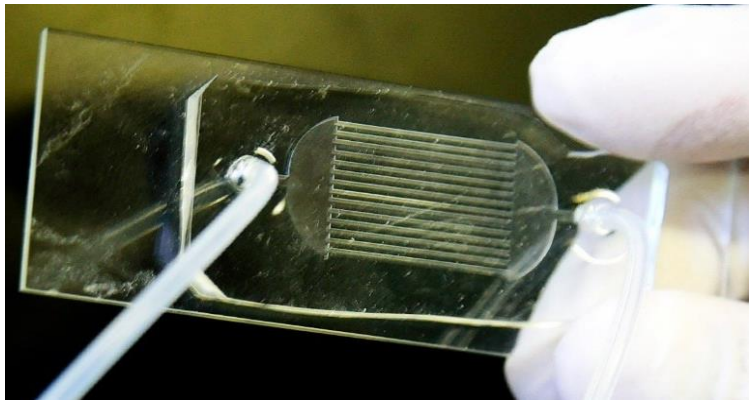
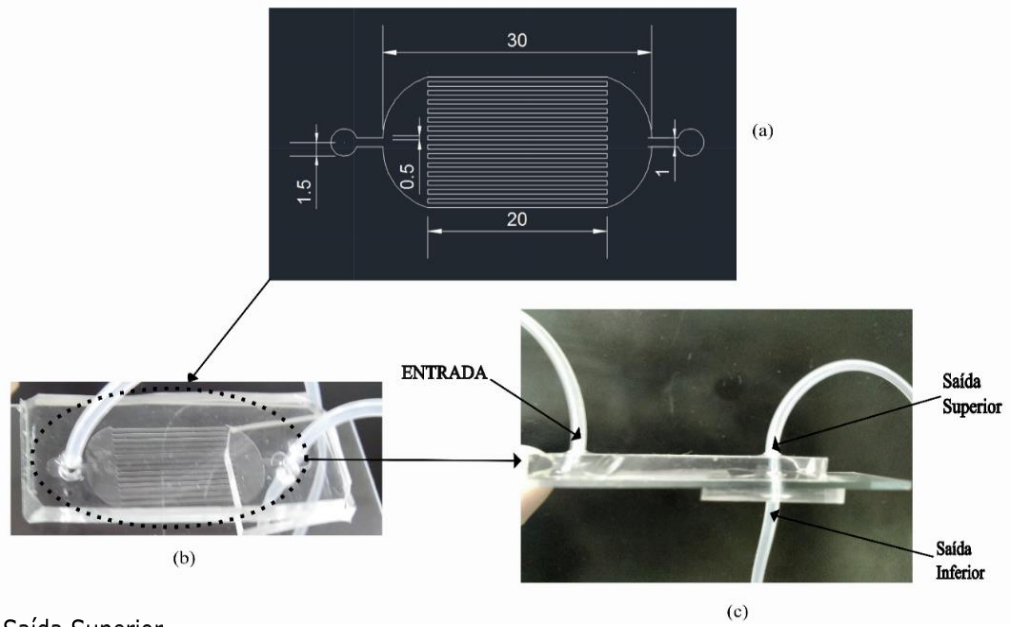
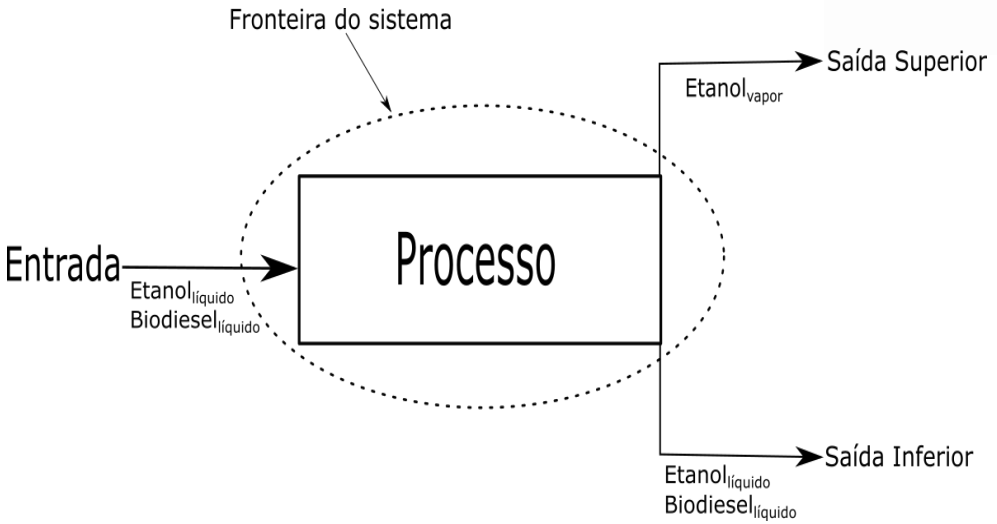
❖Desenvolvimento de microdispositivos para operações unitárias!







$$Perda\ de\ massa\ (\%) = \frac{m - m'}{m} 100$$

m: Massa total - Entrada
m': Massa total - Saída Inferior

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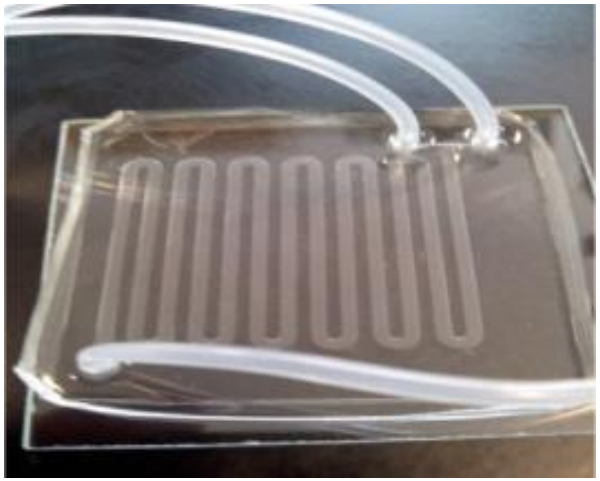
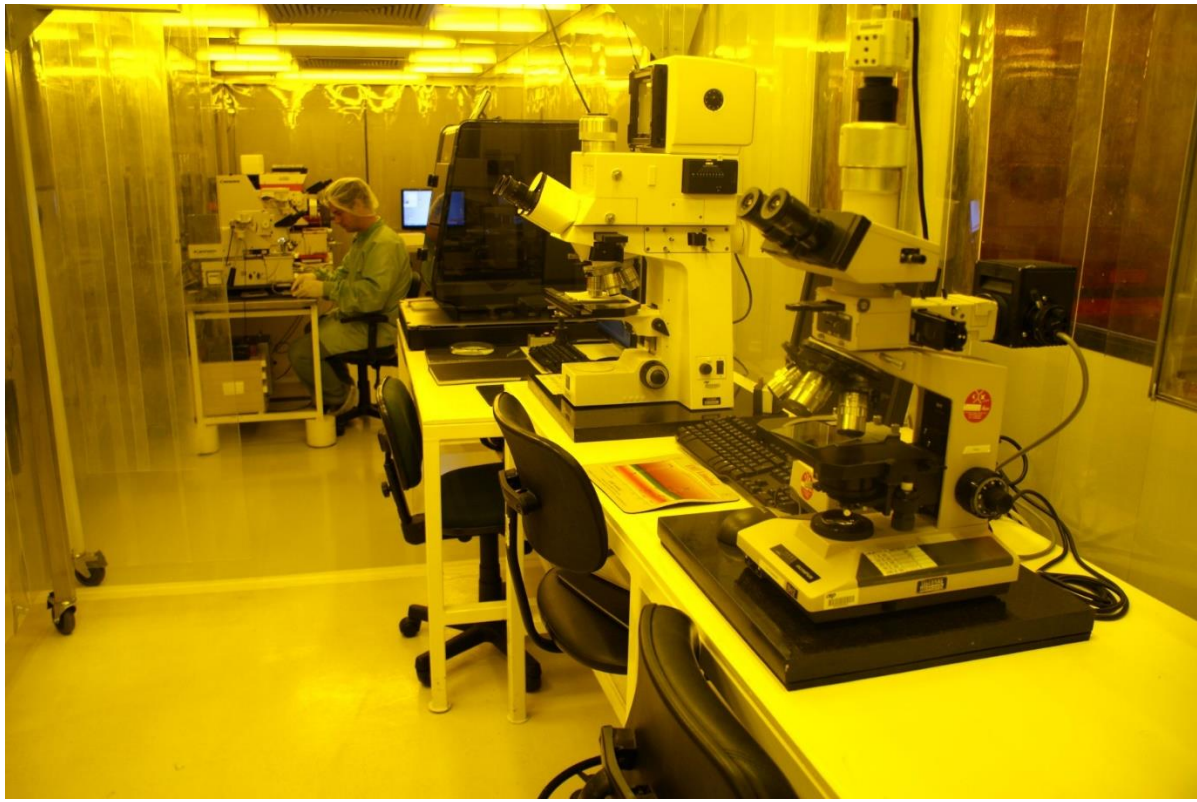
- E os resultados experimentais?
- Como fabricar os dispositivos?

LNNano





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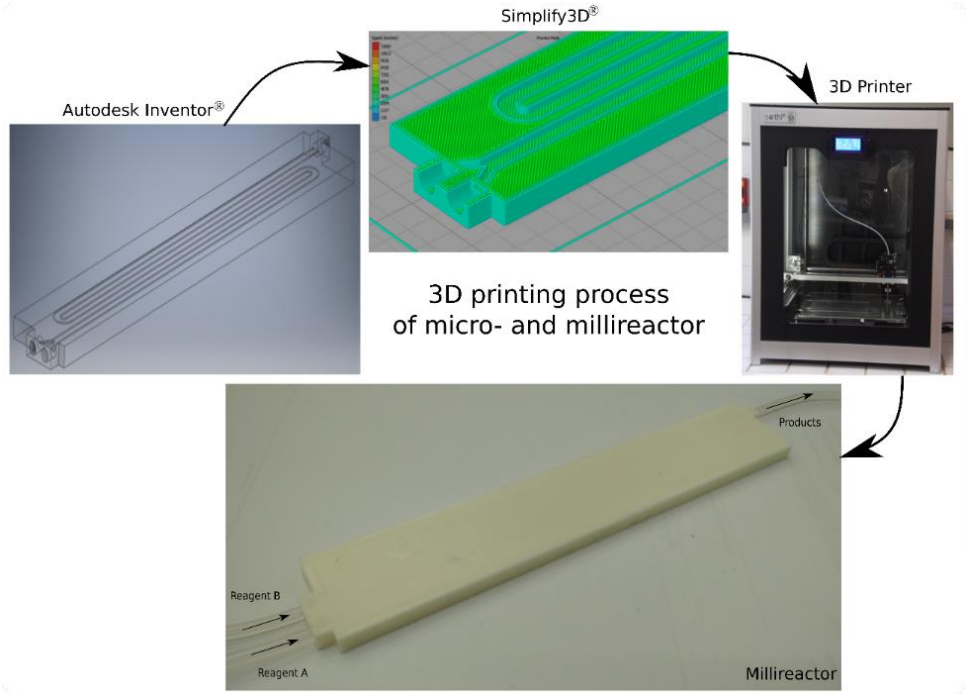
Automatizando a Manufatura

- A impressão em 3D (ou manufatura aditiva) é uma técnica que fabrica objetos físicos de modelos digitais por processos aditivos através dos quais sucessivas camadas de material são depositadas para produzir o objeto final.



Processo de impressão 3D de micro- milirreatores para reações químicas.
Santana et al., *Chinese Journal of Chemical Engineering*, 2019.

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4Qanos
Engenharia Química
UNICAMP

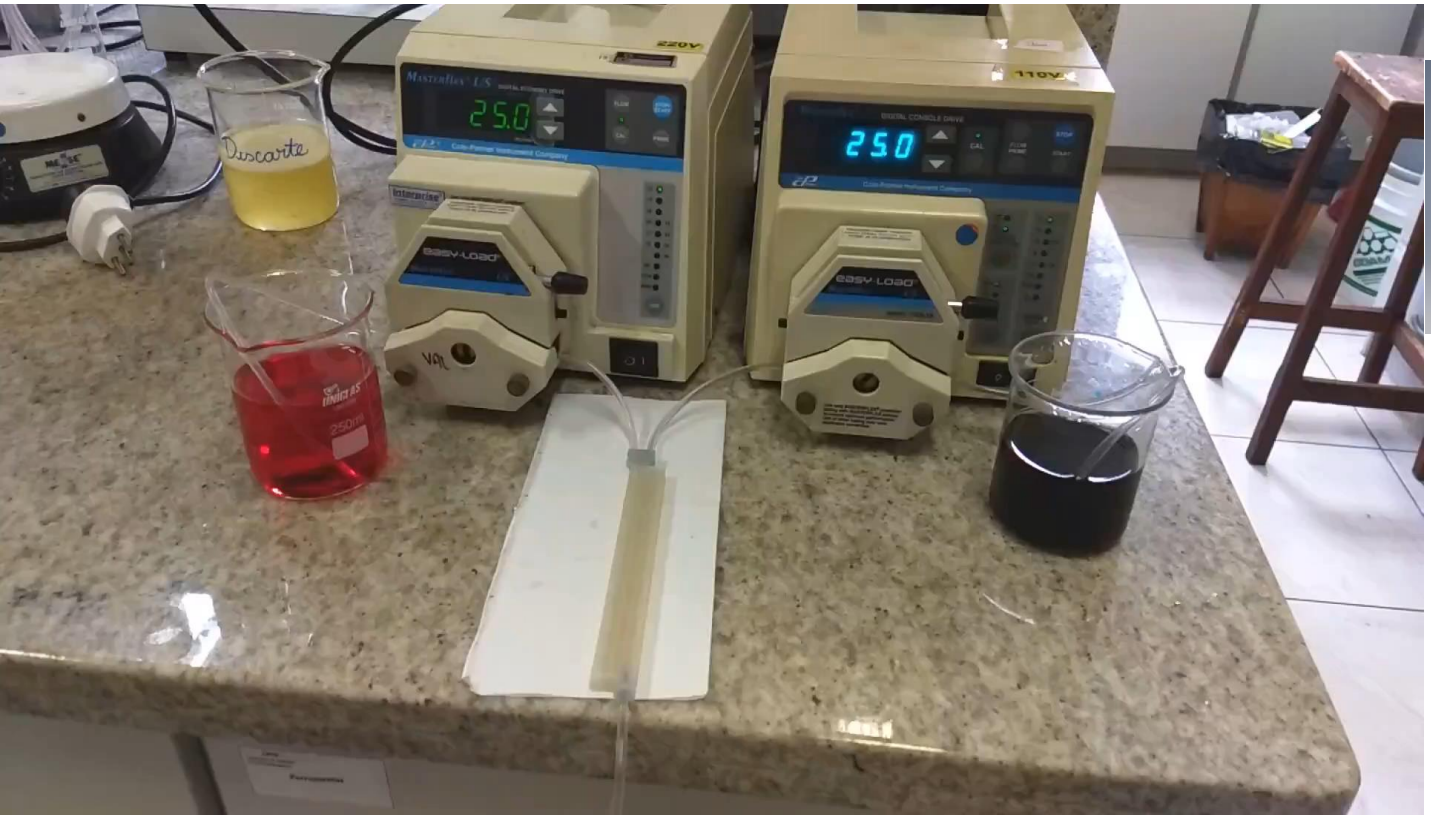
3D printed millireactors for process intensification

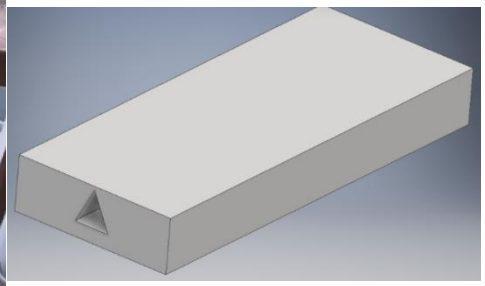
Harrson Santana, Alan Rodrigues, Mariana Lopes,
Felipe Russo, João Lameu and Osvaldir Taranto

Chinese Journal of Chemical Engineering

Video by: Harrson Santana and Adriano Paixão

✓ Dispositivos impressos para elevadas vazões!





Mariana G. M. Lopes

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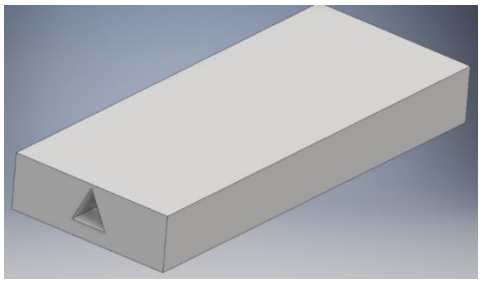
✓ Dispositivos impressos para elevadas vazões!



MTM_1Canal - Bloco de notas

Arquivo Editar Formatar Exibir Ajuda

```
M190 S60.000000
M109 S205.000000
;Basic settings: Layer height: 0.1 Walls: 1.5 Fill: 100

;Print time: 3 hours 37 minutes

;Filament used: 9.32m 27.0g

;Filament cost: None

;M190 S60 ;Uncomment to add your own bed temperature line

;M109 S205 ;Uncomment to add your own temperature line

M104 S205 T0;aquecimento do bico

M140 S60 ;aquecimento rapido mesa

M190 S60  ;espera aqueciento da mesa

M109 S205 ;espera aquecimento bico

G21        ;metric values
```

```
;TYPE:WALL-INNER
G1 F2400 E7.98243
G1 F1200 X152.750 Y26.250 E8.21110
G1 X152.750 Y21.250 E8.31503
G1 X158.250 Y21.250 E8.42937
G1 X158.250 Y173.750 E11.59947
G1 X149.250 Y173.750 E11.78656
G1 X149.250 Y178.750 E11.89050
G1 X141.750 Y178.750 E12.04641
G1 X141.750 Y26.250 E15.21651
G0 F4200 X141.250 Y25.750
G1 F1200 X152.250 Y25.750 E15.44518
G1 X152.250 Y20.750 E15.54911
G1 X158.750 Y20.750 E15.68423
G1 X158.750 Y174.250 E18.87513
G1 X149.750 Y174.250 E19.06221
G1 X149.750 Y179.250 E19.16615
G1 X141.250 Y179.250 E19.34285
G1 X141.250 Y25.750 E22.53374
G0 F4200 X140.750 Y25.250
;TYPE:WALL-OUTER
G1 F1200 X151.750 Y25.250 E22.76240
```

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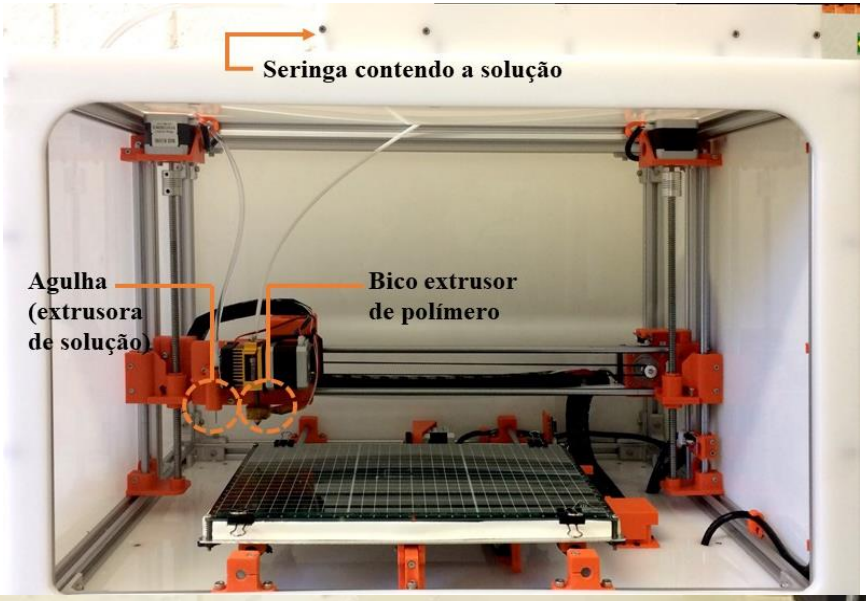
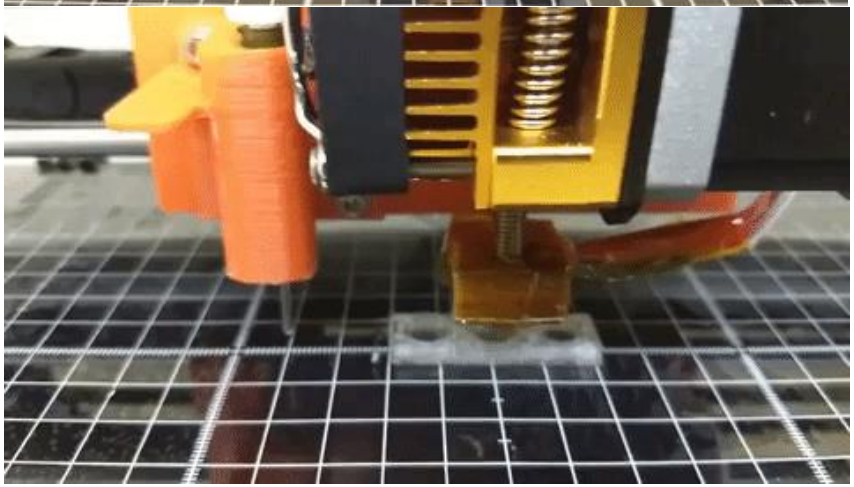
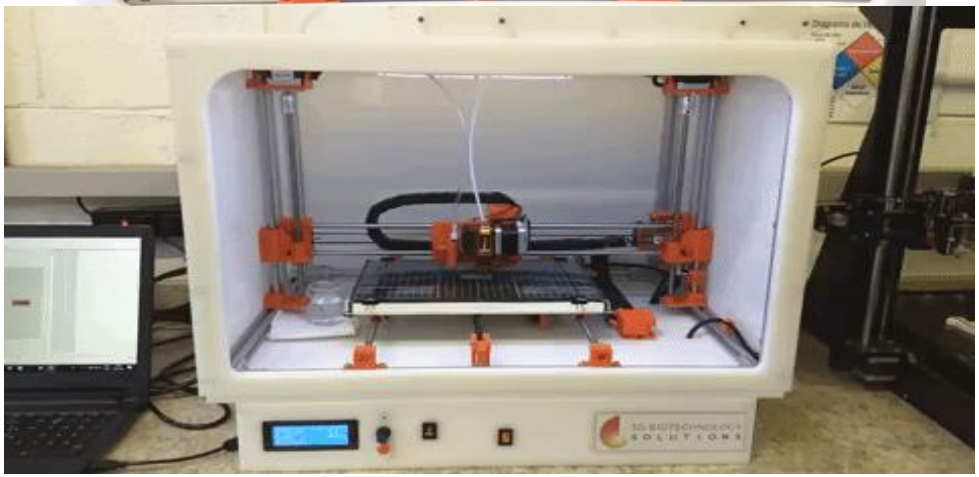
Sistemas robóticos







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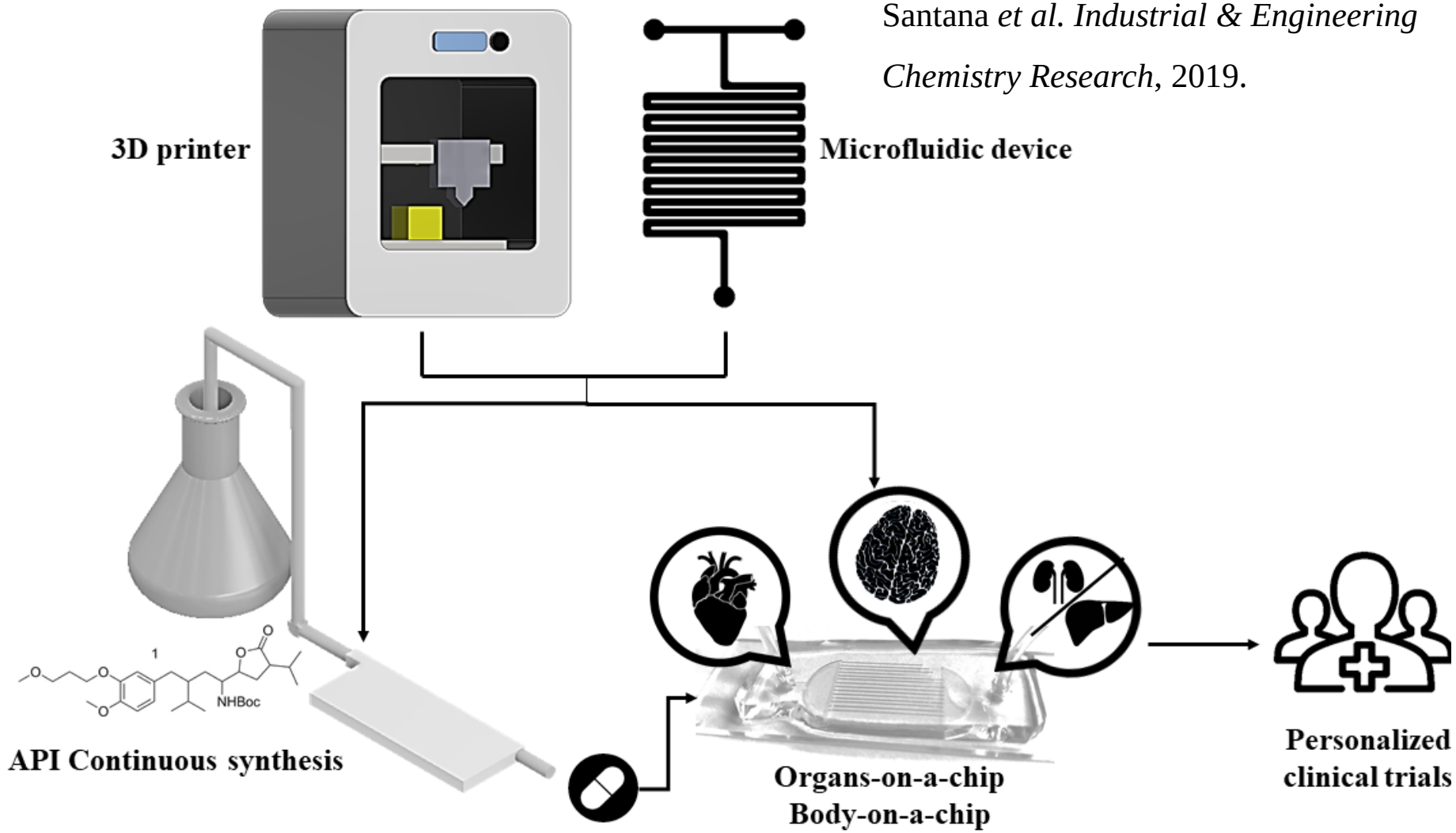
Biotecnologia

❖ Dispositivos microfluídicos e impressão 3D para triagem de medicamentos

Santana *et al. Industrial & Engineering Chemistry Research*, 2019.



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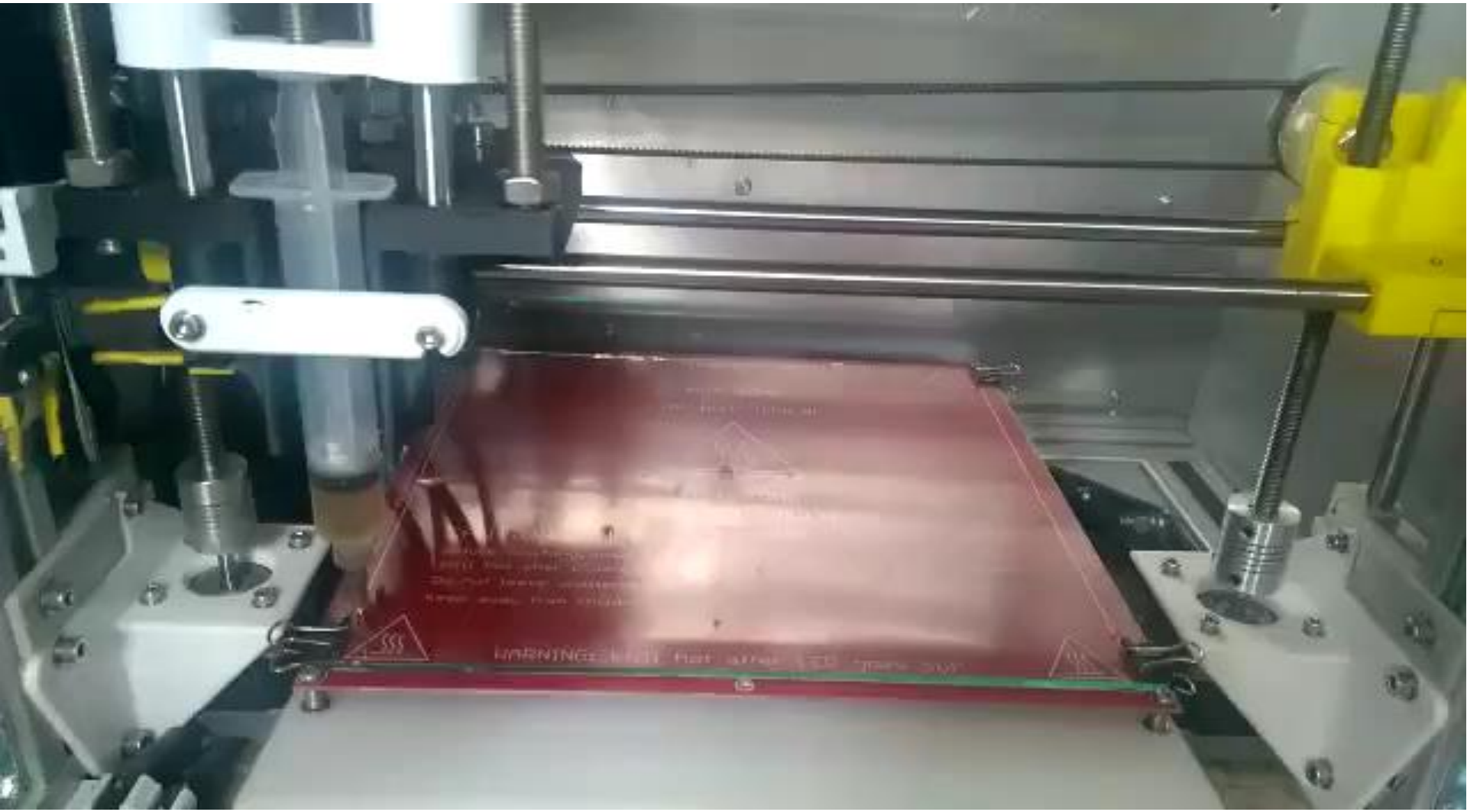
Bioimpressão



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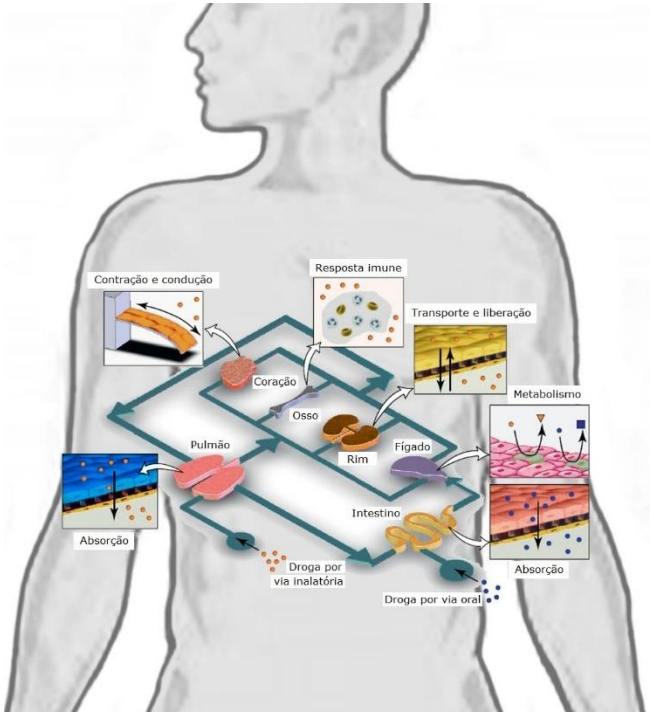
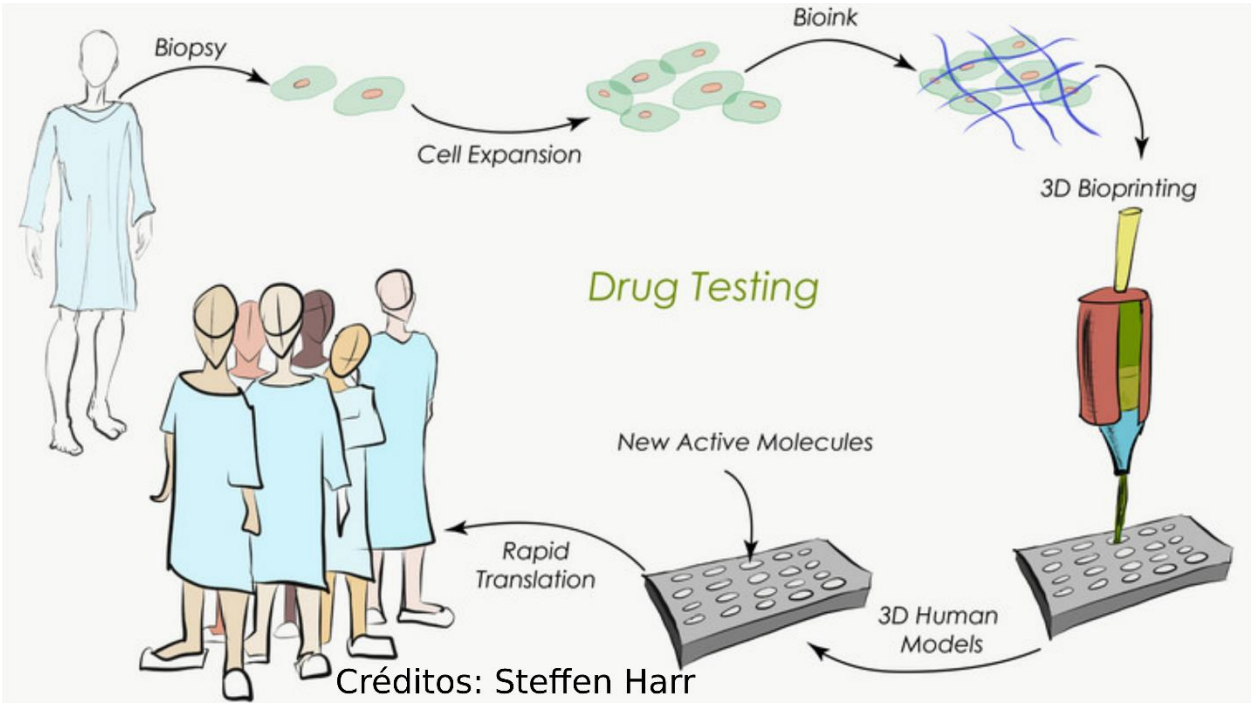
Bioimpressão

❖ **Orgão-em-chip**: dispositivos que visam à mimetização de padrões fisiológicos de órgãos





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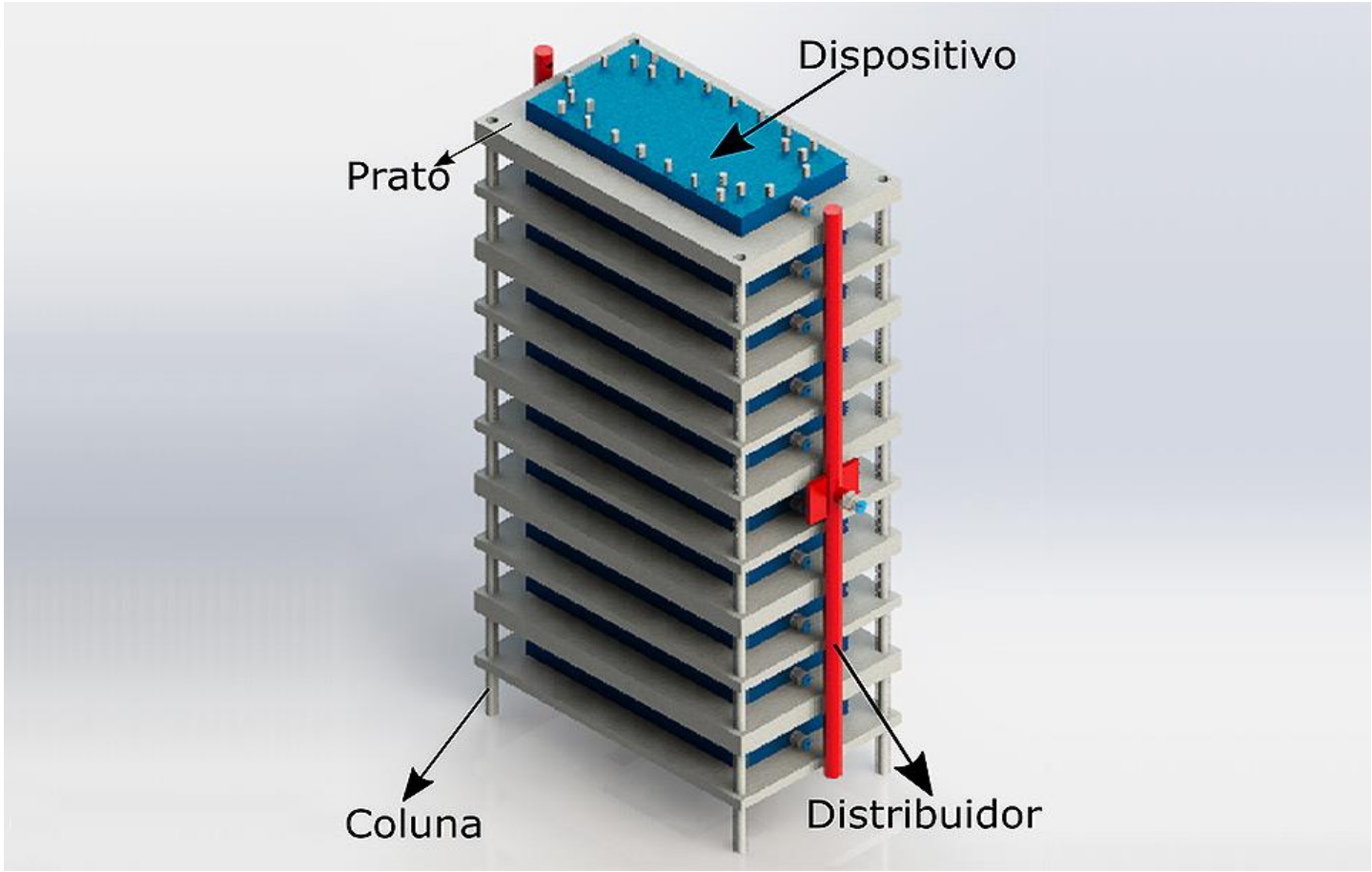
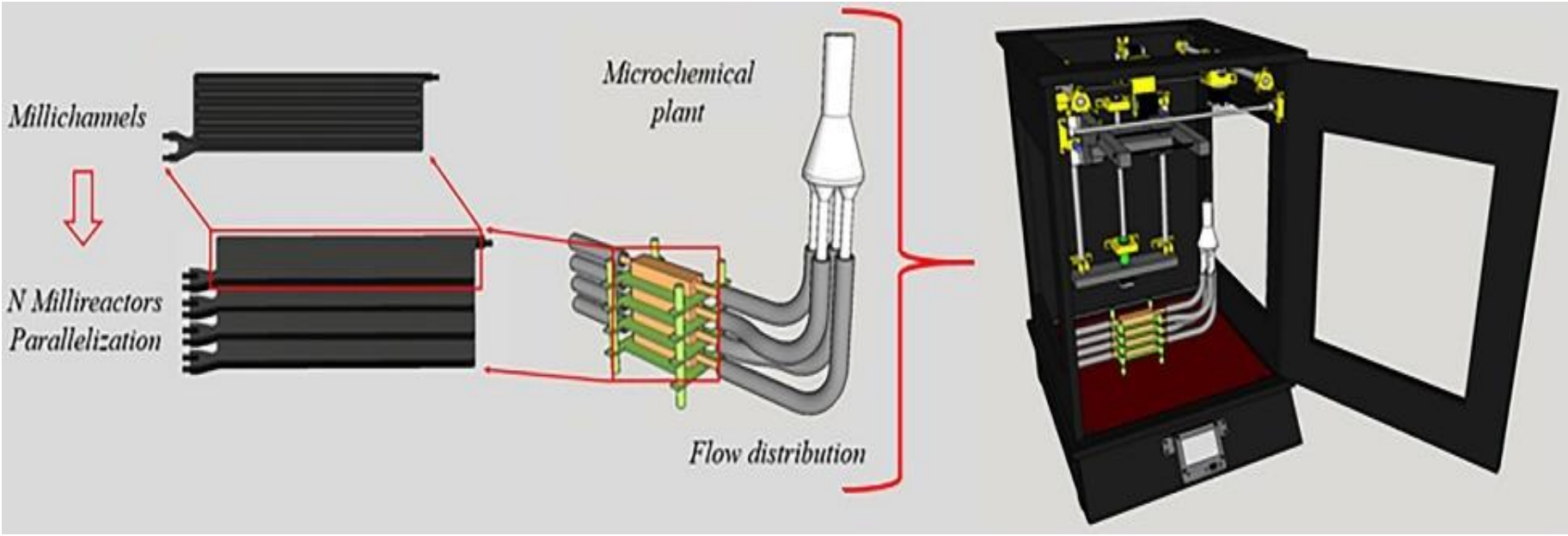
Escalonamento

- Como imprimir uma planta química?



- Imprima a sua própria microplanta química e produza seus produtos químicos.



Lopes *et al. Energy Conversion and Management*, v. 184, p. 475-487, 2019.

Lopes *et al. Energy Conversion and Management*, v. 184, p. 475-487, 2019.

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