COMUNICAÇÃO TÉCNICA

Nº 179279

CFD study to scale -up of W/O emulsions with LTCC parallelized vortex micromixer

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Palestra apresentada no LATIN AMERICAN MICROFLUIDSICS CONFERENCE, 1., 2024, São Carlos. Lecture... 26 slides.

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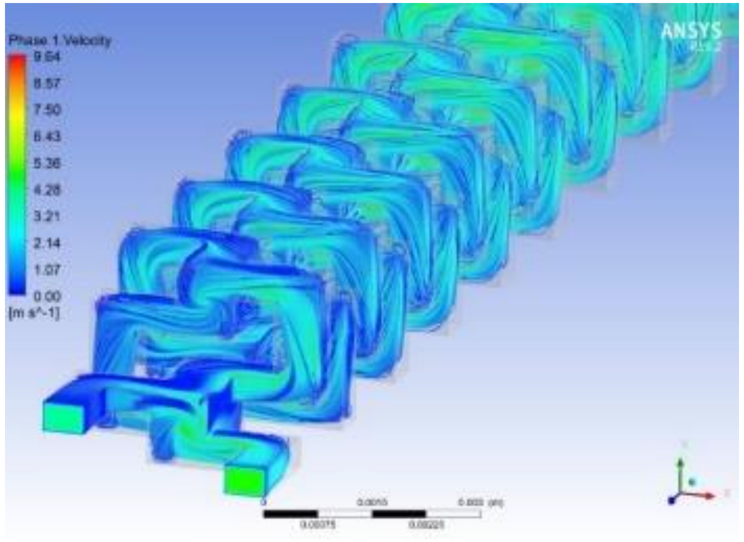
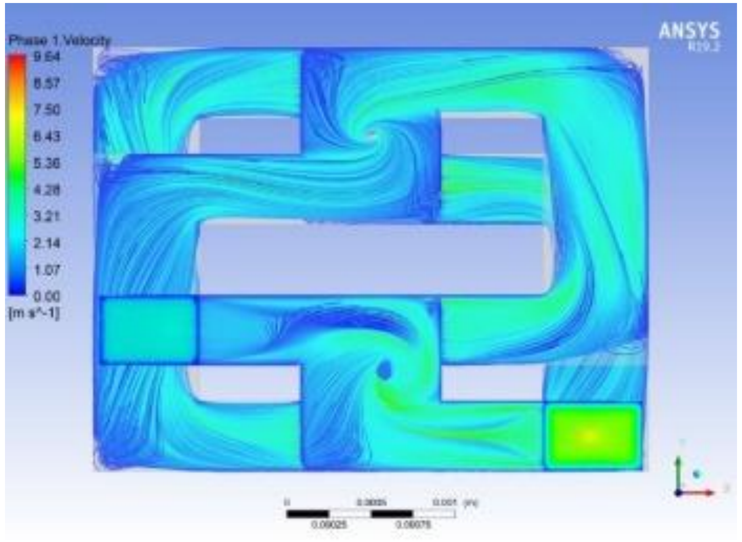
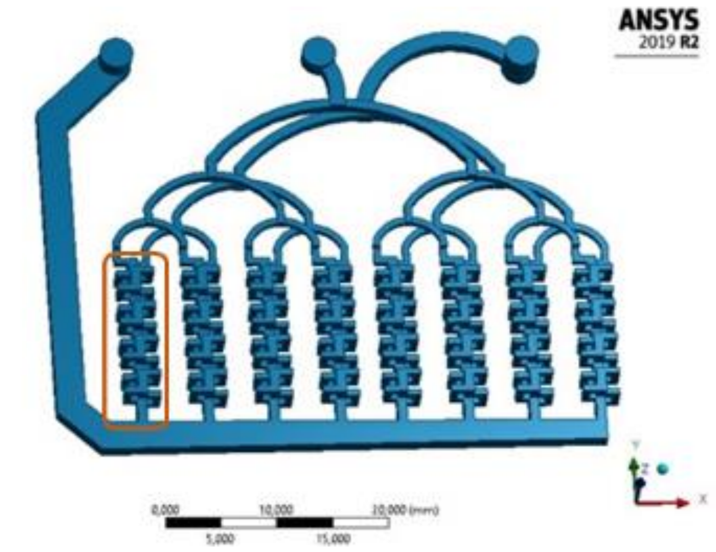
CFD STUDY TO SCALE-UP OF W/O EMULSIONS WITH LTCC PARALLELIZED VORTEX MICROMIXER

Martha Lucia Mora-Bejarano(R)[a*], Aline Furtado Oliveira(R)[a], Adriano Marim de Oliveira(R)[a], Mario Ricardo Gongora-Rubio(R)[a]

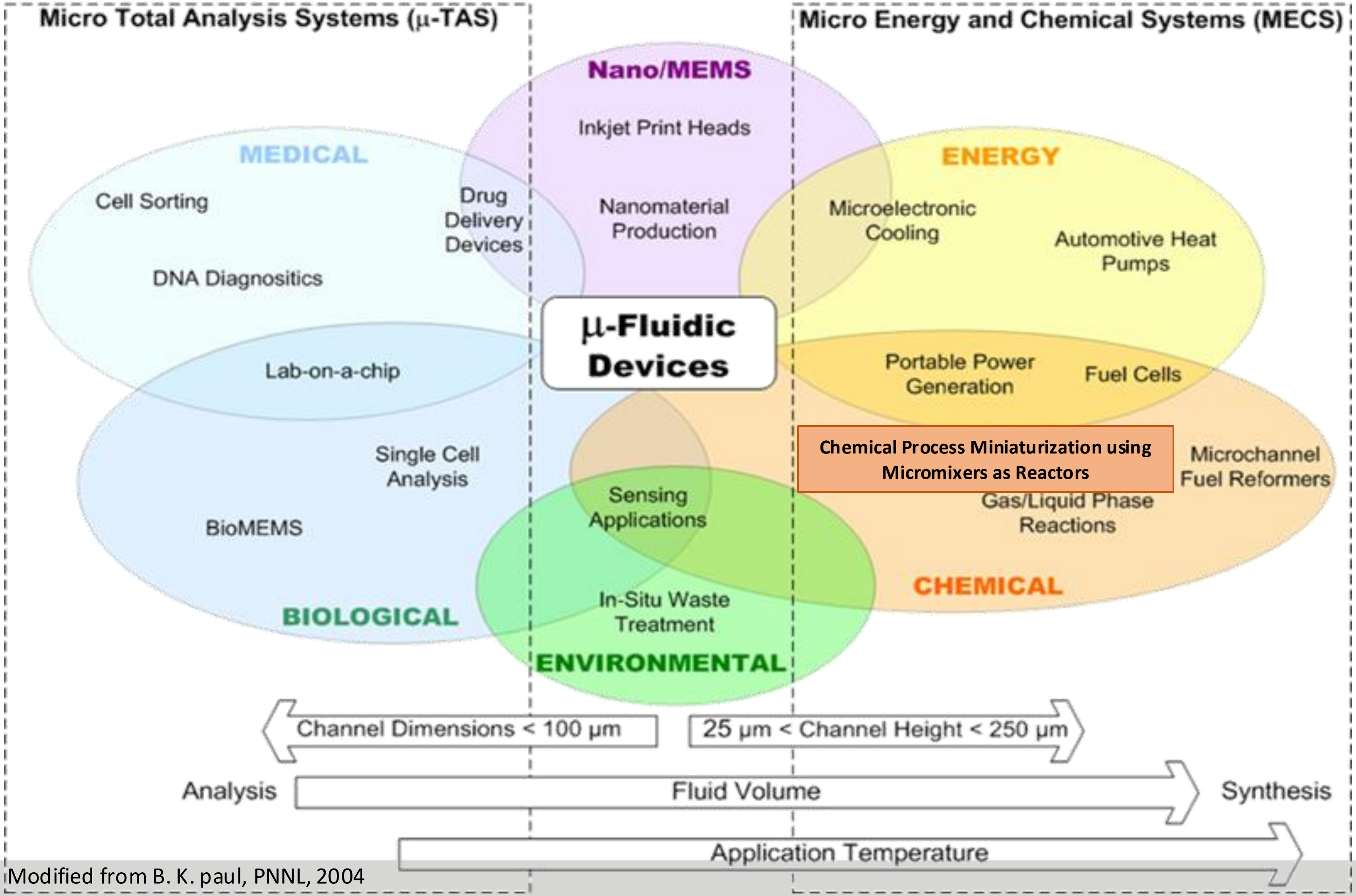
*[a] Institute for Technological Research (IPT), Bionano/ LMI, São Paulo, SP, Brazil, *e-mail: mmorabejarano@ipt.br*





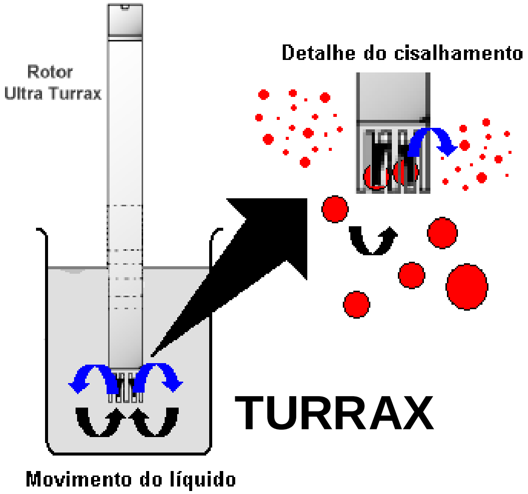


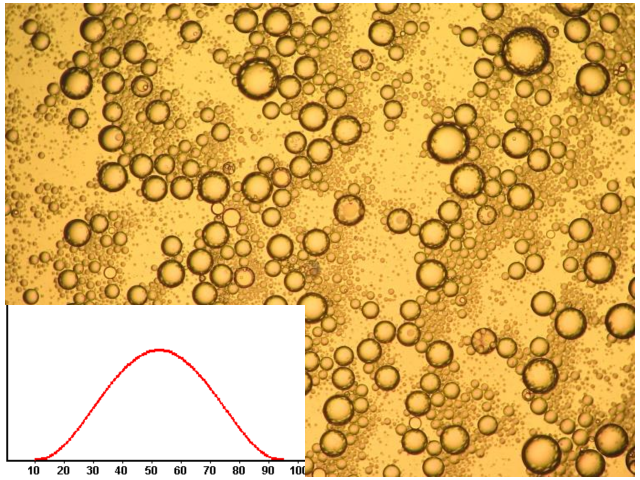
MICROFLUIDICS APPLICATIONS

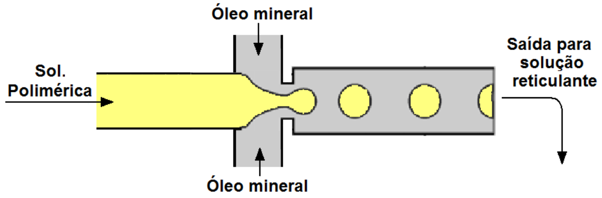


Modified from B. K. paul, PNNL, 2004

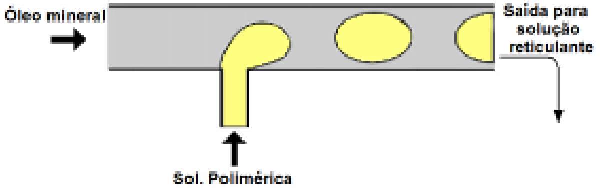
SINGLE EMULSIONS USING MICROFLUIDIC DEVICES

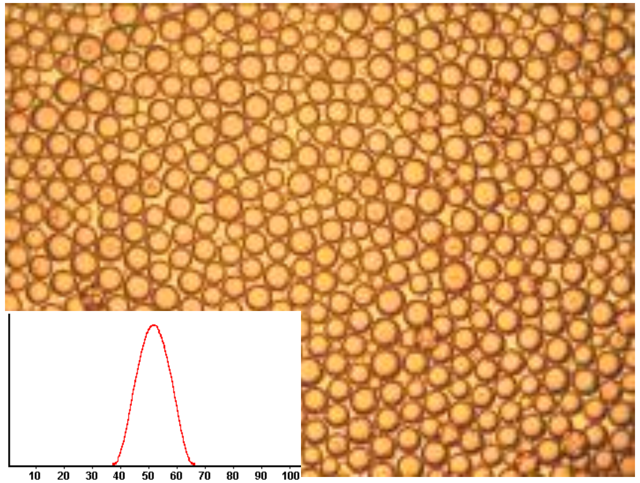


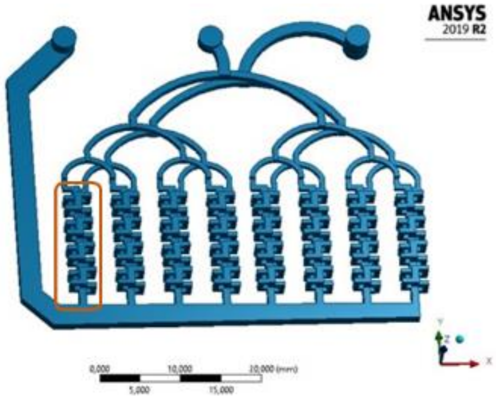




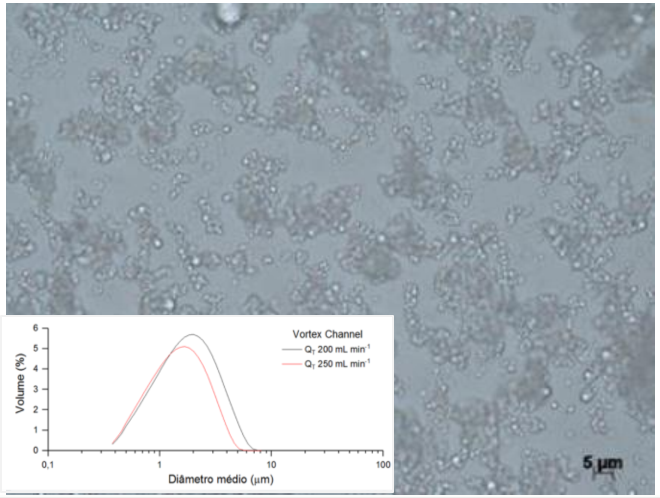
MICROFLUÍDIC DEVICES



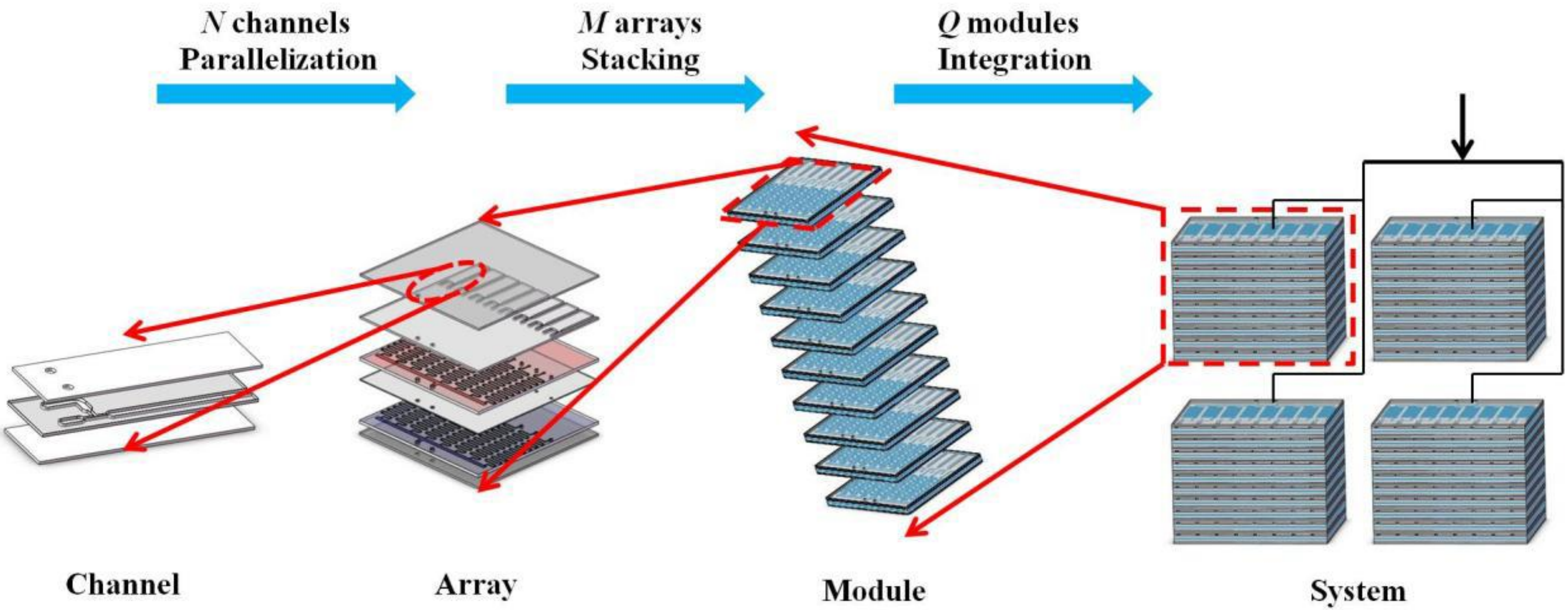




PARALLELIZED MICROMIXERS



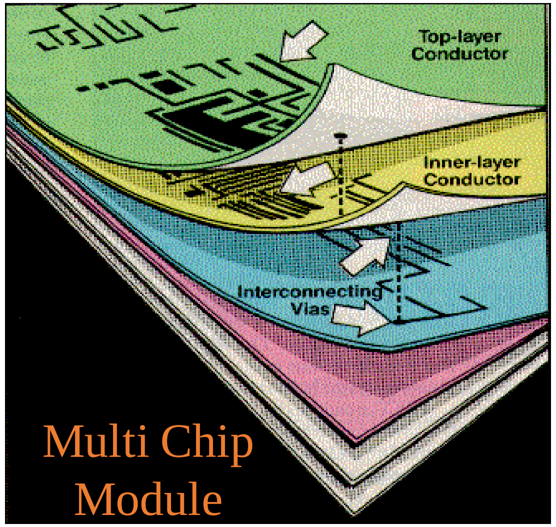
MICRODEVICE SCALE-UP STRATEGY

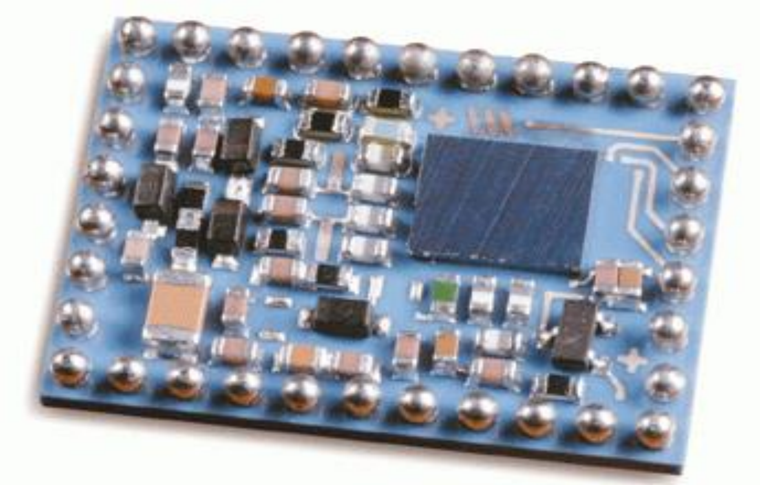


Source: **(DOI):**10.1016/j.cej.2017.06.028

WHAT IS LTCC ?

- LTCC (Low Temperature Cofired Ceramics) technology was originally developed by Hughes and DuPont for Military Systems, using Glass-Ceramic Composite Materials & thick film technology.
- The (LTCC) technology can be defined as a way to produce multilayer circuits with the help of single tapes, which are to be used to apply conductive, dielectric and / or resistive pastes on. These single sheets have to be laminated together and fired in one step all.





Bluetooth Interface (National)

- Nowdays LTCC is a Microsystem technology integrating Microelectronics, Microfluidics, Microwave & Sensors in a single package.

LTCC PROCESS AT LMI

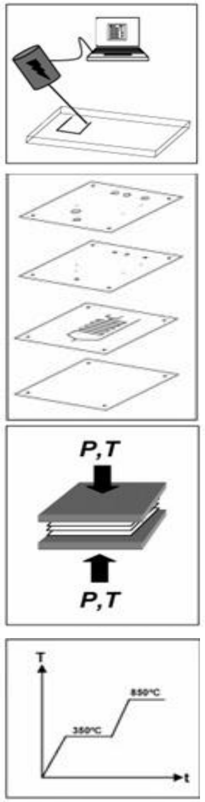
Micromachining
(Laser)

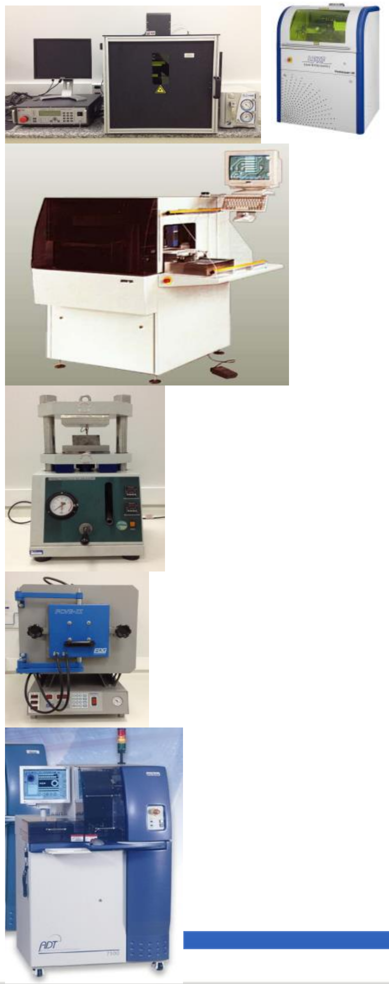
Thick Film Deposition
(Screen Printer)

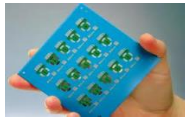
Lamination

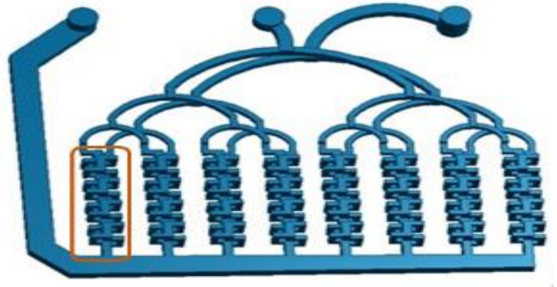
Sintering

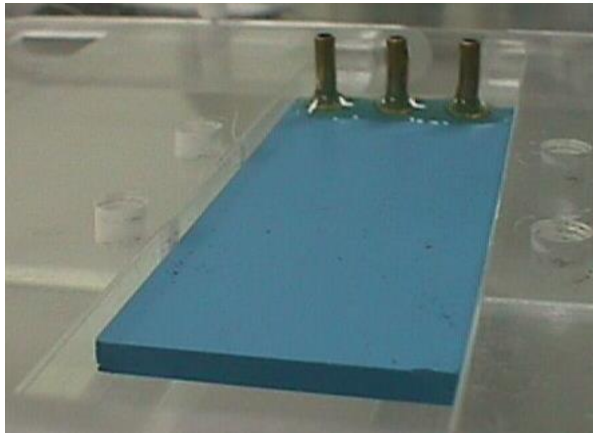
Dicing





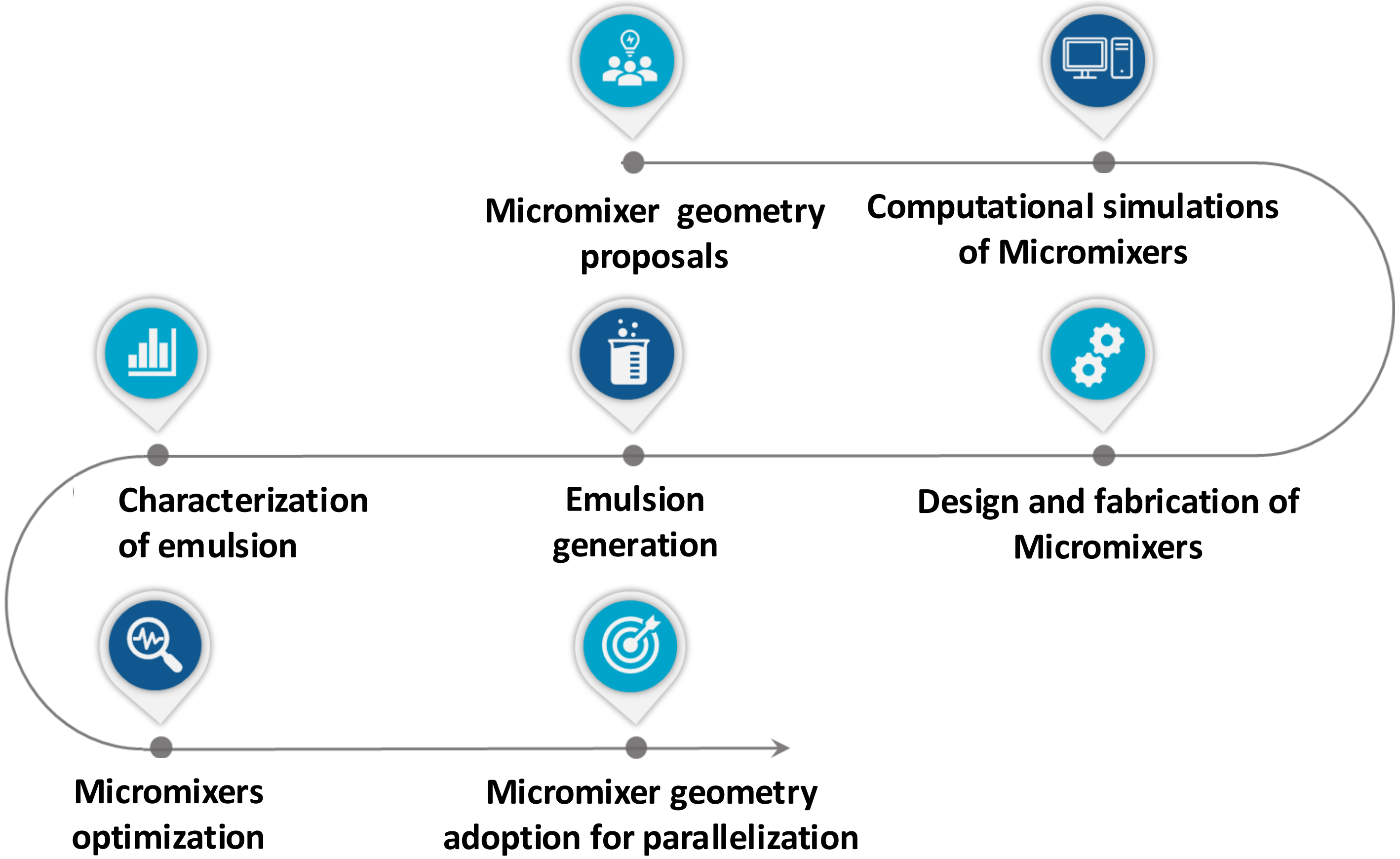






LTCC Micromixing Device and its internal parallelized geometry

EVALUATION OF SINGLE MICROMIXERS



PROCESS CONDITIONS, MODELS AND HYPOTHESES

- Non-Newtonian fluid
- Multiphase flow
- Implicit Euler – Euler, 2nd order, model
- Homogeneous distribution of the fluid at the micromixer inlet
- Constant velocity at the inlet
- Atmospheric pressure at the micromixer outlet

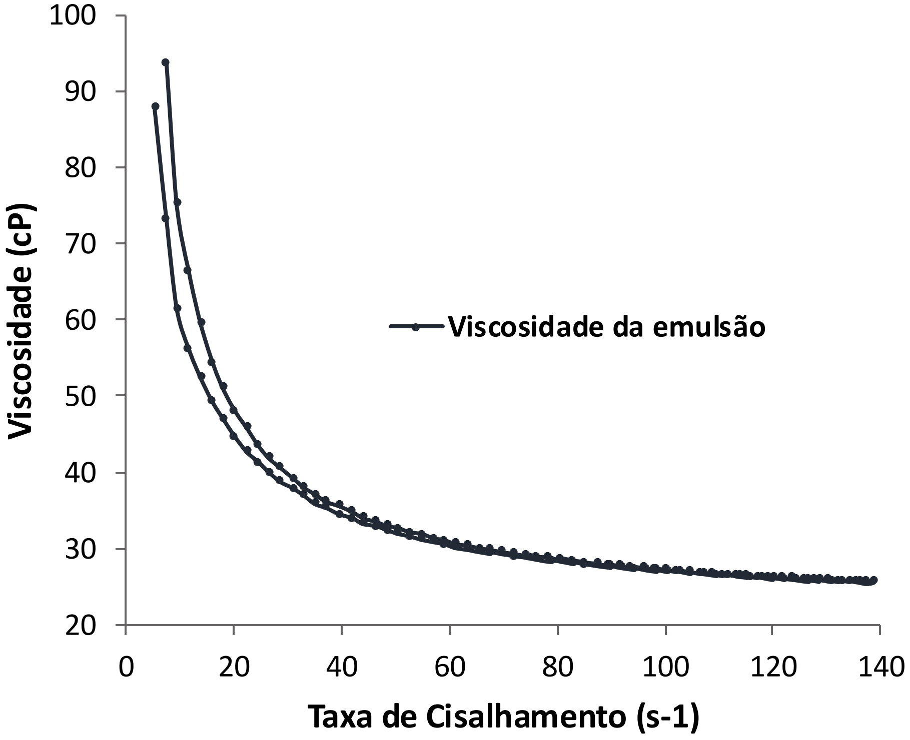
PHYSICAL AND CHEMICAL PROPERTIES

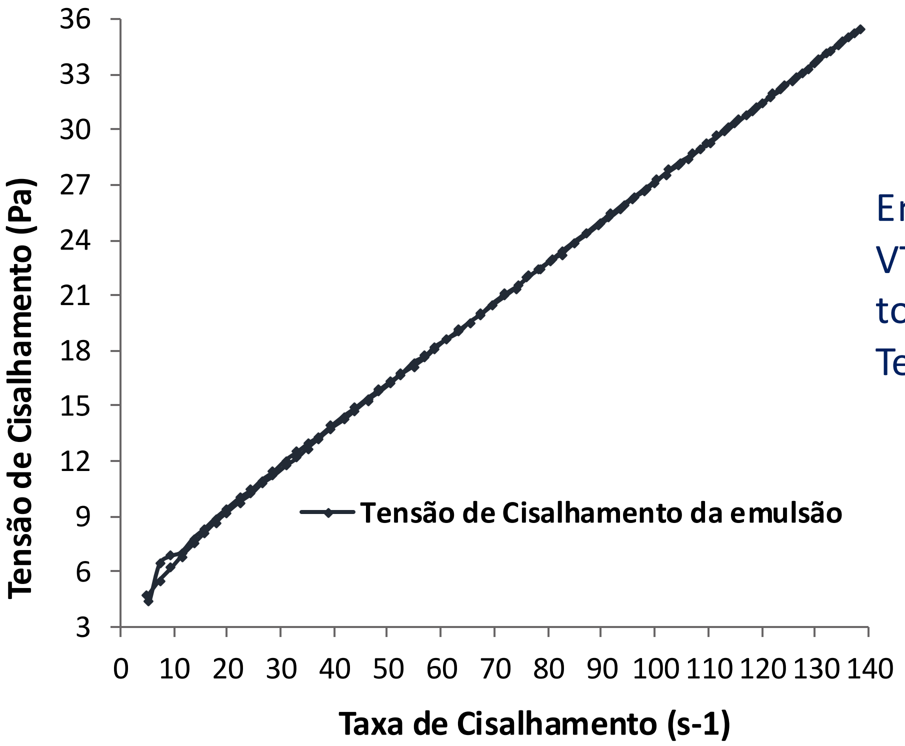
Property	Oily phase	Aqueous phase	Emulsion W/O
Viscosidade (kg $m^{-1}.s^{-1}$)	0,00396	0,00144	Non-Newtonian Power Law model
Densidade (kg.m^{-3})	781,0	1127,3	980,0
Tensão superficial	0,026535	0,07197	

Emulsion composition:

- Aqueous phase: 40%
- Oily phase: 60%
- Aqueous phase: 4 M hydrochloric acid solution + 3.5% w/w NaCl
- Oil phase: hexadecene + 2% w/w Cybermul® lipophilic surfactant

RHEOLOGICAL BEHAVIOR OF THE W/O EMULSION

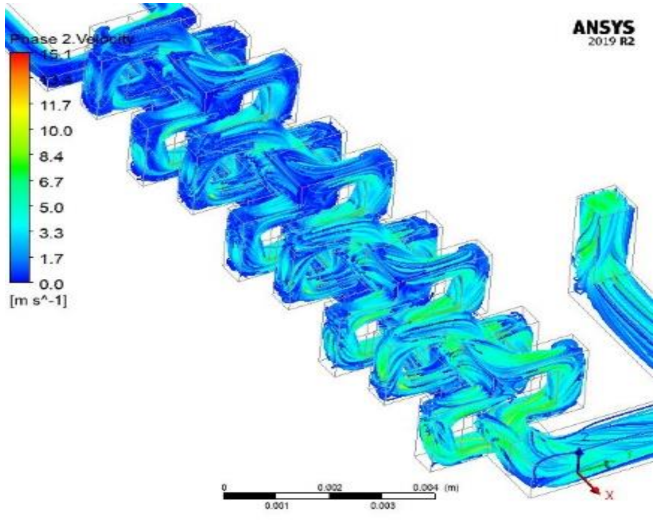


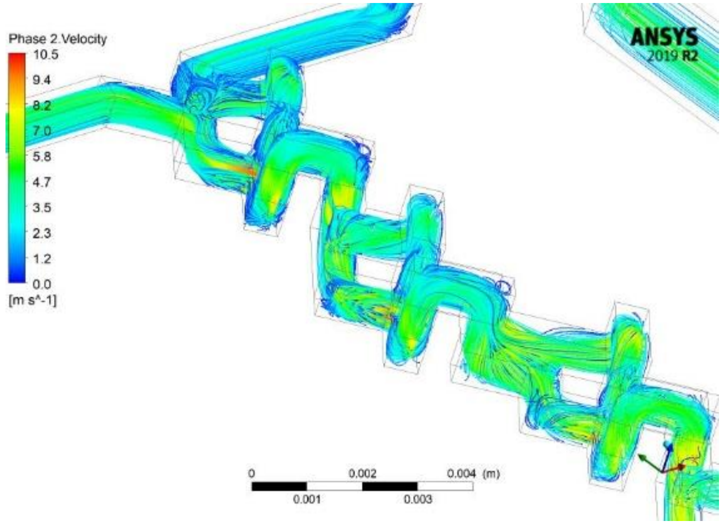


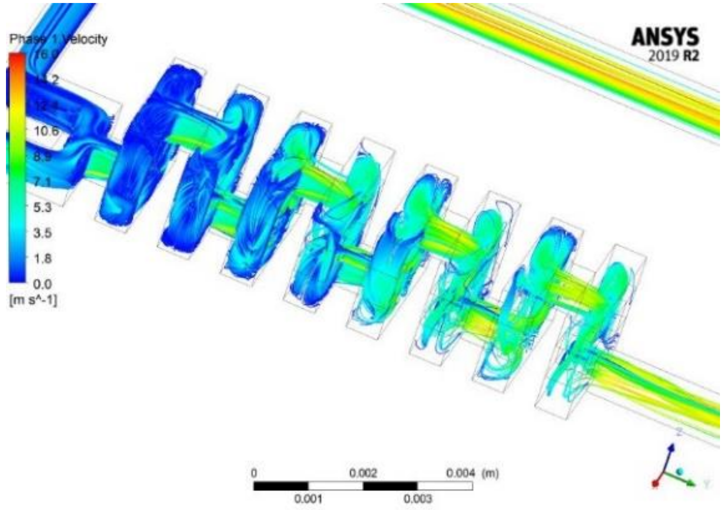
Emulsion sample prepared in VT micromixer;
total flow rate: 200 mL.min-1
Temperature: 23°C

Viscosity (η) can be calculated by the Power Law model, with k = 0.11608; n = 0.684. $\eta = \mathbf{k}\dot{\gamma}^{n-1}$

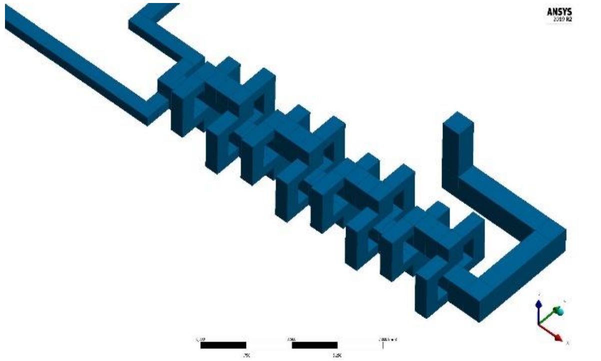
COMPUTATIONAL FLUID DYNAMICS (CFD) STUDY OF THE SINGLE MICROMIXERS

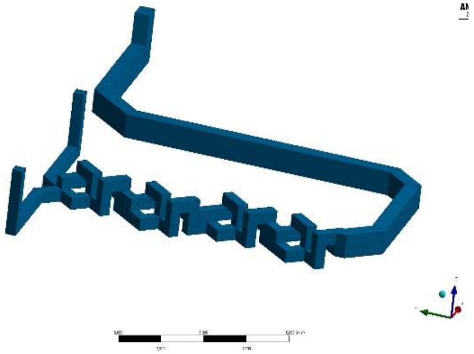


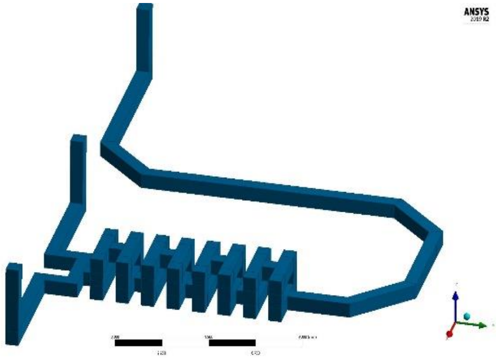


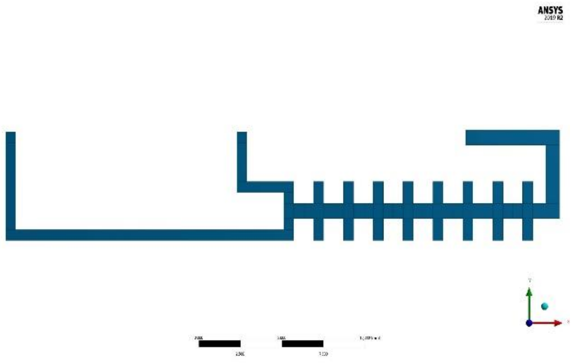


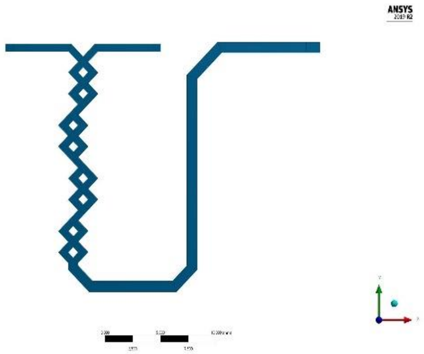
CALCULATION DOMAIN OF MICROMIXERS

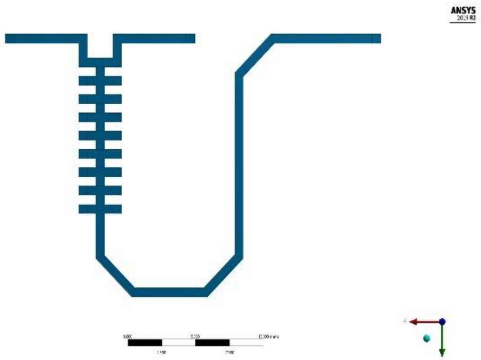










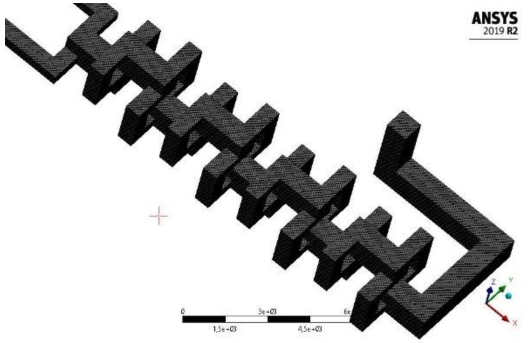


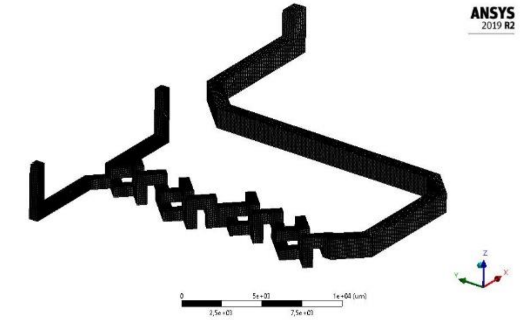
Vortex (VT)
Hydraulic Diameter (µm)
Main Channel 930
Lateral Channel 600

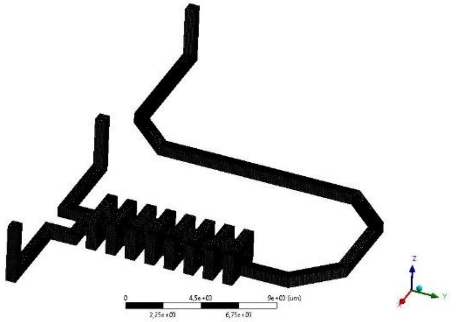
Crossing Channel (CC)
Hydraulic Diameter (µm)
652

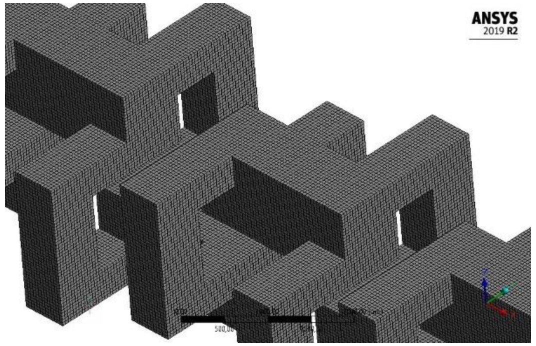
HH-Channel
Hydraulic Diameter (µm)
652

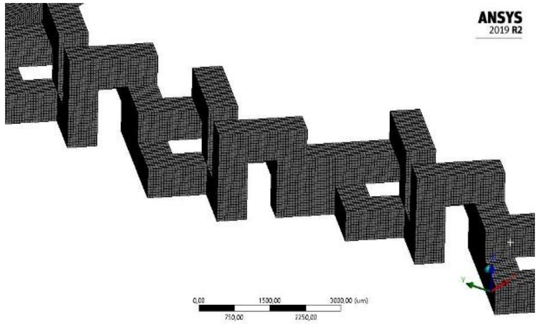
GEOMETRY DISCRETIZATION: DETAILS OF THE VORTEX-FORMING ASSEMBLIES AND GENERATED HEXAHEDRAL MESH

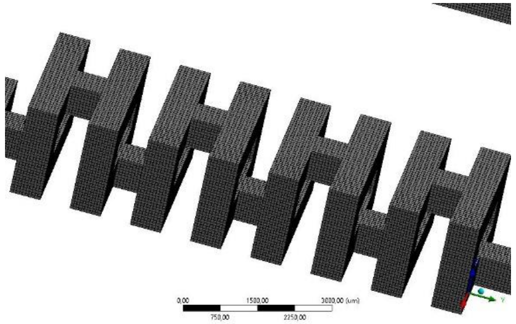












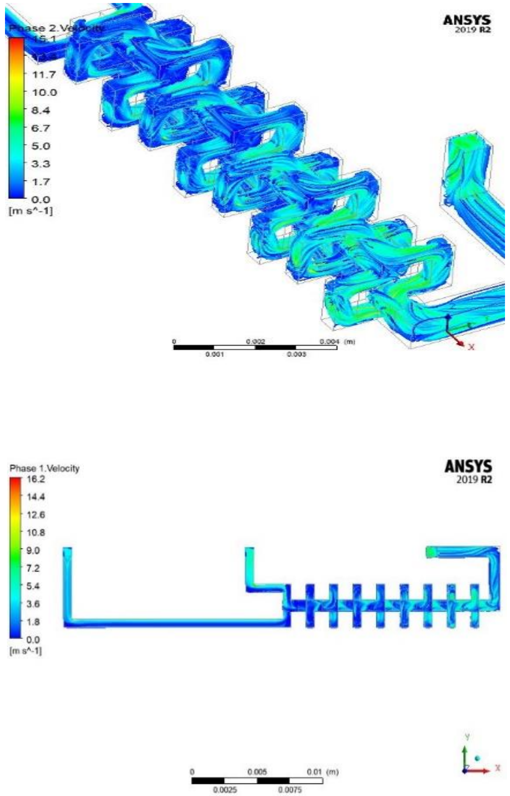
Skewness: 0,3

Vortex (VT)

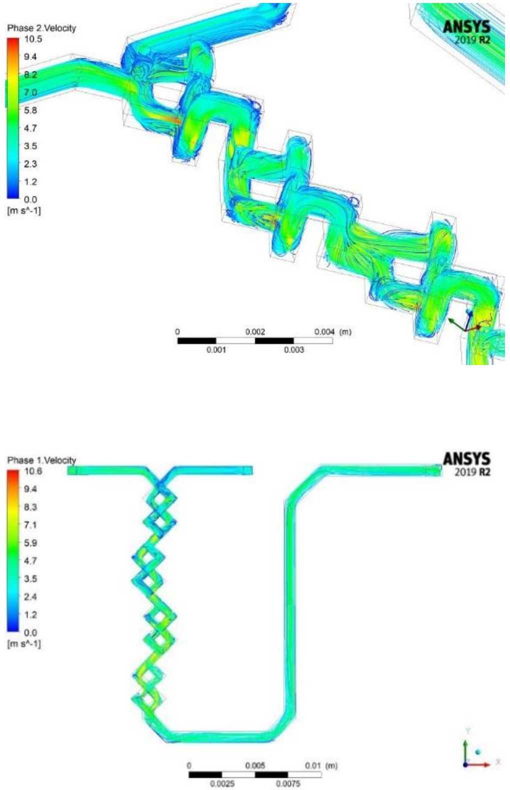
Crossing Channels (CC)

HH-Channels

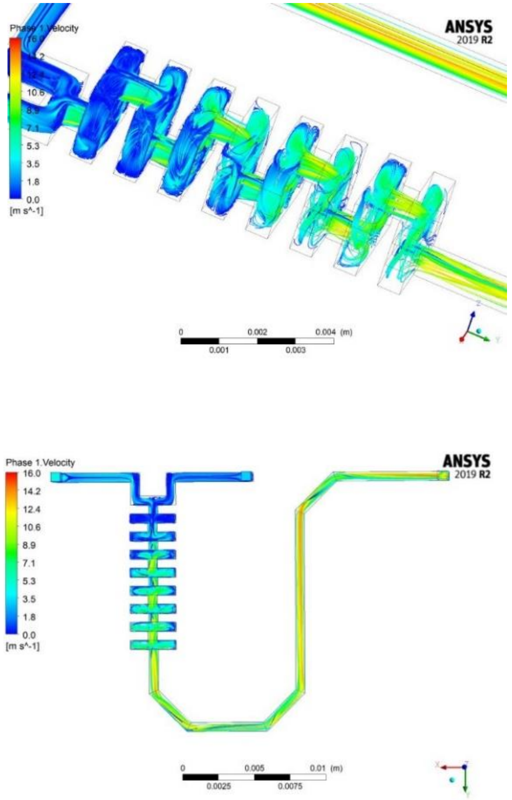
COMPUTATIONAL FLUID DYNAMICS (CFD) RESULTS CURRENT LINES COLORED BY THE VELOCITY MAGNITUDE



Vortex (VT)



Crossing Channels (CC)



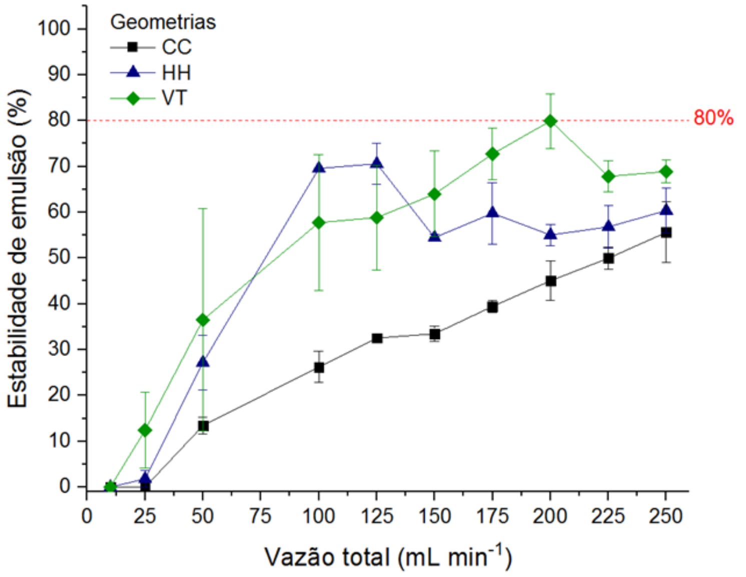
HH-Channels

No preferential paths were observed

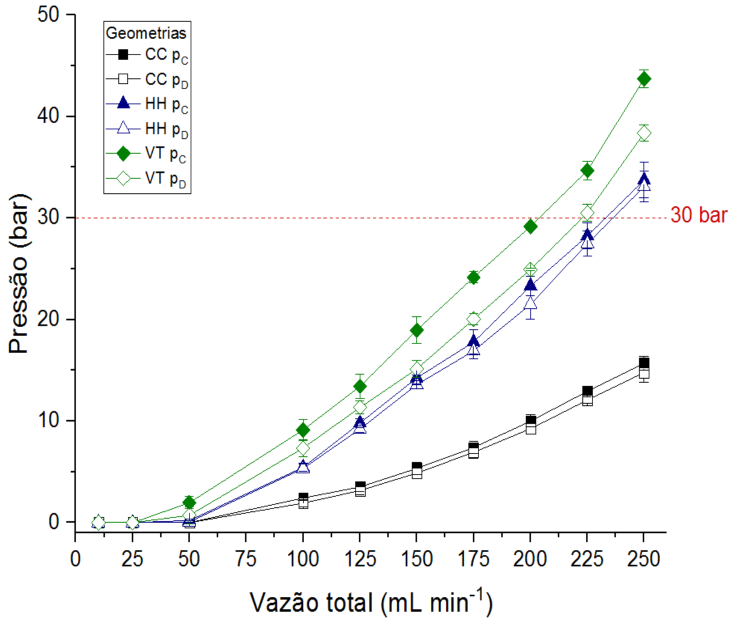
Total flow rate: 200 mL.min-1

SINGLE MICROMIXERS EVALUATION PARAMETERS

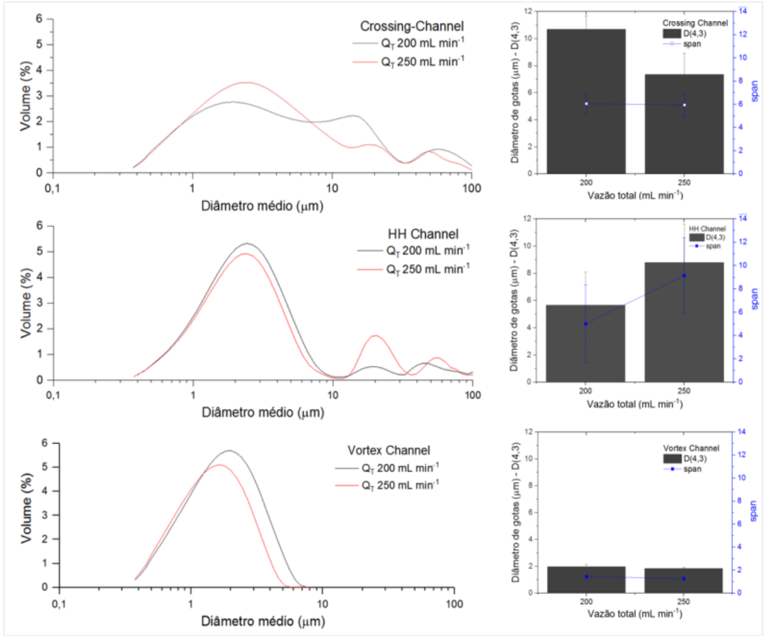
Emulsion stability



Pressure drop



Average droplet diameter

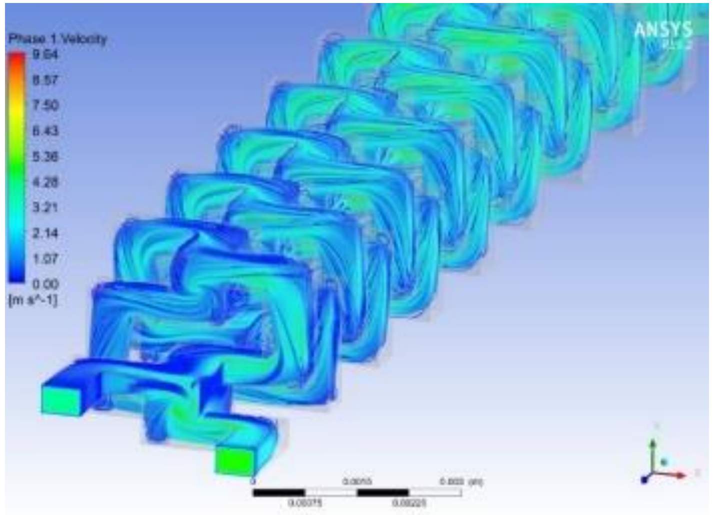


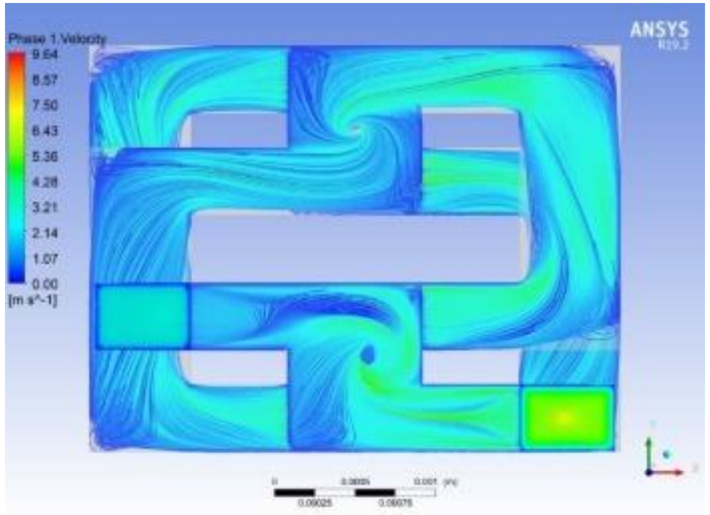
Vortex Channel (VT) micromixer had the best results in terms of stability, droplet sizes and pressure drop values. Pressure drop values were validated with those obtained in laboratory tests.

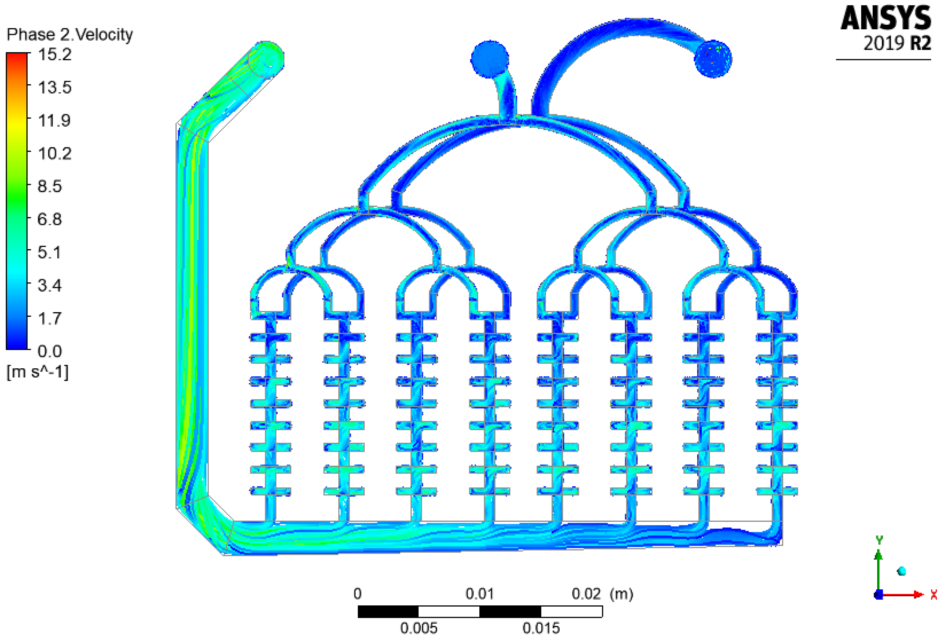
SCALE-UP OF W/O EMULSIONS WITH LTCC PARALLELIZED VORTEX MICROMIXER

- Design of the experimental apparatus on a production model scale
- Design of the Parallelized Micromixer
- Computational simulations of Parallelized Micromixer
- Operational tests Parallelized Micromixer
- Production of emulsion Parallelized Micromixer
- Characterization of emulsion
- Production of emulsion Production model scale

COMPUTATIONAL FLUID DYNAMICS (CFD) STUDY OF THE PARALLELIZED MICROMIXER







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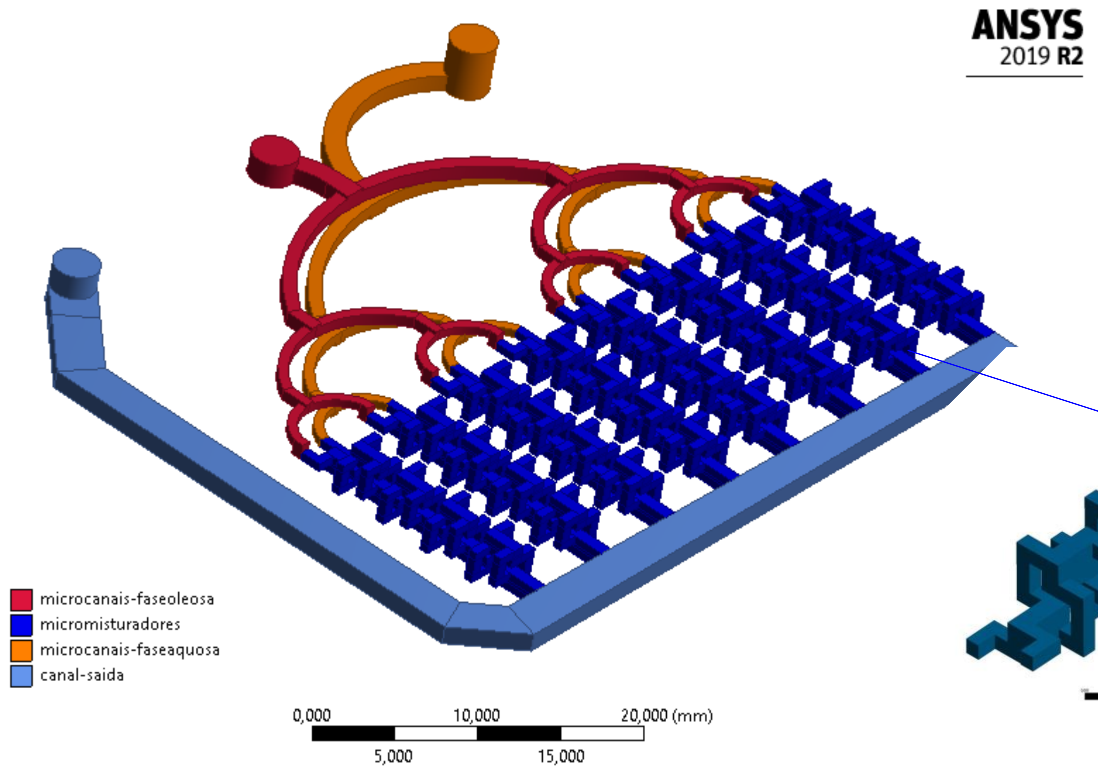
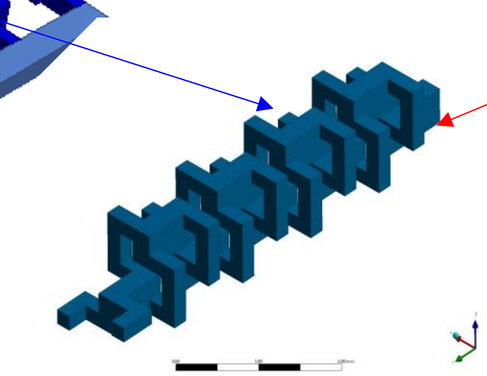
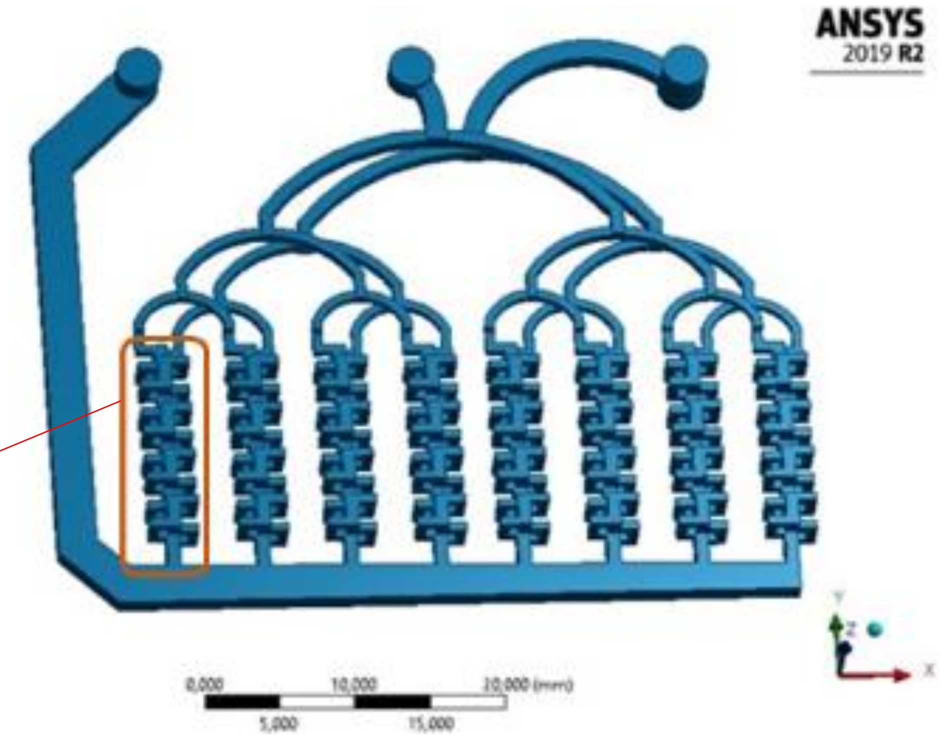
GOVERNO DO ESTADO

CALCULATION DOMAIN OF INTERNAL PARALLELIZED VT MICROMIXER

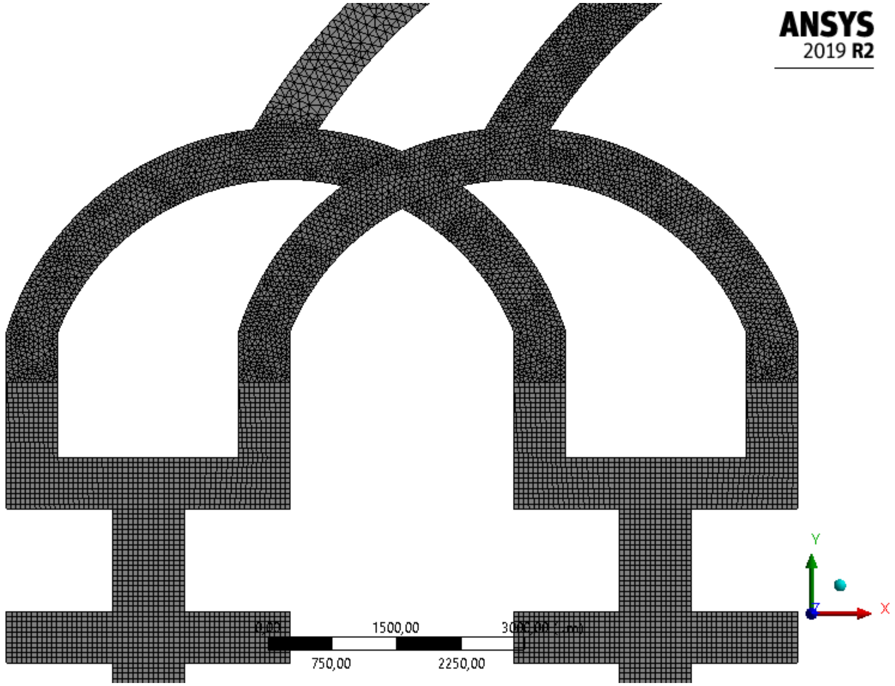


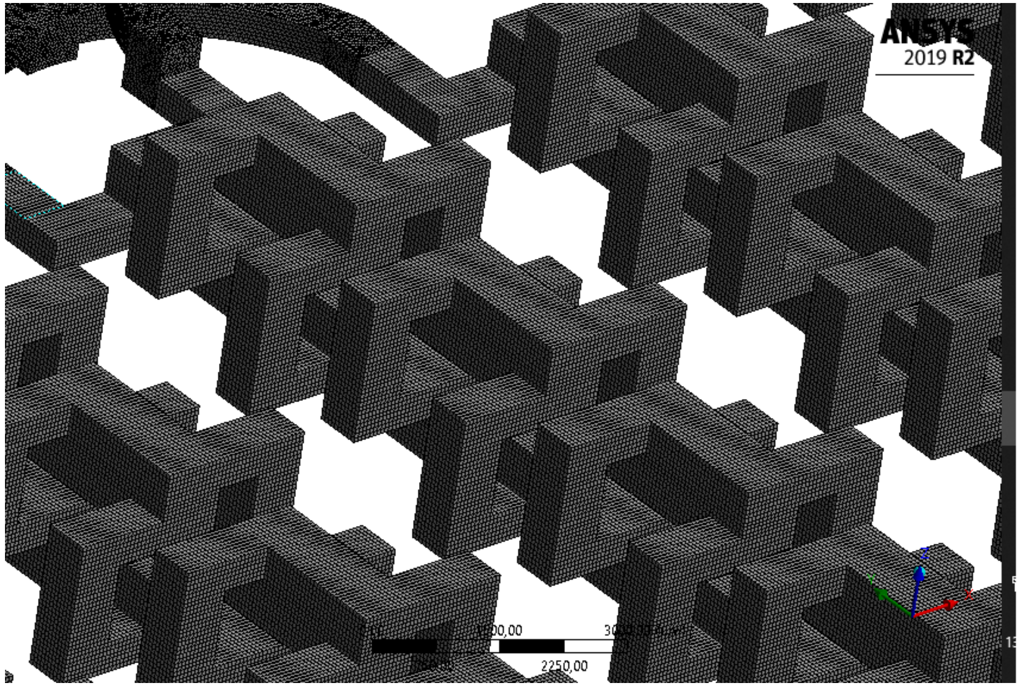




Simple VT Micromixer

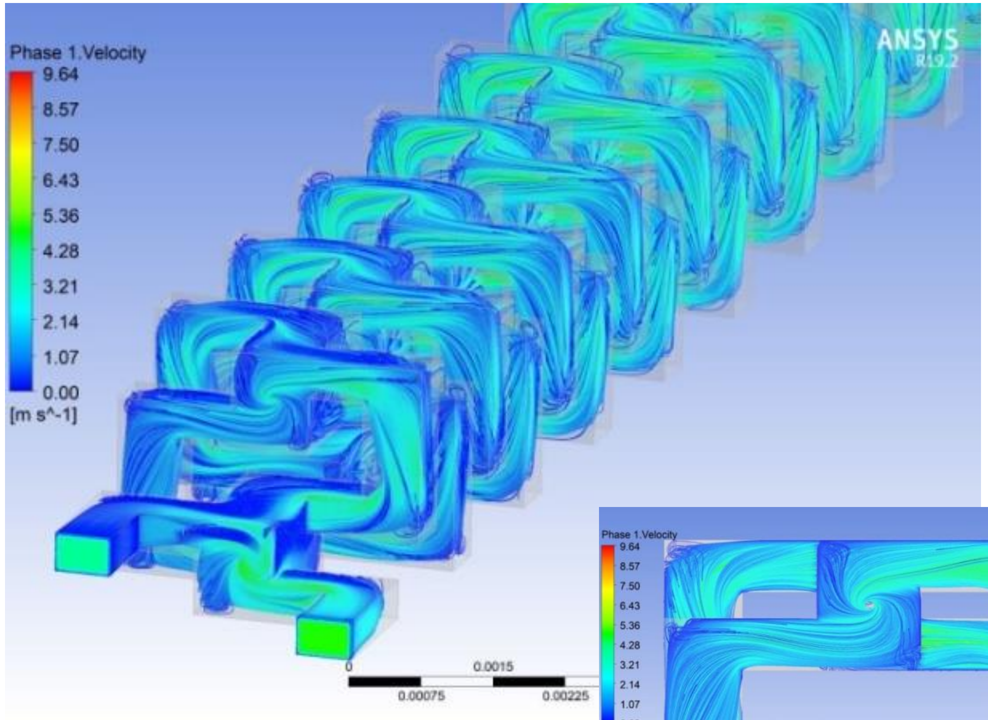
GEOMETRY DISCRETIZATION: DETAILS OF THE VORTEX-FORMING ASSEMBLIES AND GENERATED HEXAHEDRAL AND TETRAHEDRAL MESH

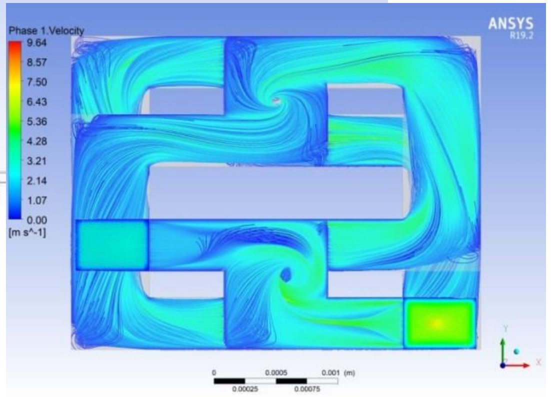


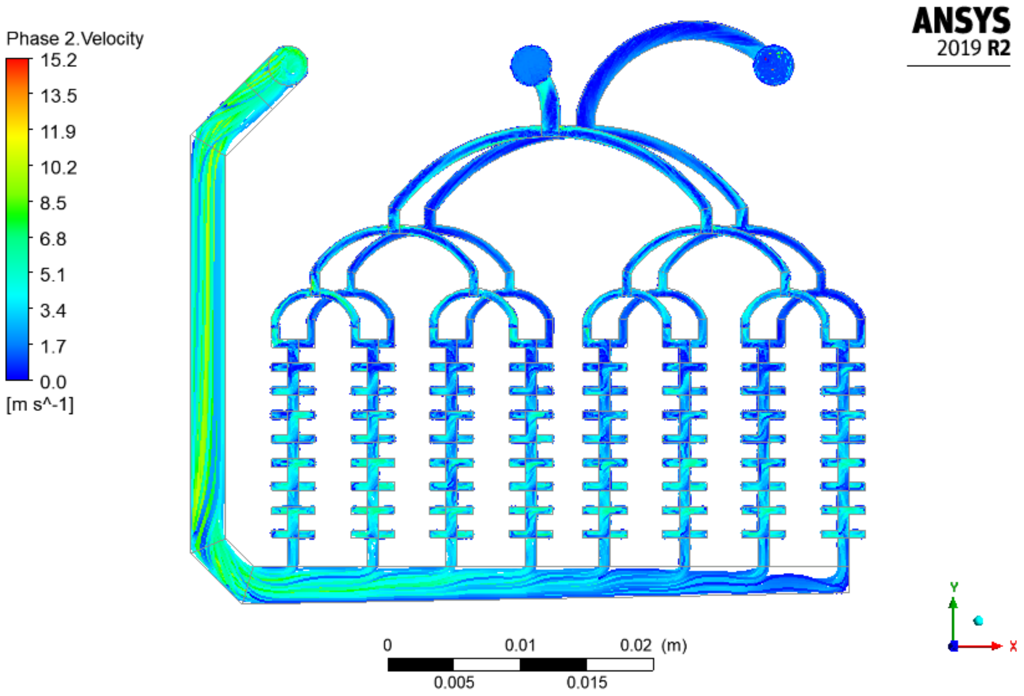


Element average size of approx: 60 to 200 µm. The mesh volumes number was around 3.900.000. Average skewness value: 0.3 and standard deviation values: 0.11

COMPUTATIONAL FLUID DYNAMICS (CFD) RESULTS CURRENT LINES COLORED BY THE VELOCITY MAGNITUDE







Total flow rate:
1.25 L.min-1

DESIGN OF THE EXPERIMENTAL APPARATUS ON A PRODUCTION MODEL SCALE: PROCESS FLOW DIAGRAM

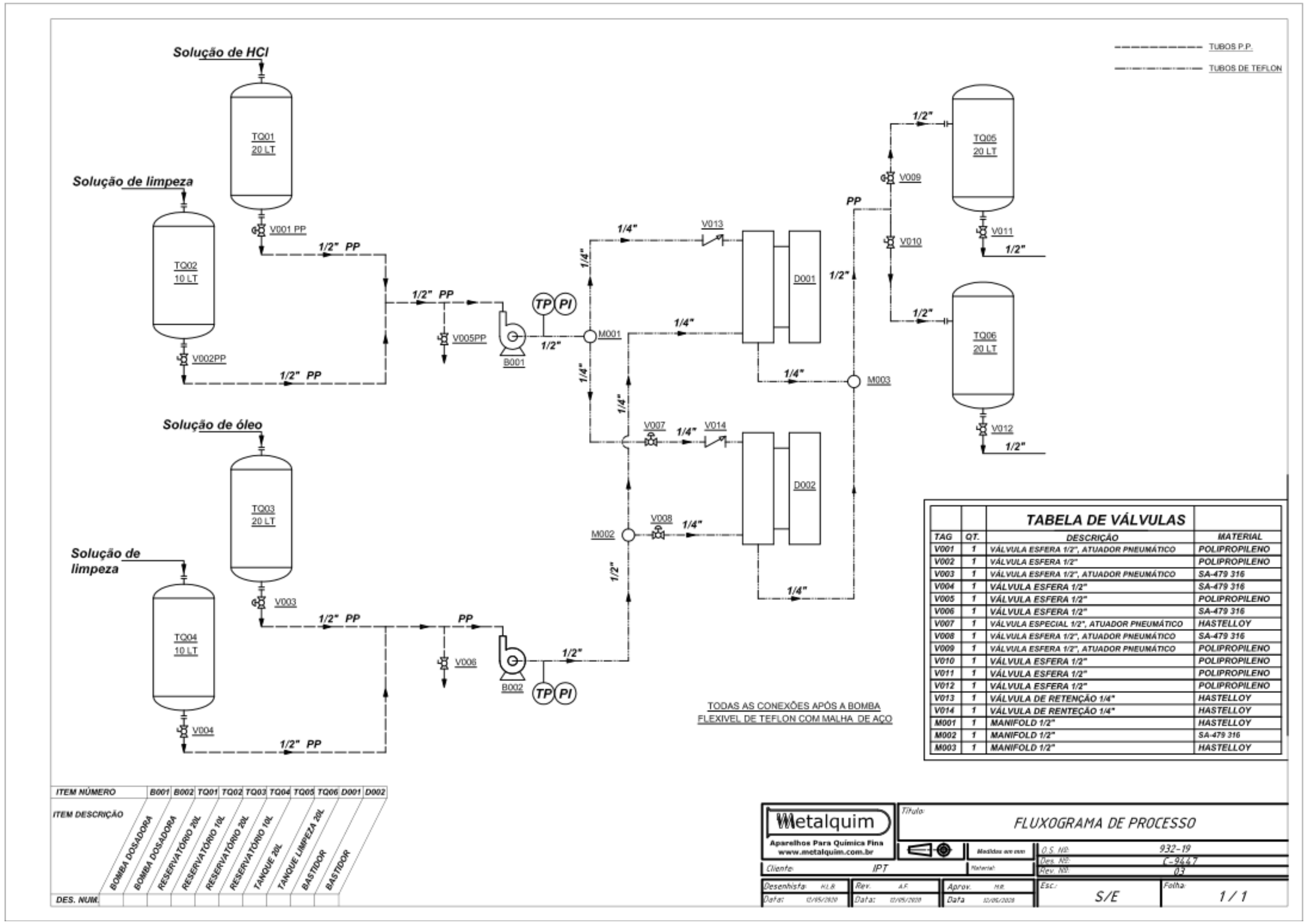
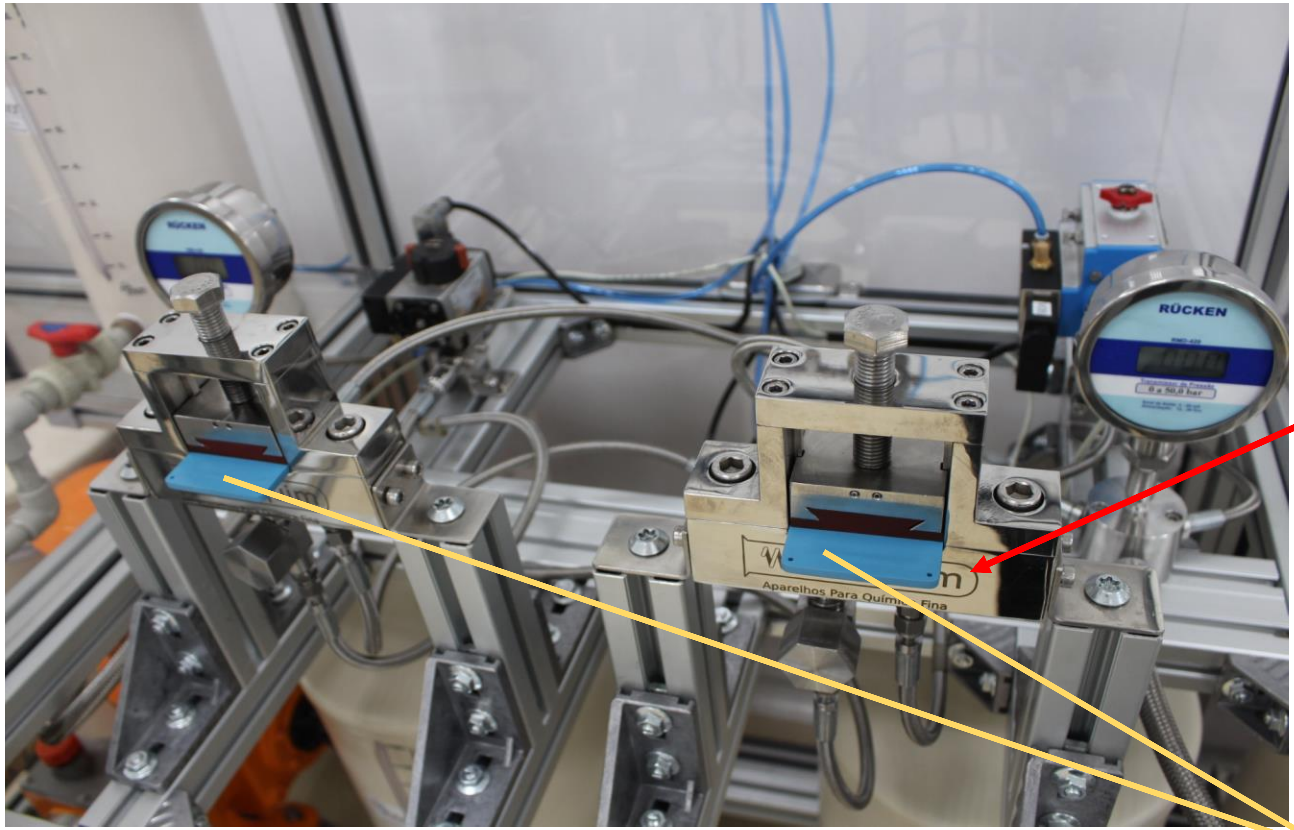


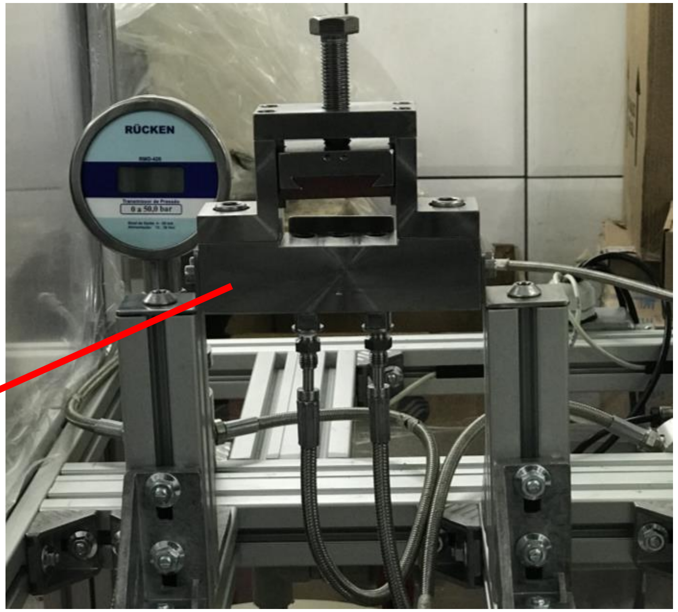
TABELA DE VÁLVULAS

TAG	QT.	DESCRIÇÃO	MATERIAL
V001	1	VÁLVULA ESFERA 1/2", ATUADOR PNEUMÁTICO	POLIPROPILENO
V002	1	VÁLVULA ESFERA 1/2"	POLIPROPILENO
V003	1	VÁLVULA ESFERA 1/2", ATUADOR PNEUMÁTICO	SA-479 316
V004	1	VÁLVULA ESFERA 1/2"	SA-479 316
V005	1	VÁLVULA ESFERA 1/2"	POLIPROPILENO
V006	1	VÁLVULA ESFERA 1/2"	SA-479 316
V007	1	VÁLVULA ESPECIAL 1/2", ATUADOR PNEUMÁTICO	HASTELLOY
V008	1	VÁLVULA ESFERA 1/2", ATUADOR PNEUMÁTICO	SA-479 316
V009	1	VÁLVULA ESFERA 1/2", ATUADOR PNEUMÁTICO	POLIPROPILENO
V010	1	VÁLVULA ESFERA 1/2"	POLIPROPILENO
V011	1	VÁLVULA ESFERA 1/2"	POLIPROPILENO
V012	1	VÁLVULA ESFERA 1/2"	POLIPROPILENO
V013	1	VÁLVULA DE RETENÇÃO 1/4"	HASTELLOY
V014	1	VÁLVULA DE RENTEÇÃO 1/4"	HASTELLOY
M001	1	MANIFOLD 1/2"	HASTELLOY
M002	1	MANIFOLD 1/2"	SA-479 316
M003	1	MANIFOLD 1/2"	HASTELLOY

EXPERIMENTAL APPARATUS FOR PRODUCTION MODEL SCALE

EXTERNAL PARALLELIZATION OF VT MICROMIXERS





Rack supports fixes and connects the micromixer to the integrated system

LTCC Parallelized micromixers

CFD SIMULATIONS RESULTS

- The results showed that for total flow rates of 1 and 1,250 L.min-1, the parallelized VT micromixer developed showed a homogeneous distribution of the fluid in the channels between the eight VT micromixers and no preferential paths was observed.
- It was also possible to observe that for these flow rate values, vortices were formed in the main channels and in the side channels, which participate in the process of splitting and recombination of currents, inducing chaotic advection in the channels of the parallelized micromixer.
- The application of the Hydraulic Resistance Minimization methodology to calculate the dimensions of the microchannels in the feed network led to a ΔP reduction of microchannels and consequently in the ΔPtotal of the parallelized micromixer.
- The average pressure differential (ΔP) of the eight VT micromixers was 3.6 ± 0.13 bar for 1 L.min-1 and 3.8 ± 0.13 bar for 1,250 L.min-1. The total ΔP of the parallelized micromixer was 7.7 and 8.1 bar for 1 and 1,250 L.min-1, respectively.

RESULTS OF OPERATIONAL TESTS

- Finally, the acid-in-oil (W/O) emulsion generation process using the (internal & External) parallelized micromixers was validated at a total flow rate of 1 L min-1, generating an emulsion with a stability of 82.69 ± 4.61 % in 0.5 h and 60.92 ± 15.80 % in 1 h, with droplets with an average diameter of 21.60 ± 1.52 µm, but still a high polydispersity, given by the span value of 6.73 ± 0.32.
- Although it was noted that studies are still needed to explore the optimum condition for emulsion generation by the parallelized micromixer at high flow rates, the process proved capable of generating W/O emulsions with a wide range of possible applications.

Thanks for your attention!

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