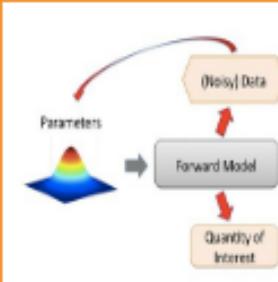


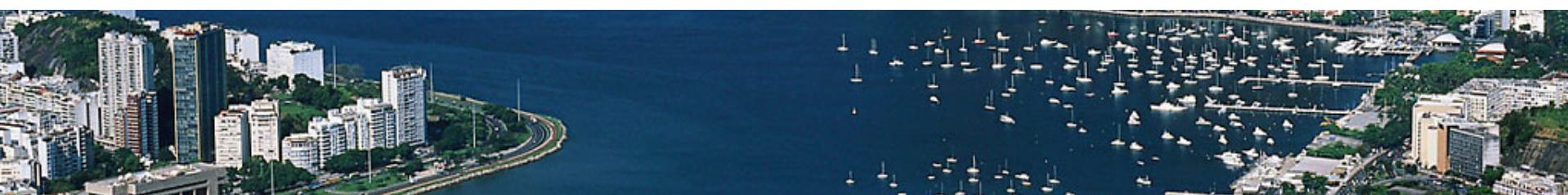
Thematic Program on Parameter identification in mathematical models

IMPA, Rio de Janeiro, Brazil

October 2nd to November 30th, 2017



Experimental-Theoretical Analysis of Biodiesel Synthesis in Micro-reactors with Inverse Problem Solution for Parameter Estimation



Assoc. Prof. Carolina P. Naveira Cotta

Laboratory of Nano and Microfluidics and Micro-Systems – LabMEMS

Mechanical Engineering Program – PEM/COPPE
Engineering of Nanotechnology Program – PENT/COPPE

Universidade Federal do Rio de Janeiro - UFRJ



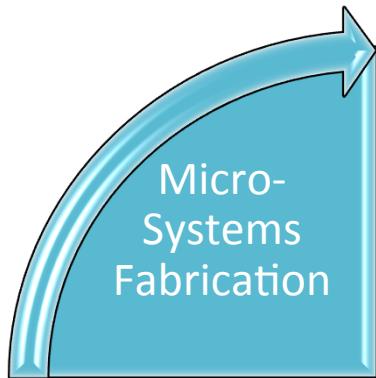
Fields/Areas:

- Heat & Mass Transfer and Fluid Flow in Micro and Nano Scale
- Continuum Mechanics and Complex Fluids



Fields/Areas:

- Heat & Mass Transfer and Fluid Flow in Micro and Nano Scale
- Continuum Mechanics and Complex Fluids

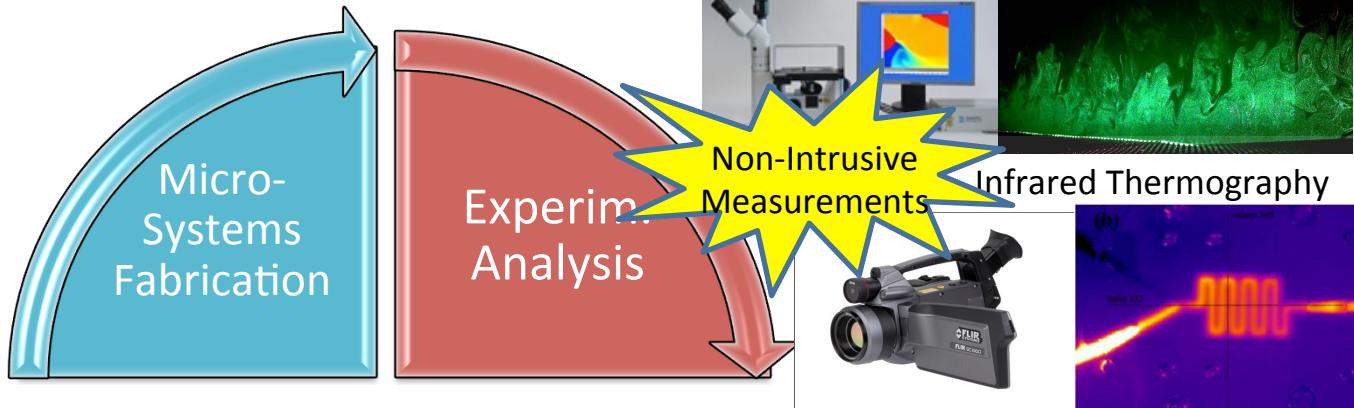




Fields/Areas:

- Heat & Mass Transfer and Fluid Flow in Micro and Nano Scale
- Continuum Mechanics and Complex Fluids

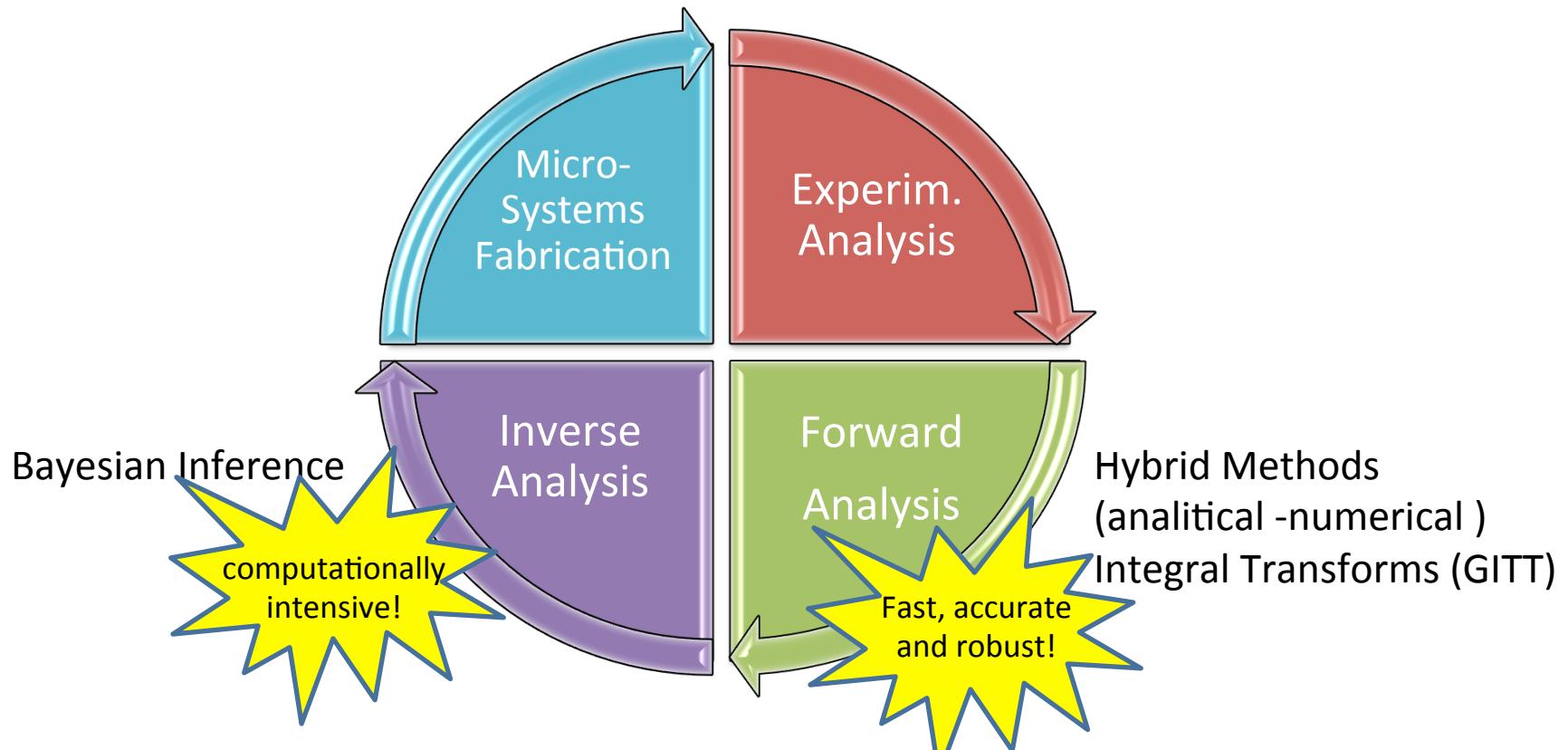
μ -PIV : Particle Image Velocimetry
 μ -LIF : Laser Induced Fluorescence





Fields/Areas:

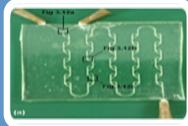
- Heat & Mass Transfer and Fluid Flow in Micro and Nano Scale
- Continuum Mechanics and Complex Fluids



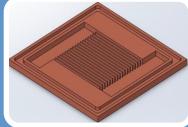
Application Areas



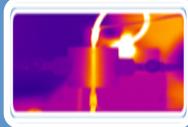
Nanocomposites and Nanofluids



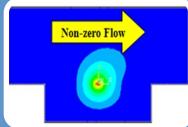
Micro reactors



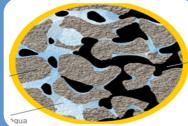
Micro-Heat Exchangers



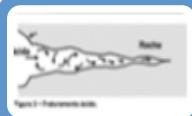
Micro-Heat Spreaders



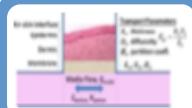
Micro-Sensors



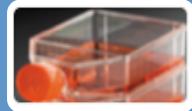
Micro-Models of Porous Media



EOR – Enhanced Oil Recovery



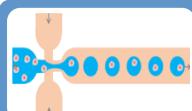
Human on a chip (cell toxicology)



Cell culture



Cell separation

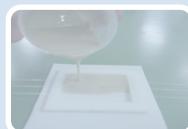


Cell encapsulation

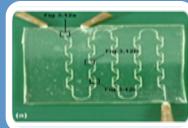


Bio-printing

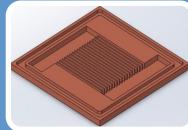
Application Areas



Nanocomposites and Nanofluids



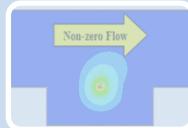
Micro reactors



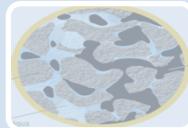
Micro-Heat Exchangers



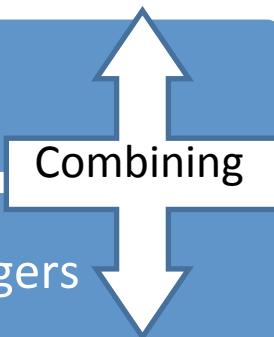
Micro-Heat Spreaders



Micro-Sensors



Micro-Models of Porous Media



EOC – Enhanced Oil Recovery



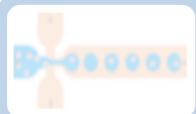
Human on a chip (cell toxicology)



Cell culture



Cell separation

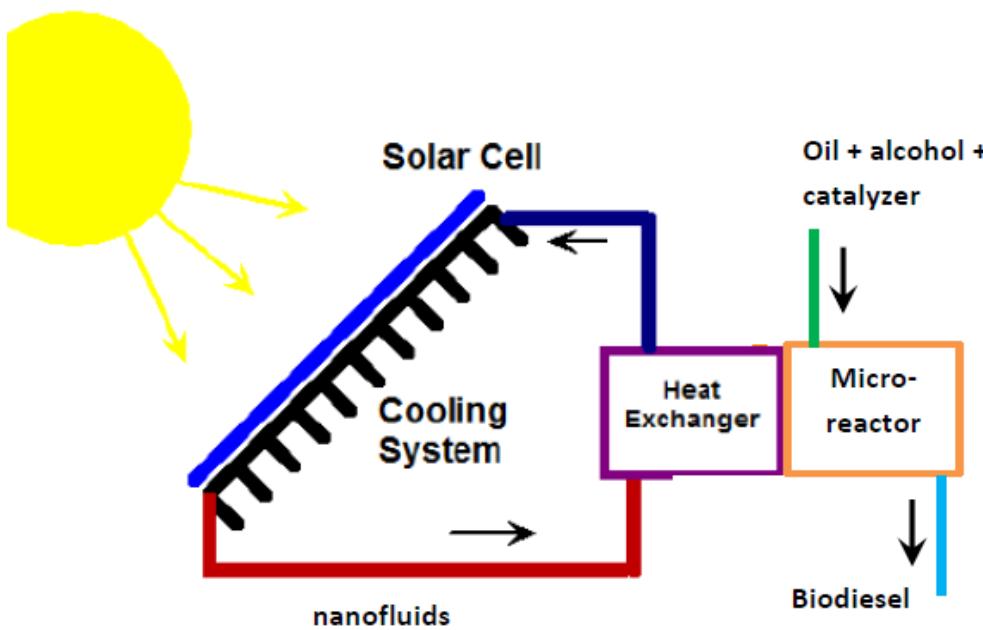


Cell encapsulation



Bio-printing

R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

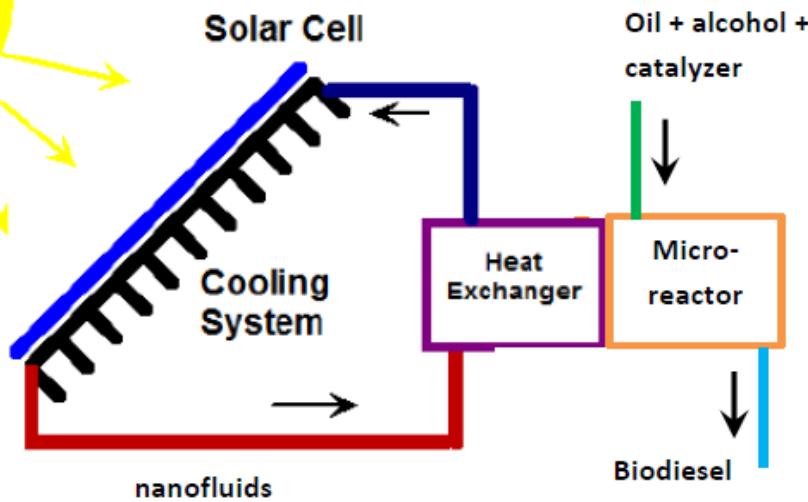


- Rejected heat can be used for other purposes (desalination, heating, cooling, **biodiesel production**, etc) ;

R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

Network !!!

**UCL & COPPE/UFRJ
Project**

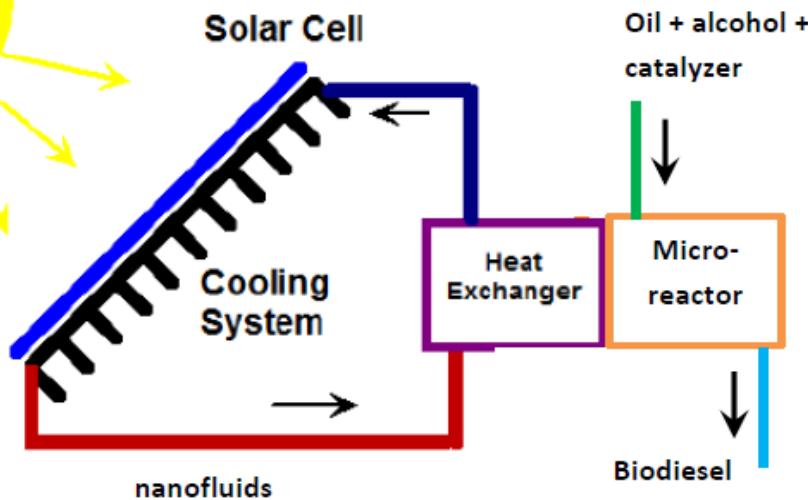


- Rejected heat can be used for other purposes (desalination, heating, cooling, **biodiesel production**, etc) ;

R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

Network !!!

**UCL & COPPE/UFRJ
Project**

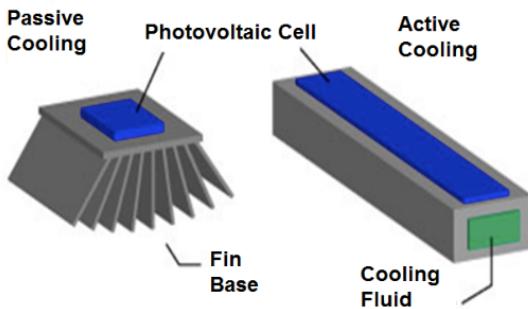


- Rejected heat can be used for other purposes (desalination, heating, cooling, biodiesel production, etc) ;

HCPV system

High Concentration: 800 suns

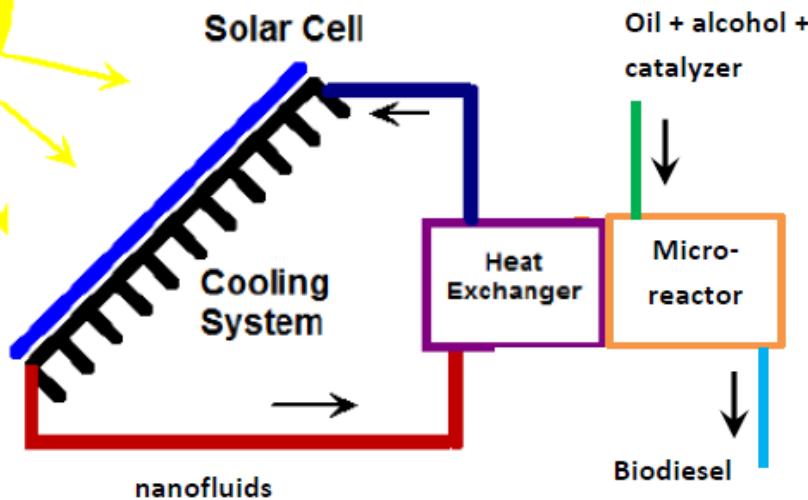
Power Generation: 1.5kVA



R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

Network !!!

**UCL & COPPE/UFRJ
Project**

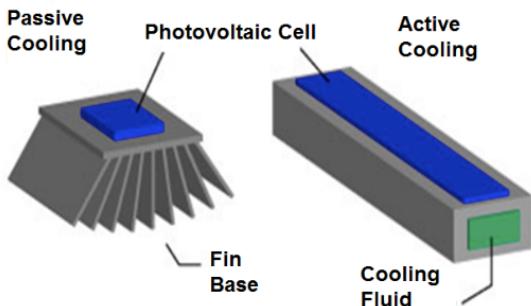


- Rejected heat can be used for other purposes (desalination, heating, cooling, **biodiesel production**, etc) ;

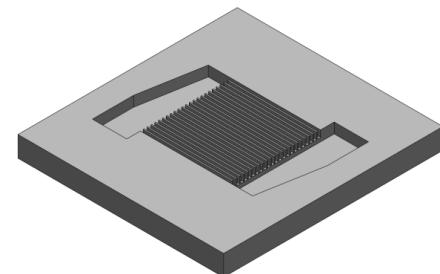
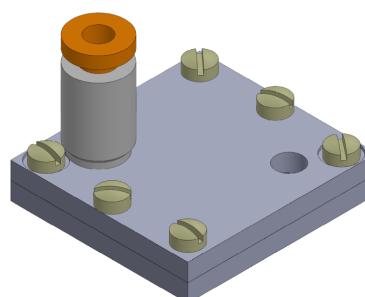
HCPV system

High Concentration: 800 suns

Power Generation: 1.5kVA



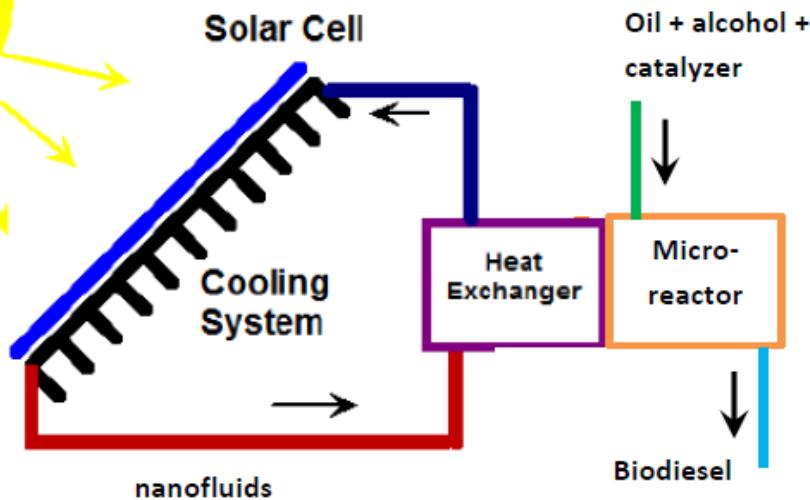
Optimized
Micro Heat Exchanger
For the HCPV cooling system



R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

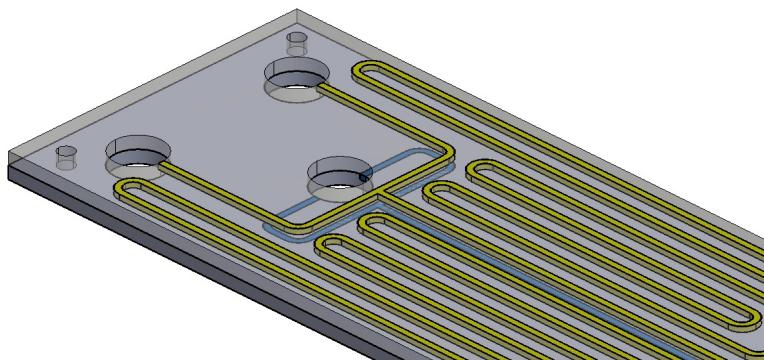
Network !!!

**UCL & COPPE/UFRJ
Project**

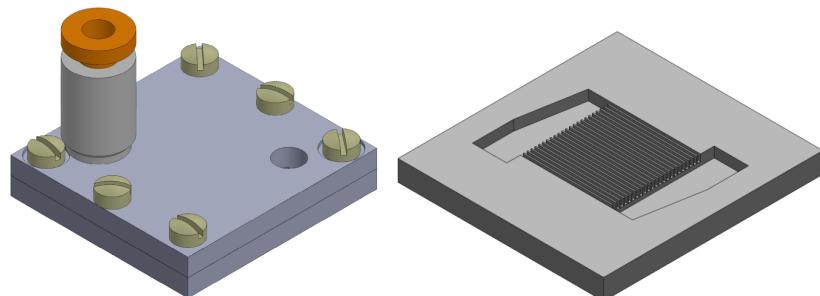


- Rejected heat can be used for other purposes (desalination, heating, cooling, **biodiesel production**, etc) ;

Integrated micro-heat exchanger and micro reactor;



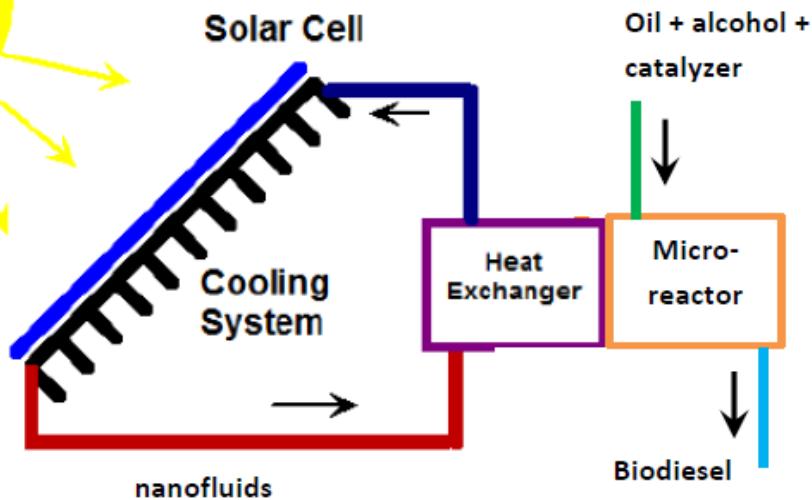
Optimized
Micro Heat Exchanger
For the HCPV cooling system



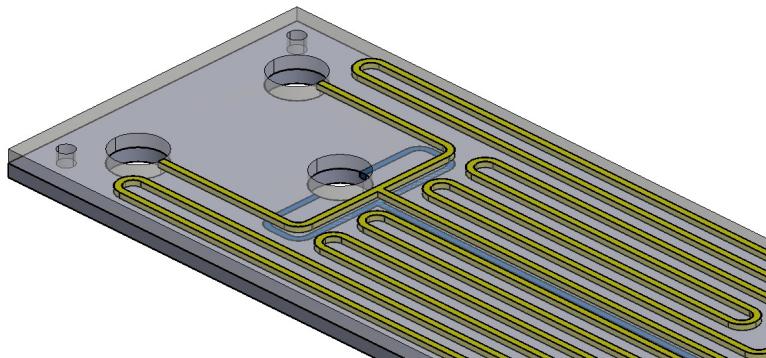
R&D Challenges : Biodiesel Production Intensification with Heat Recovery from High Concentration Photovoltaic Cells (HCPV)

Network !!!

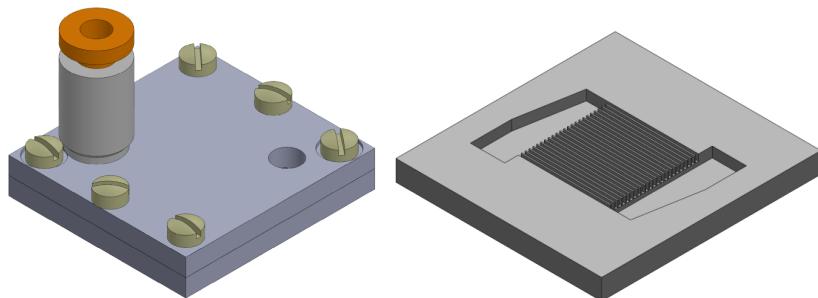
**UCL & COPPE/UFRJ
Project**



Integrated micro-heat exchanger and micro reactor;



Optimized
Micro Heat Exchanger
For the HCPV cooling system



R&D Challenges : Biodiesel Production in micro reactors

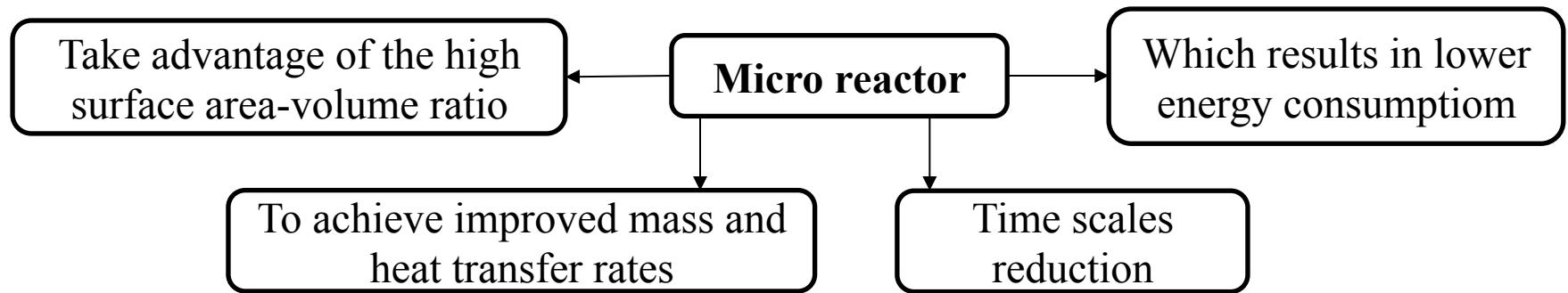


Fig. : Advantages of microreactors in reactional systems.

R&D Challenges : Biodiesel Production in micro reactors

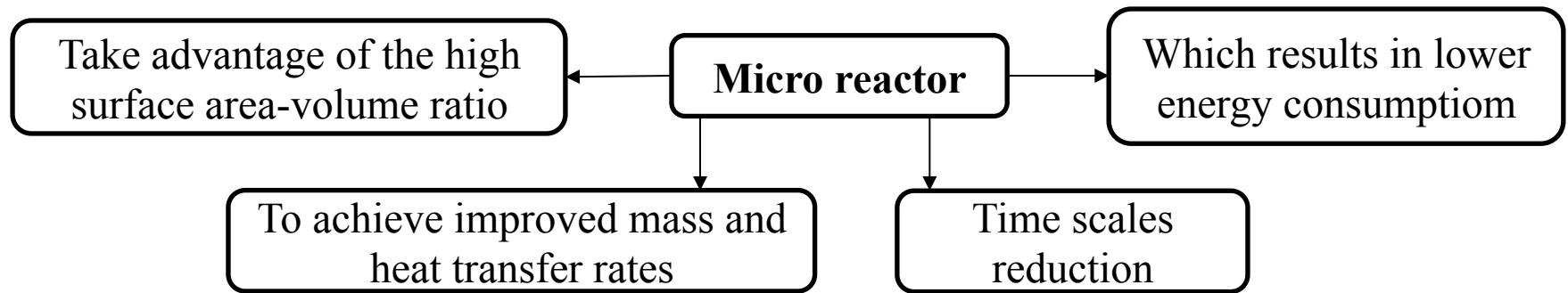


Fig. : Advantages of microreactors in reactional systems.

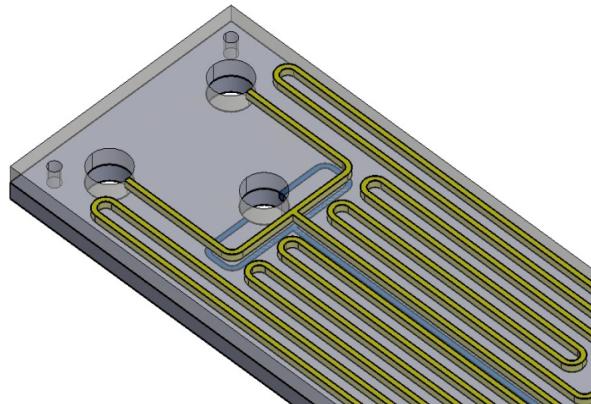


Fig. Single micro reactor;

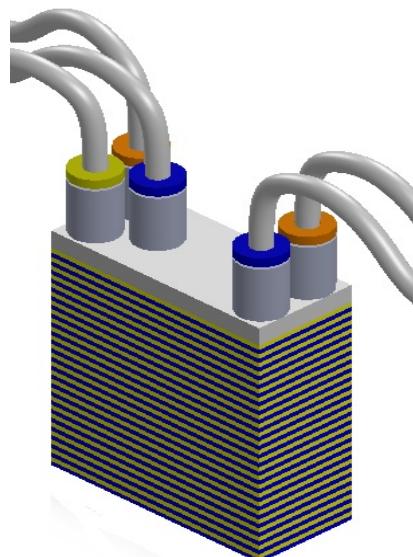


Fig. Module of micro reactors

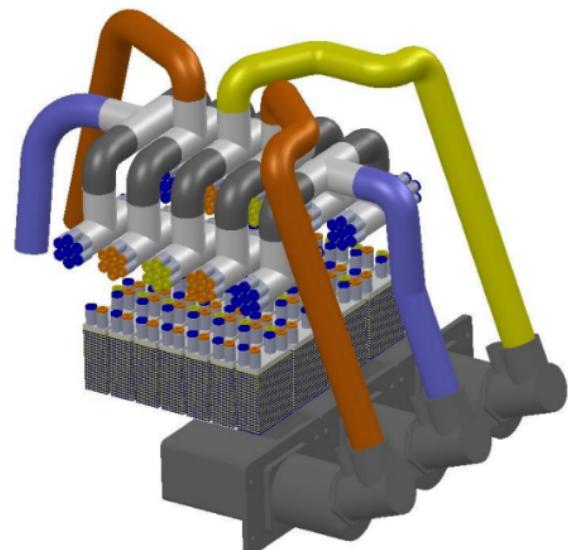
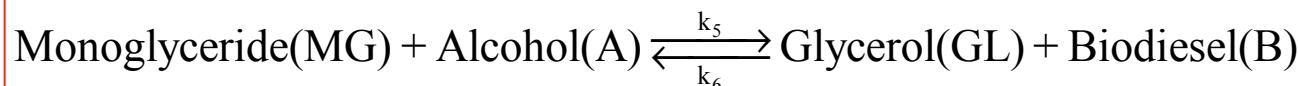
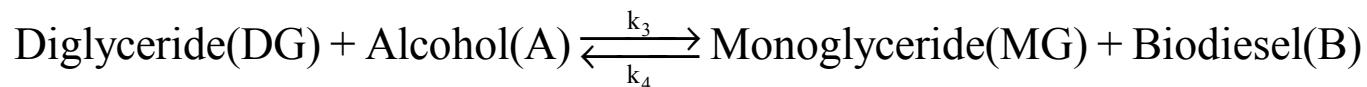
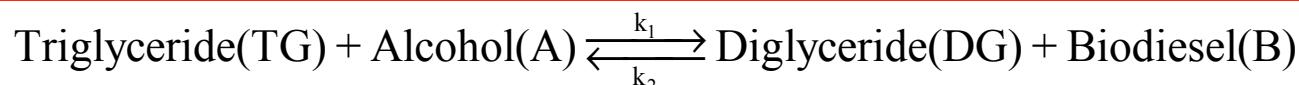
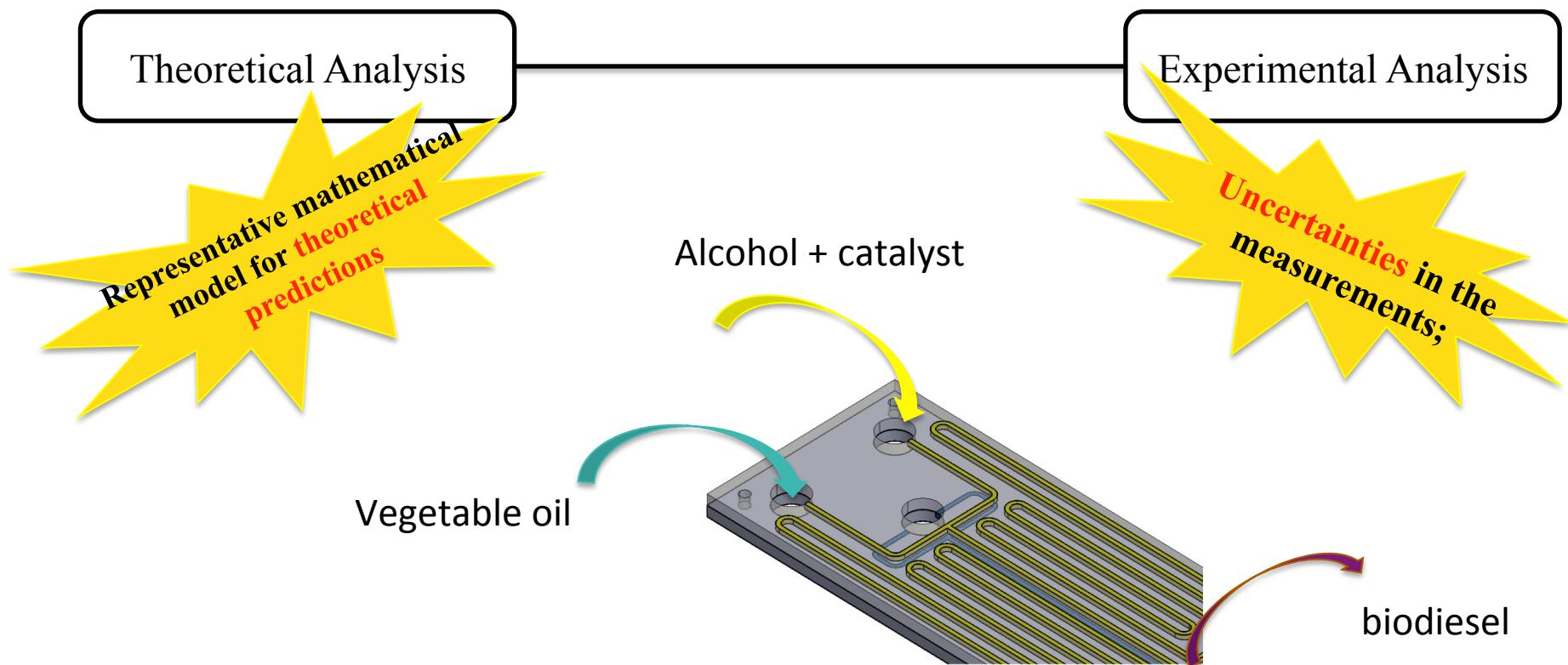


Fig. Complete manifold of micro reactors

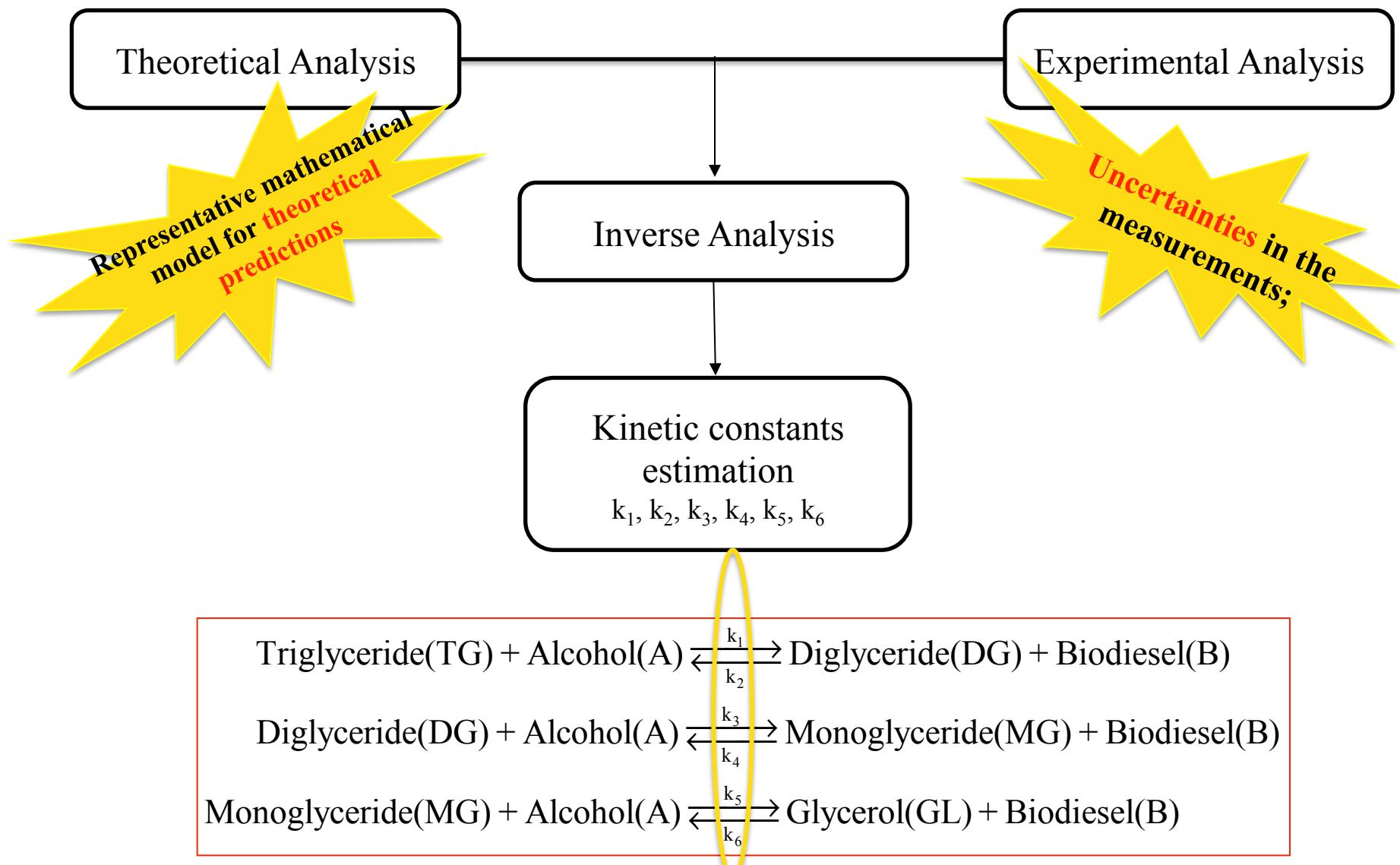
R&D Challenges : Biodiesel Production in micro reactors

➤ Design of optimized micro-reactor



R&D Challenges : Biodiesel Production in micro reactors

➤ Design of optimized micro-reactor



R&D Challenges : Biodiesel Production in micro reactors

➤ Design of optimized micro-reactor

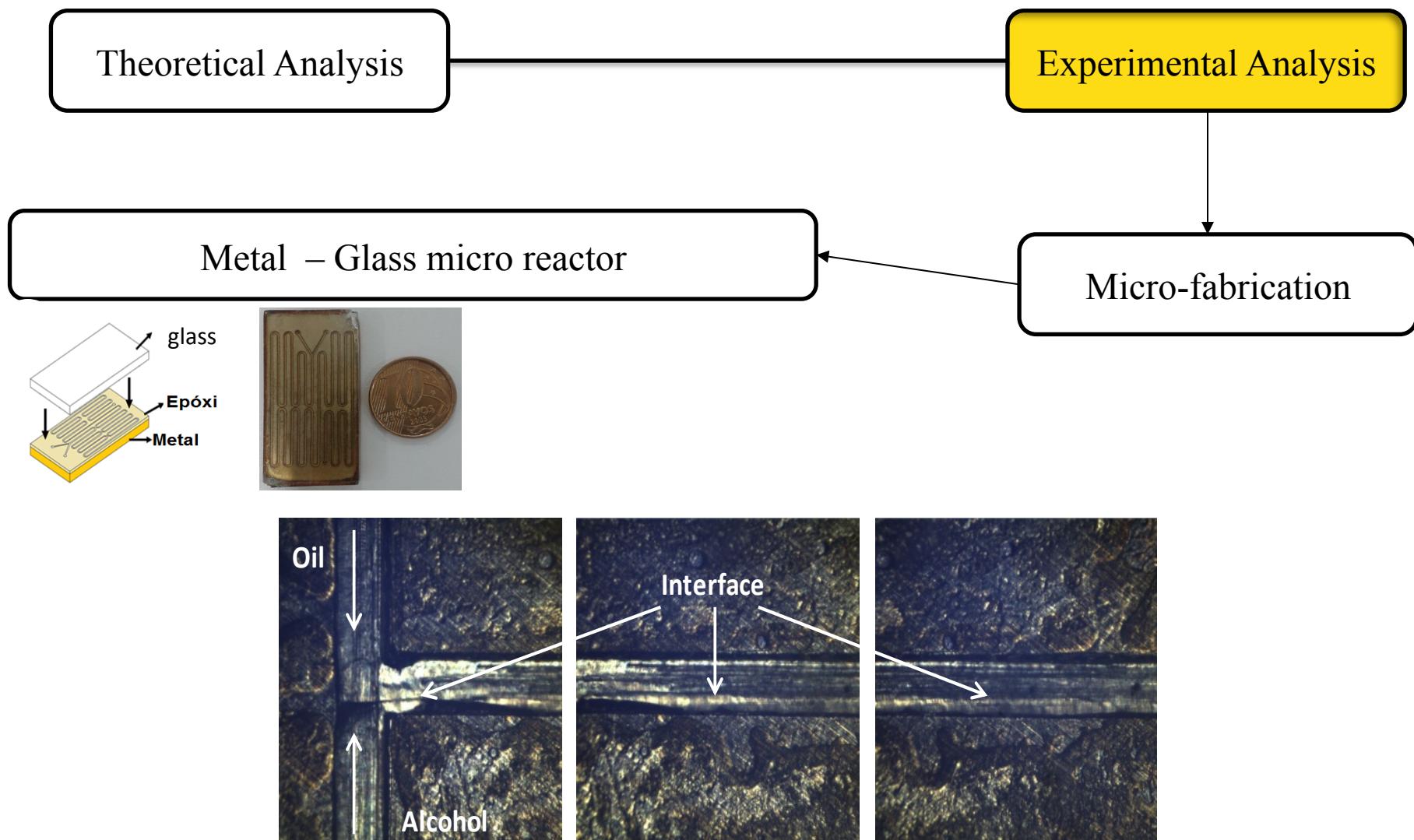
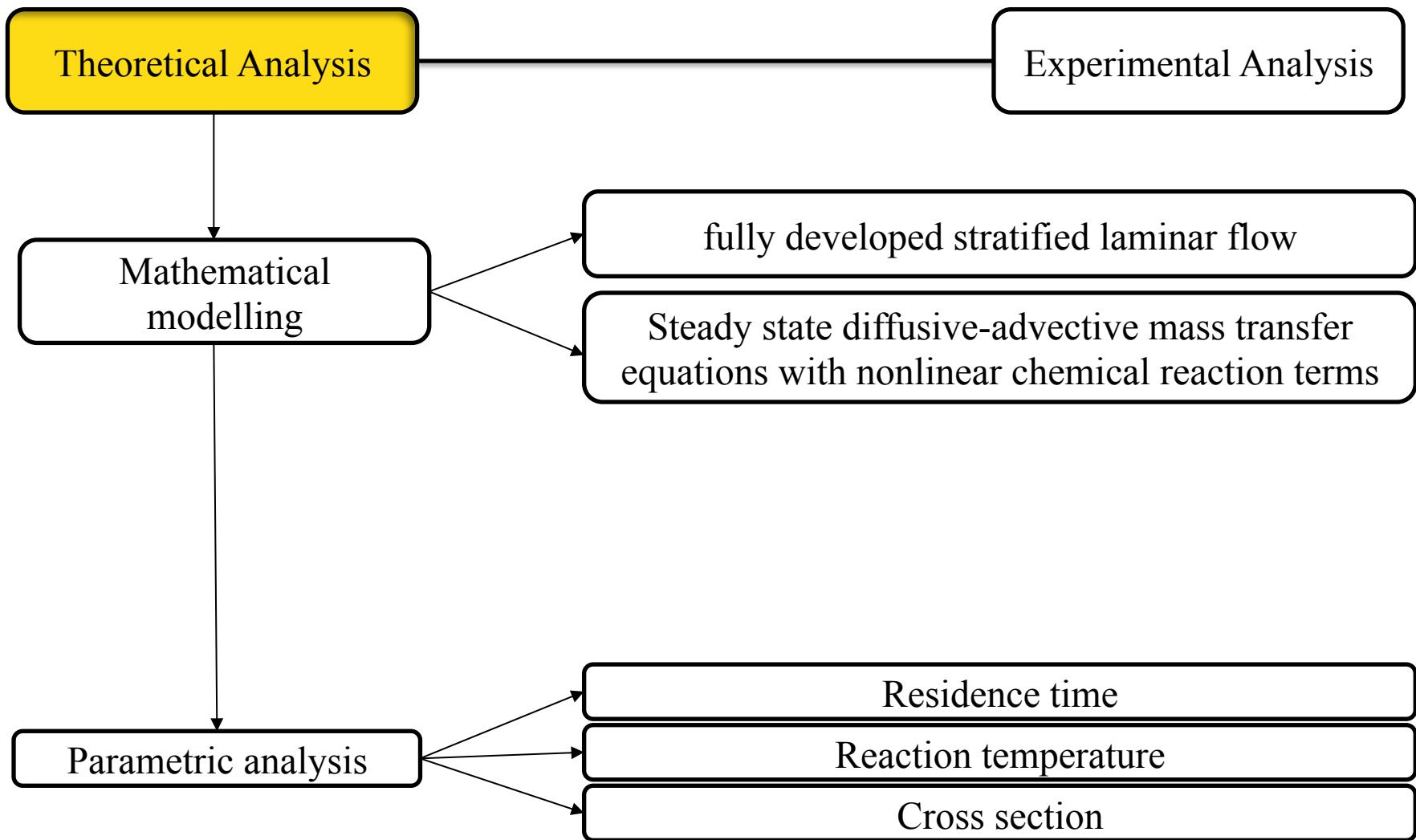


Fig.: Exp. observation of stratified flow pattern formed by the alcohol and the vegetable oil.

R&D Challenges : Biodiesel Production in micro reactors

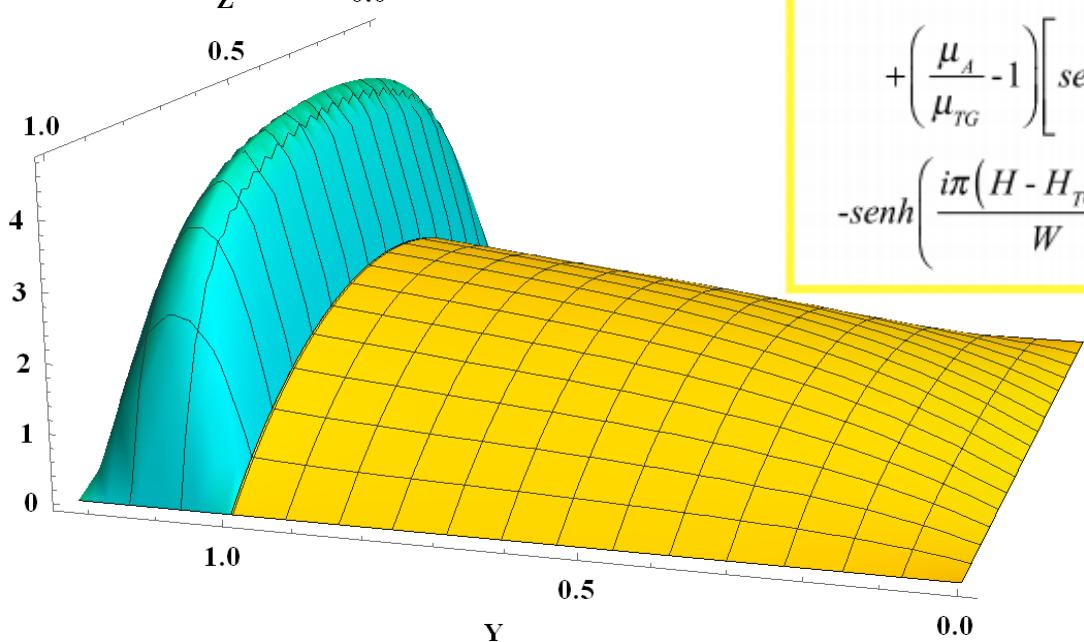
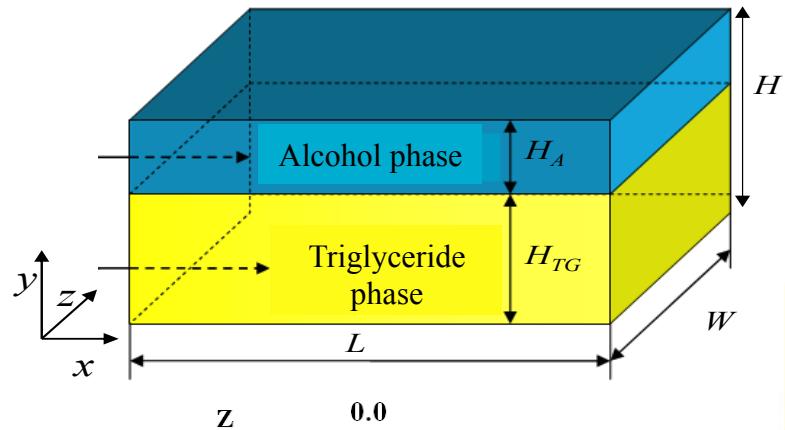
➤ MODELLING



R&D Challenges : Biodiesel Production in micro reactors

➤ FLOW PROBLEM: FORMULATION AND SOLUTION

Velocity profiles
for stratified flow:



$$u_A(y,z) = \sum_{i=1}^{\infty} \tilde{\Psi}_{vel,i}(z) S5_i \left\{ \left(1 + \frac{\mu_{TG}}{\mu_A} \right) \left[-\sinh\left(\frac{Hi\pi}{W}\right) + \sinh\left(\frac{i\pi y}{W}\right) \right] + \left(1 - \frac{\mu_{TG}}{\mu_A} \right) \left[\sinh\left(\frac{(H-2H_{TG})i\pi}{W}\right) + \sinh\left(\frac{i\pi(2H_{TG}-y)}{W}\right) \right] - \sinh\left(\frac{i\pi(H-H_{TG}-y)}{W}\right) - \sinh\left(\frac{i\pi(H+H_{TG}-y)}{W}\right) \right\} + 2 \sinh\left(\frac{i\pi(H-y)}{W}\right)$$

$$u_{TG}(y,z) = \sum_{i=1}^{\infty} \tilde{\Psi}_{vel,i}(z) S5_i \left\{ \left(1 + \frac{\mu_A}{\mu_{TG}} \right) \left[-\operatorname{senh}\left(\frac{Hi\pi}{W}\right) + \operatorname{senh}\left(\frac{i\pi(H-y)}{W}\right) \right] + \left(\frac{\mu_A}{\mu_{TG}} - 1 \right) \left[\operatorname{senh}\left(\frac{(H-2H_{TG})i\pi}{W}\right) + \operatorname{senh}\left(\frac{i\pi(H-H_{TG}+y)}{W}\right) \right] - \operatorname{senh}\left(\frac{i\pi(H-H_{TG}-y)}{W}\right) - \operatorname{senh}\left(\frac{i\pi(H-2H_{TG}+y)}{W}\right) \right\} + 2 \operatorname{senh}\left(\frac{i\pi y}{W}\right)$$

$$U = \frac{u(y,z)}{U_{TGAv}}$$

R&D Challenges : Biodiesel Production in micro reactors

➤ MASS TRANSFER MODELLING

Dimensionless reaction-convection-diffusion :

3D Model:

$$U_{TG}(Y, Z) \frac{\partial F_s(X, Y, Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X, Y, Z)}{\partial X^2} + \frac{\partial^2 F_s(X, Y, Z)}{\partial Y^2} + \delta \frac{\partial^2 F_s(X, Y, Z)}{\partial Z^2} \right) + \xi G_s$$

Table: Dimensionless kinetic relations for the species in the transesterification reaction.

<i>Species</i> F_s	<i>Reaction terms</i> G_s
TG	$-k_1 F_{TG} F_A + k_2 F_{DG} F_B$
A	$(-k_1 F_{TG} - k_3 F_{DG} - k_5 F_{MG}) F_A + (k_2 F_{DG} + k_4 F_{MG} + k_6 F_{GL}) F_B$
DG	$(k_1 F_{TG} - k_3 F_{DG}) F_A + (-k_2 F_{DG} + k_4 F_{MG}) F_B$
MG	$(k_3 F_{DG} - k_5 F_{MG}) F_A + (-k_4 F_{MG} + k_6 F_{GL}) F_B$
GL	$k_5 F_{MG} F_A - k_6 F_{GL} F_B$
B	$(k_1 F_{TG} + k_3 F_{DG} + k_5 F_{MG}) F_A + (-k_2 F_{DG} - k_4 F_{MG} - k_6 F_{GL}) F_B$

R&D Challenges : Biodiesel Production in micro reactors

➤ MASS TRANSFER MODELLING

- Solved though GITT (Generalized Integral Transform Technique)

Hybrid numerical-analytical solution with automatic error control

STEPS in the Generalized Integral Transform Technique (G.I.T.T.)

1 - Choose the associated eigenvalue problem.

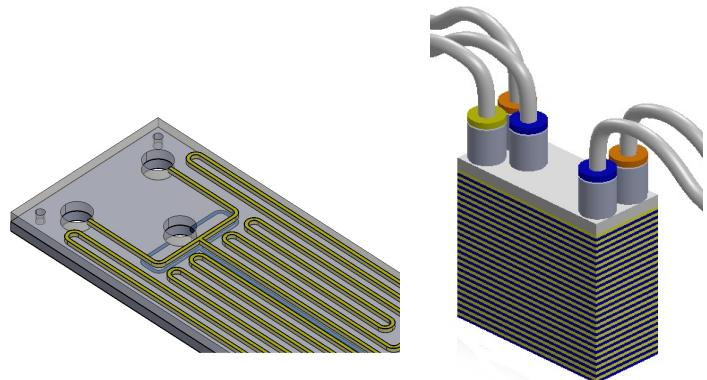
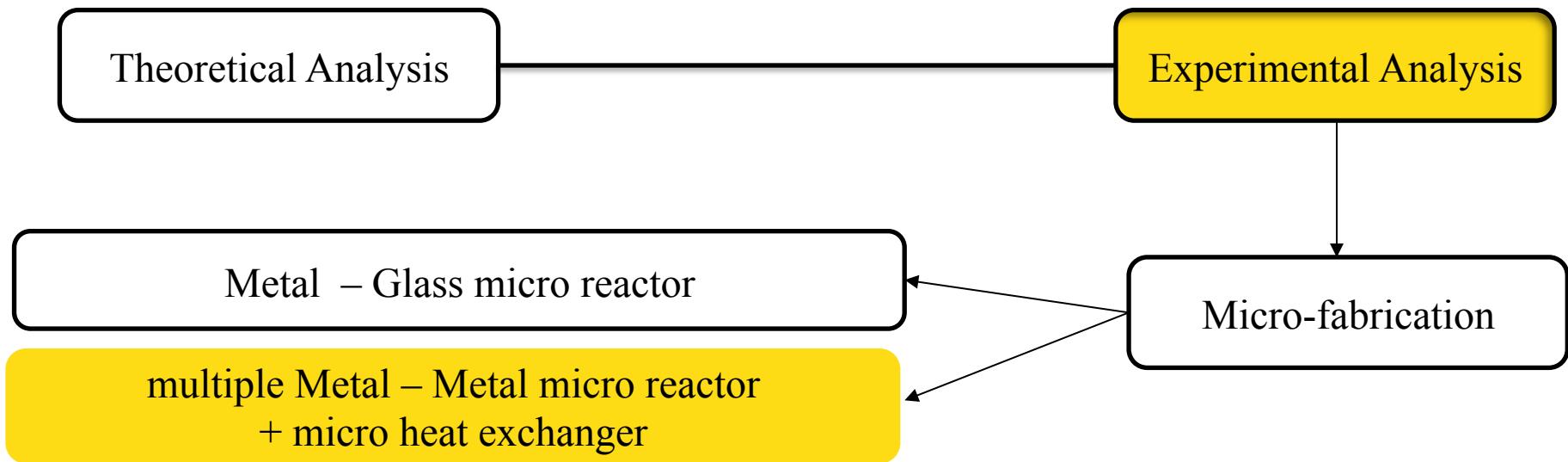
2 - Develop the integral transform pair.

3 - Integral transform the original PDE.

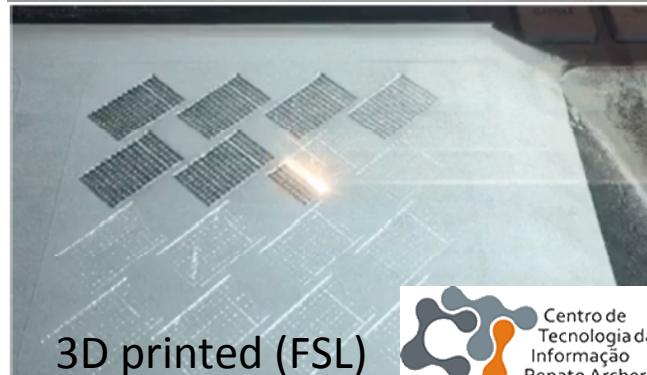
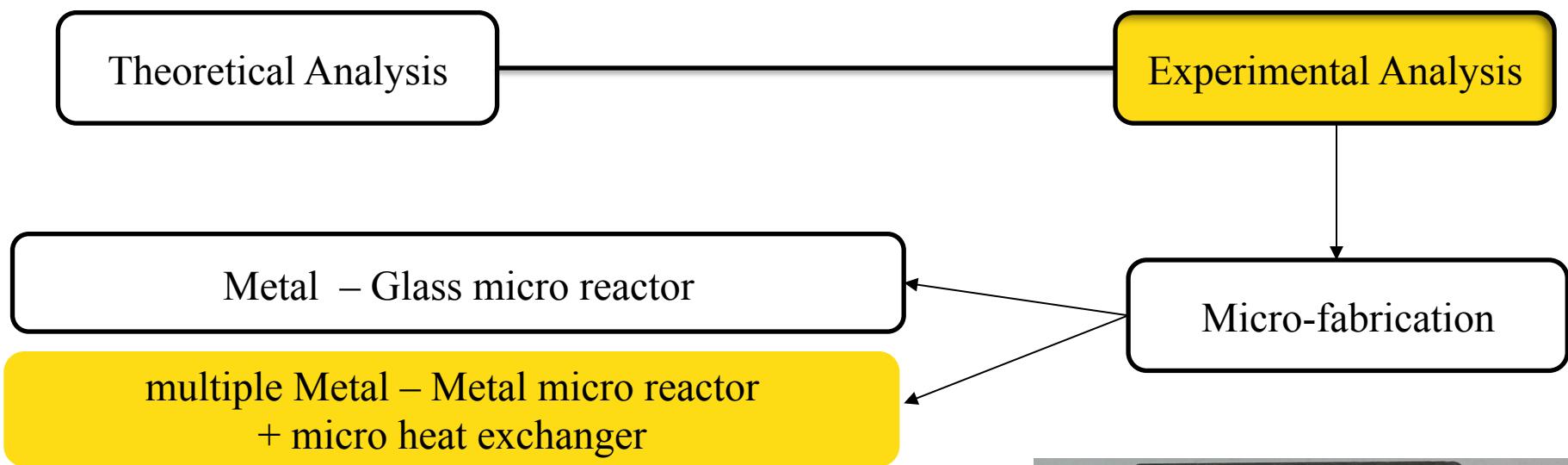
4 - Numerically (or analytically) solve the resulting coupled ODE system for the transformed potentials.

5 - Recall the analytical inversion formula to reconstruct the desired potential.

R&D Challenges : Biodiesel Production in micro reactors



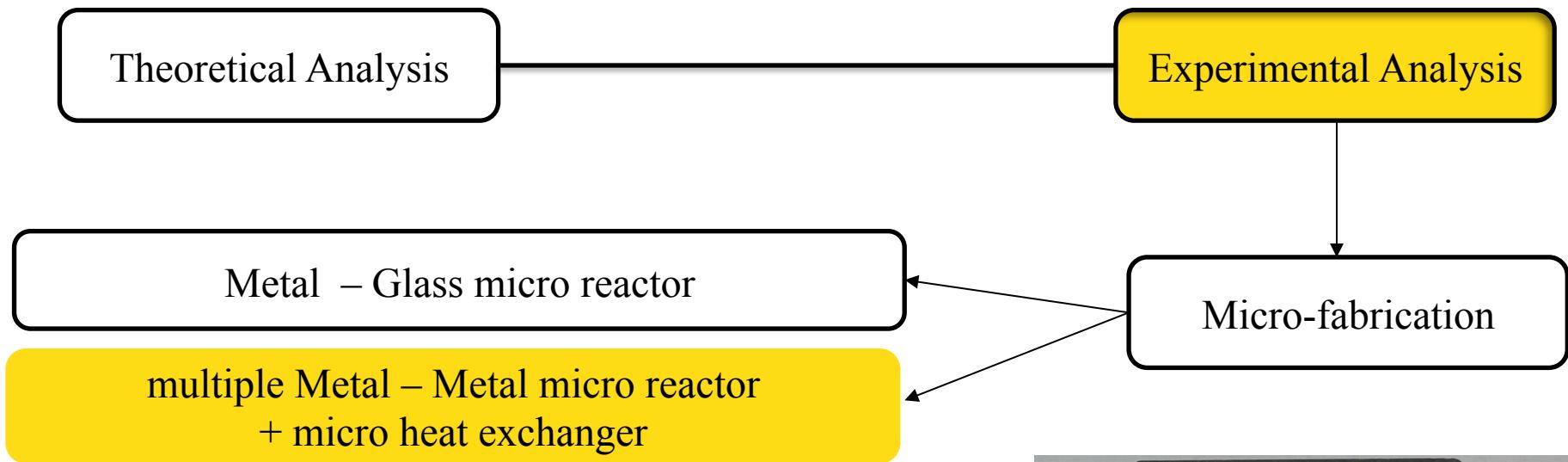
R&D Challenges : Biodiesel Production in micro reactors



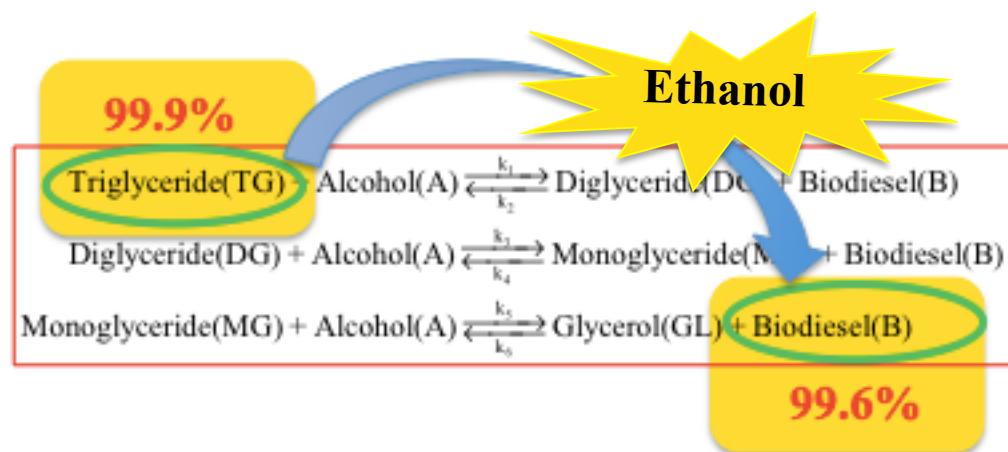
Features of the Device:

- Composed of 10 micro reactors
- Composed of 11 micro-heat exchanger
- Total Dimensions 2,5cm x 4cm x 1.27cm.
- Microchannels with square section 400µmX400µm**
- Total Length of the microchannel of the reactor of 43.26 cm.

R&D Challenges : Biodiesel Production in micro reactors

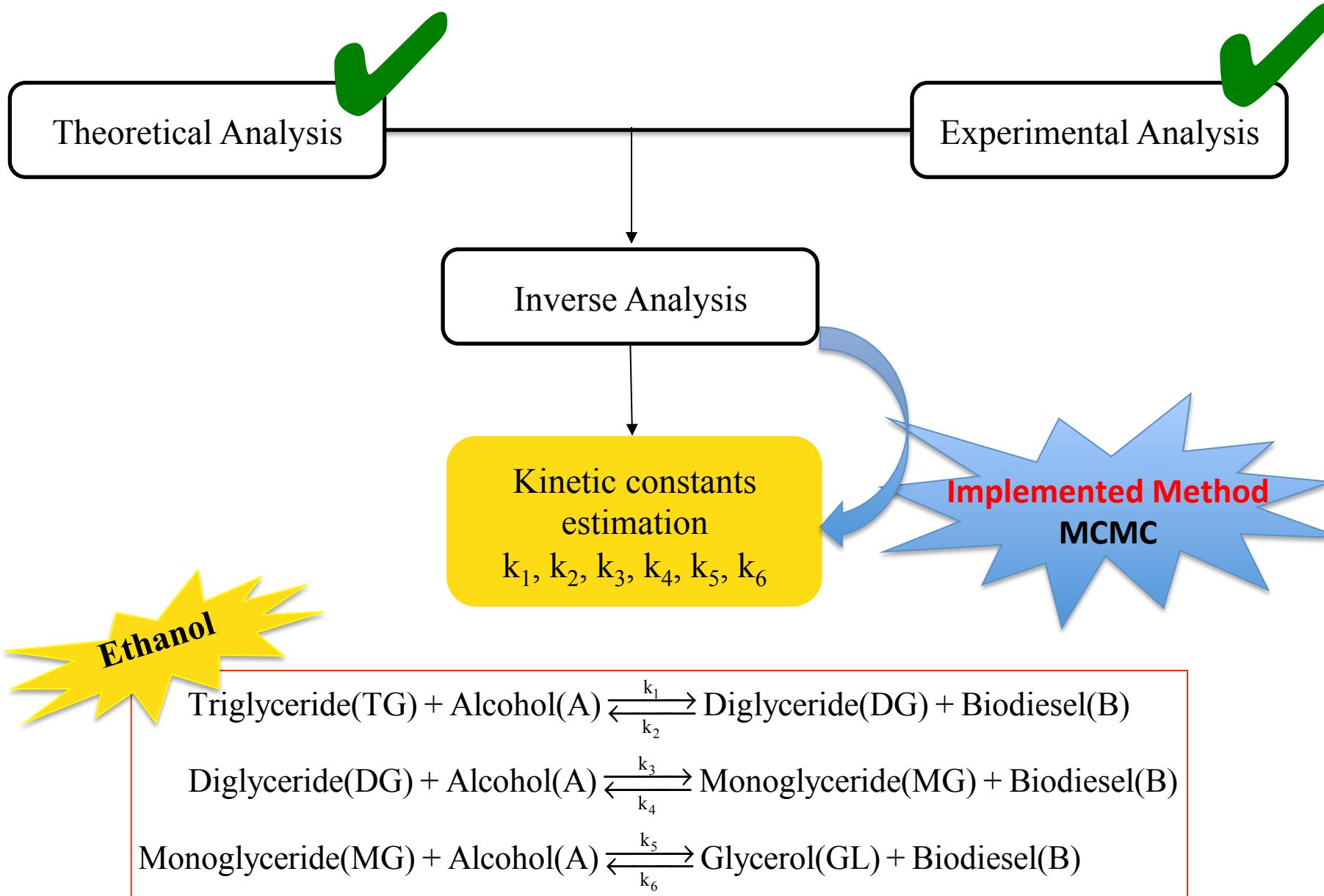


3D printed (FSL)



Ethanol/Soybean Oil ratio: 20:1
Catalyst: NaOH 1,5% wt oil
Reaction temperature: 64,9°C
Residence time: 35 seconds

R&D Challenges : Biodiesel Production in micro reactors



R&D Challenges : Biodiesel Production in micro reactors

➤ SENSITIVITY ANALYSIS

1

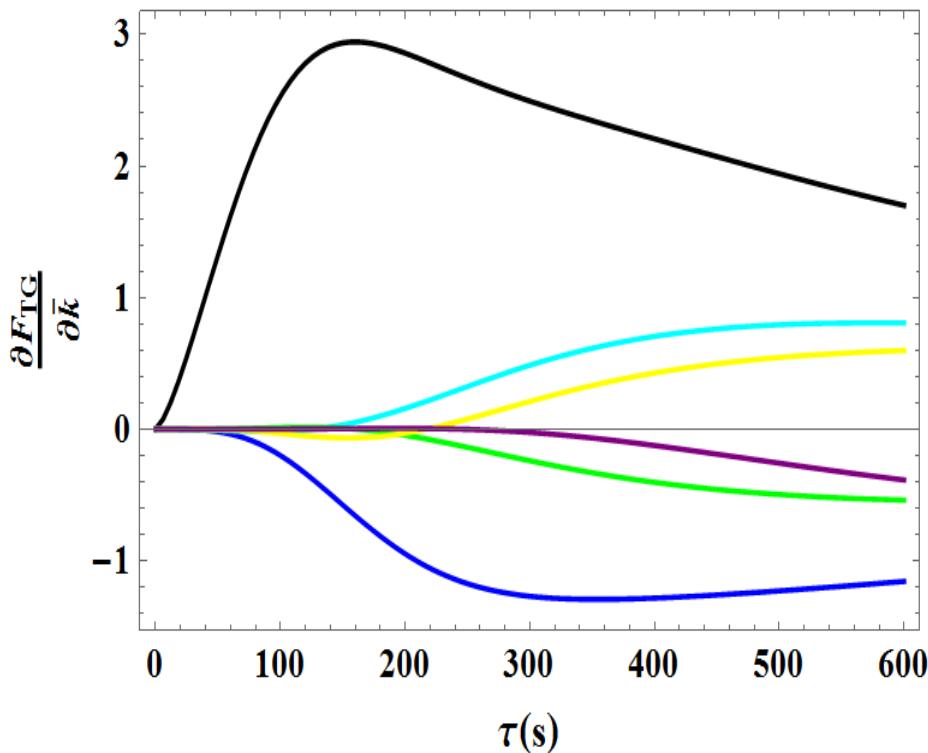
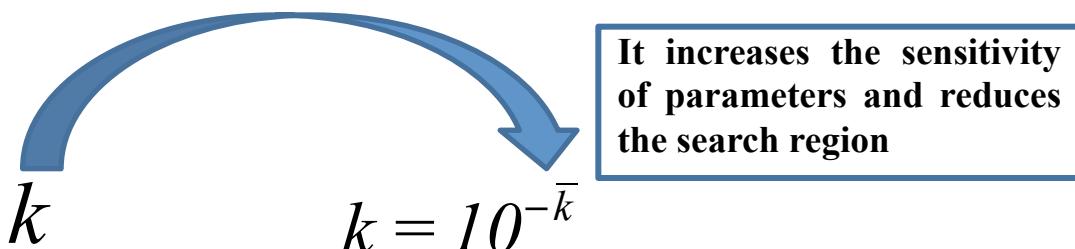
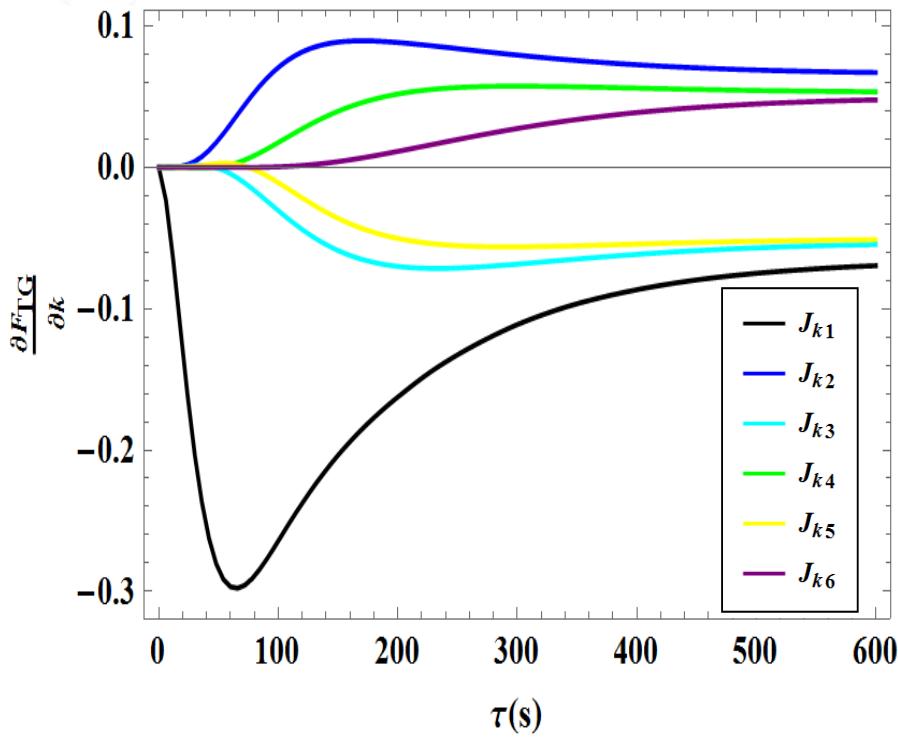


Figure: Reduced sensitivity coefficients.

Range of search:

$$k : 10^{-9} \text{ to } 10^{-1}$$

Range of search :

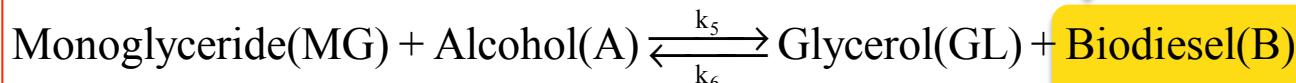
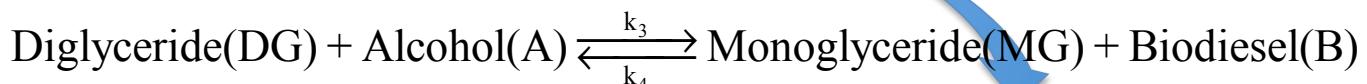
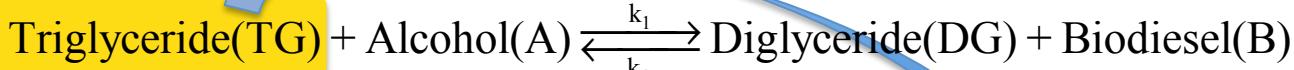
$$\bar{k} : 1 \text{ to } 9$$

R&D Challenges : Biodiesel Production in micro reactors

➤ SENSITIVITY ANALYSIS

Table – Cases for each set of measures of the species used in the analysis of the $|J^T J|$.

Cases	Meas. Species	Determinant $J^T J$
Case 1	B	6.922×10^{-3}
Case 2	B and TG	2258
Case 3	B, TG, DG and MG	3.821×10^7
Case 4	B, TG, DG, MG and GL	8.073×10^7
Case 5	B, TG, DG, MG, GL and A	8.074×10^7



Good Exp.

R&D Challenges : Biodiesel Production in micro reactors

➤ SENSITIVITY ANALYSIS

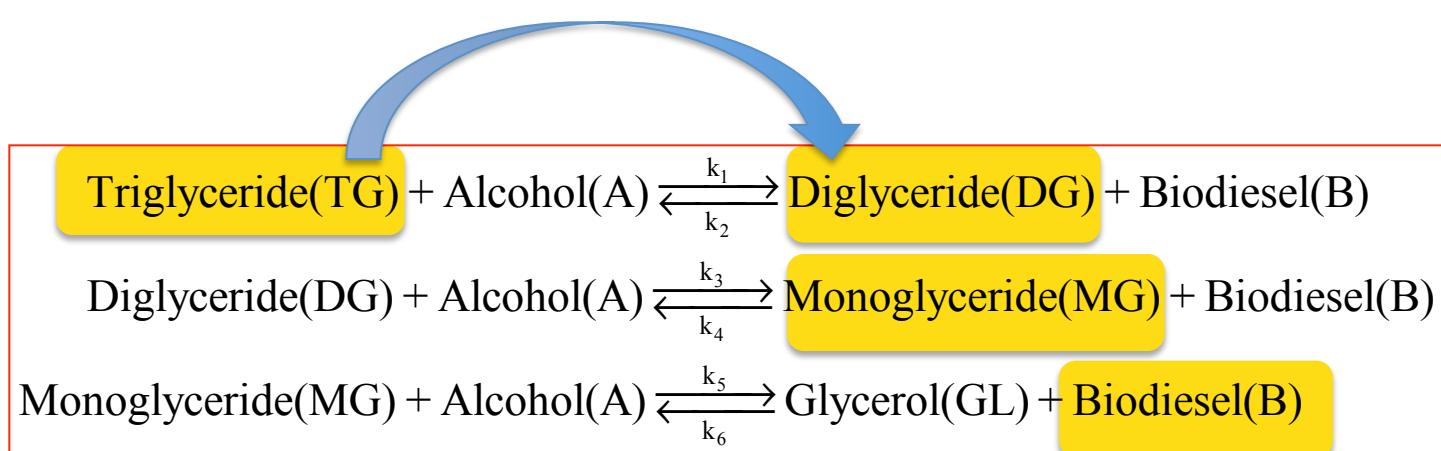
2

Table – Cases for each set of measures of the species used in the analysis of the $J^T J$.

Cases	Meas. Species	Determinant $J^T J$
Case 1	B	6.922×10^{-3}
Case 2	B and TG	2258
Case 3	B, TG, DG and MG	3.821×10^7
Case 4	B, TG, DG, MG and GL	8.073×10^7
Case 5	B, TG, DG, MG, GL and A	8.074×10^7



“Bad” Exp.



R&D Challenges : Biodiesel Production in micro reactors

3

➤ MASS TRANSFER MODELLING

Dimensionless reaction-convection-diffusion :

3D Model:

$$U_{TG}(Y,Z) \frac{\partial F_s(X,Y,Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X,Y,Z)}{\partial X^2} + \frac{\partial^2 F_s(X,Y,Z)}{\partial Y^2} + \delta \frac{\partial^2 F_s(X,Y,Z)}{\partial Z^2} \right) + \zeta G_s$$

$s = TG, MG, DG, B, GL, A$

2D - Parallel plates :

$$U_{TG}(Y,Z) \frac{\partial F_s(X,Y,Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X,Y,Z)}{\partial X^2} + \frac{\partial^2 F_s(X,Y,Z)}{\partial Y^2} \right) + \zeta G_s$$

Reduced Model

R&D Challenges : Biodiesel Production in micro reactors

3

➤ MASS TRANSFER MODELLING

Dimensionless reaction-convection-diffusion :

3D Model:

$$I \sum_{i=1}^{40} \dots \frac{\partial F_s(X, Y, Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X, Y, Z)}{\partial X^2} + \frac{\partial^2 F_s(X, Y, Z)}{\partial Y^2} + \delta \frac{\partial^2 F_s(X, Y, Z)}{\partial Z^2} \right) + \zeta G_s$$

$s = TG, MG, DG, B, GL, A$

2D - Parallel plates :

$$\sum_{i=1}^1 \dots \frac{\partial F_s(X, Y, Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X, Y, Z)}{\partial X^2} + \frac{\partial^2 F_s(X, Y, Z)}{\partial Y^2} \right) + \zeta G_s$$

Reduced Model

R&D Challenges : Biodiesel Production in micro reactors

3

➤ MASS TRANSFER MODELLING

Dimensionless reaction-convection-diffusion :

3D Model:

$$I \sum_{i=1}^{40} \dots \frac{\partial F_s(X, Y, Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X, Y, Z)}{\partial X^2} + \frac{\partial^2 F_s(X, Y, Z)}{\partial Y^2} + \delta \frac{\partial^2 F_s(X, Y, Z)}{\partial Z^2} \right) + \zeta G_s$$

$s = TG, MG, DG, B, GL, A$

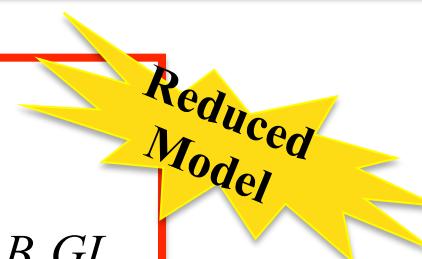
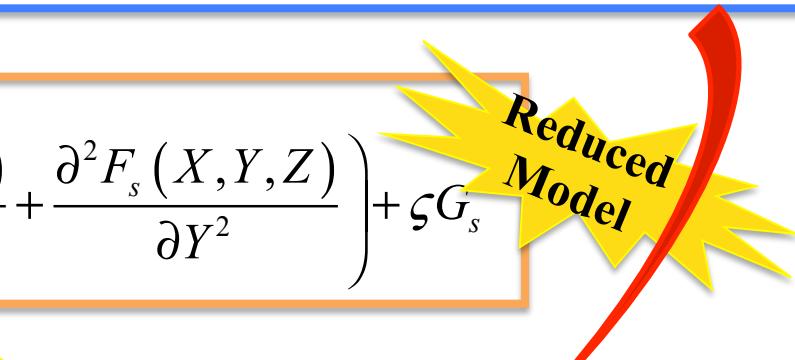
2D - Parallel plates :

$$\sum_{i=1}^1 \dots \frac{\partial F_s(X, Y, Z)}{\partial X} = \xi_s \left(\gamma \frac{\partial^2 F_s(X, Y, Z)}{\partial X^2} + \frac{\partial^2 F_s(X, Y, Z)}{\partial Y^2} \right) + \zeta G_s$$

1D - Lumped-Differential Model :

$$\bar{U}_{TG} \frac{d\bar{F}_s(X)}{dX} = \zeta \bar{G}_s , \quad s = TG, MG, DG, B, GL$$

$$\bar{U}_{TG} \frac{d\bar{F}_A(X)}{dX} = \xi_A (3P^* \bar{F}_A(X) + Q^*) + \zeta \bar{G}_A$$



CIEA - Coupled Integral
Equations Approach
(Improved Lumped Analysis)

R&D Challenges : Biodiesel Production in micro reactors

➤ BAYE'S FORMULA

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P} | \mathbf{Y}_{exp}) = \frac{\pi_{prior}(\mathbf{P})\pi(\mathbf{Y}_{exp} | \mathbf{P})}{\pi(\mathbf{Y}_{exp})}$$

posterior \propto prior x likelihood

➤ MCMC (MARKOV CHAIN MONTE CARLO METHODS)

METROPOLIS-HASTINGS ALGORITHM

1. Sample a *Candidate Point* \mathbf{P}^* from a jumping distribution $q(\mathbf{P}^*, \mathbf{P}^{(t-1)})$.
2. Calculate:
$$\alpha = \min \left[1, \frac{\pi(\mathbf{P}^* | \mathbf{Y}) q(\mathbf{P}^{(t-1)}, \mathbf{P}^*)}{\pi(\mathbf{P}^{(t-1)} | \mathbf{Y}) q(\mathbf{P}^*, \mathbf{P}^{(t-1)})} \right]$$
3. Generate a random value U which is uniformly distributed on $(0,1)$.
4. If $U < \alpha$, define $\mathbf{P}^{(t)} = \mathbf{P}^*$; otherwise, define $\mathbf{P}^{(t)} = \mathbf{P}^{(t-1)}$.
5. Return to step 1 in order to generate the sequence $\{\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \dots, \mathbf{P}^{(n)}\}$.

R&D Challenges : Biodiesel Production in micro reactors

➤ LIKELIHOOD

$$\pi(\mathbf{Y}_{\text{exp}} \mid \mathbf{P}) = (2\pi)^{-I/2} |\mathbf{W}^{-1}|^{-1/2} \exp \left[-\frac{1}{2} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}})^T \mathbf{W} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}}) \right]$$

- The exp. errors are additive, with zero mean and normally distributed.
- The statistical parameters describing the errors are known.
- There are no errors in the independent variables.
- \mathbf{P} is a random vector with known mean μ and known covariance matrix \mathbf{W} .
- \mathbf{P} is independent of \mathbf{Y}_{exp} .

R&D Challenges : Biodiesel Production in micro reactors

➤ LIKELIHOOD

$$\pi(\mathbf{Y}_{\text{exp}} \mid \mathbf{P}) = (2\pi)^{-J/2} |\mathbf{W}^{-1}|^{-1/2} \exp \left[-\frac{1}{2} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}})^T \mathbf{W} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}}) \right]$$

➤ APPROXIMATION ERROR MODEL

$$\mathbf{Y}_{\text{model}} = \mathbf{Y}_{\substack{\text{reduced} \\ \text{model}}} + \boldsymbol{\varepsilon}(\mathbf{P})$$

$$\boldsymbol{\varepsilon}(\mathbf{P}) = \boldsymbol{\varepsilon}_{\substack{\text{reduced} \\ \text{model}}}(\mathbf{P}) + \boldsymbol{\varepsilon}_{\text{exp}}$$

R&D Challenges : Biodiesel Production in micro reactors

➤ LIKELIHOOD

$$\pi(\mathbf{Y}_{\text{exp}} \mid \mathbf{P}) = (2\pi)^{-I/2} |\mathbf{W}^{-1}|^{-1/2} \exp \left[-\frac{1}{2} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}})^T \mathbf{W} (\mathbf{Y}_{\text{exp}} - \mathbf{Y}_{\text{model}}) \right]$$

➤ APPROXIMATION ERROR MODEL

$$\mathbf{Y}_{\text{model}} = \mathbf{Y}_{\text{reduced model}} + \boldsymbol{\varepsilon}(\mathbf{P})$$

$$\boldsymbol{\varepsilon}(\mathbf{P}) = \boldsymbol{\varepsilon}_{\text{reduced model}}(\mathbf{P}) + \boldsymbol{\varepsilon}_{\text{exp}}$$

$$\bar{\boldsymbol{\varepsilon}} = \bar{\boldsymbol{\varepsilon}}_{\text{reduced model}} + \bar{\boldsymbol{\varepsilon}}_{\text{exp}} + \boldsymbol{\Gamma}_{\boldsymbol{\varepsilon}_{\mathbf{P}^r}} \boldsymbol{\Gamma}_{\mathbf{P}^r}^{-1} (\mathbf{P}^r - \boldsymbol{\mu})$$

$$\tilde{\mathbf{W}} = \mathbf{W}_{\text{reduced model}} + \mathbf{W}_{\text{exp}} - \boldsymbol{\Gamma}_{\boldsymbol{\varepsilon}_{\mathbf{P}^r}} \boldsymbol{\Gamma}_{\mathbf{P}^r}^{-1} \boldsymbol{\Gamma}_{\mathbf{P}^r} \boldsymbol{\varepsilon}$$

$\bar{\boldsymbol{\varepsilon}}_{\text{exp}} \rightarrow 0$, measurement uncertainties have zero mean

$\boldsymbol{\Gamma}_{\boldsymbol{\varepsilon}_{\mathbf{P}^r}} \rightarrow 0$, neglecting the linear dependence between $\boldsymbol{\varepsilon}$ and \mathbf{P}^r

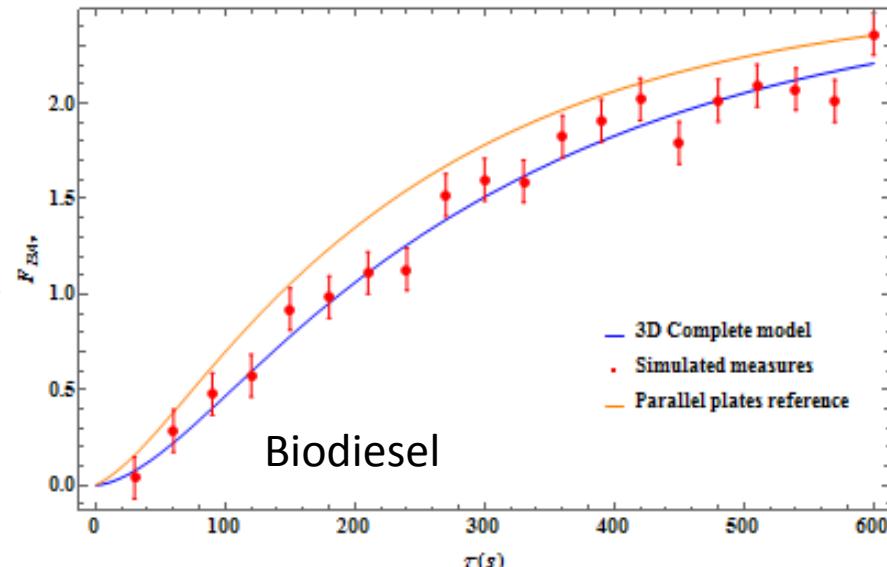
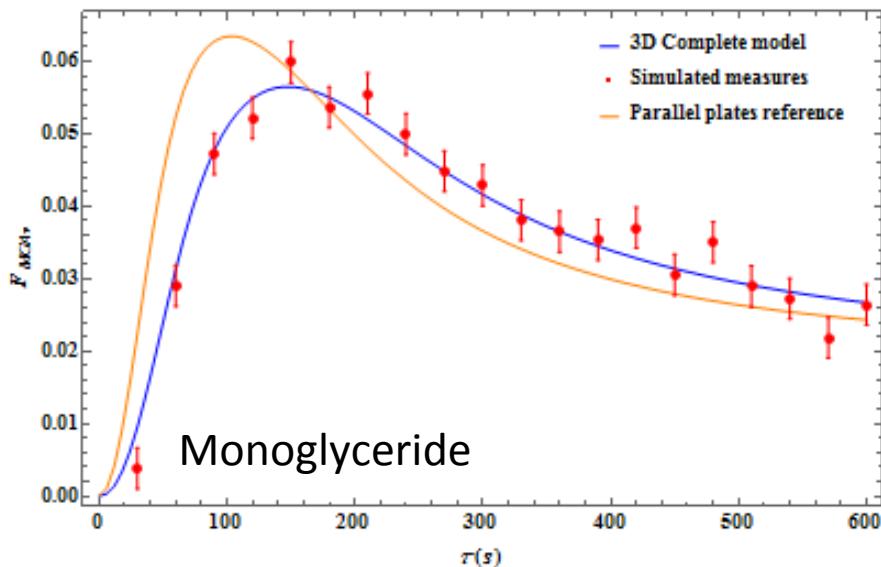
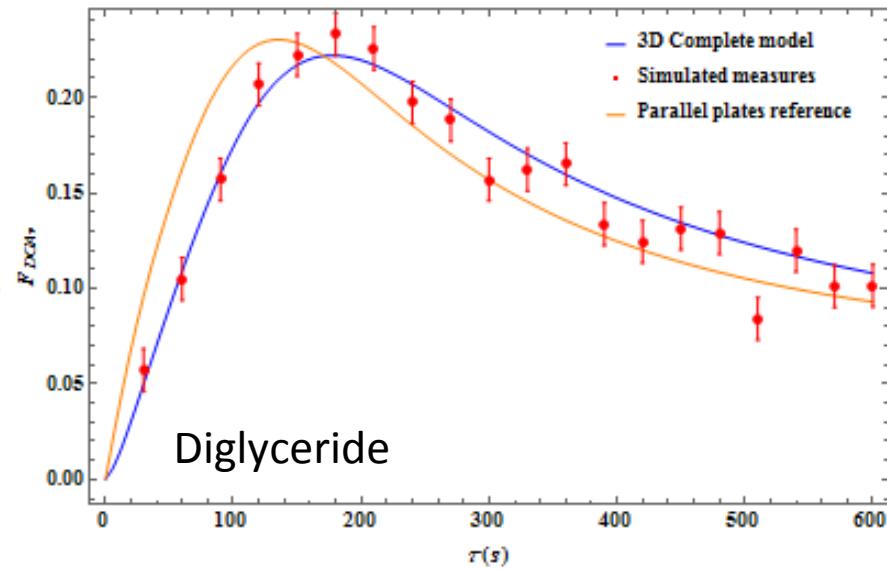
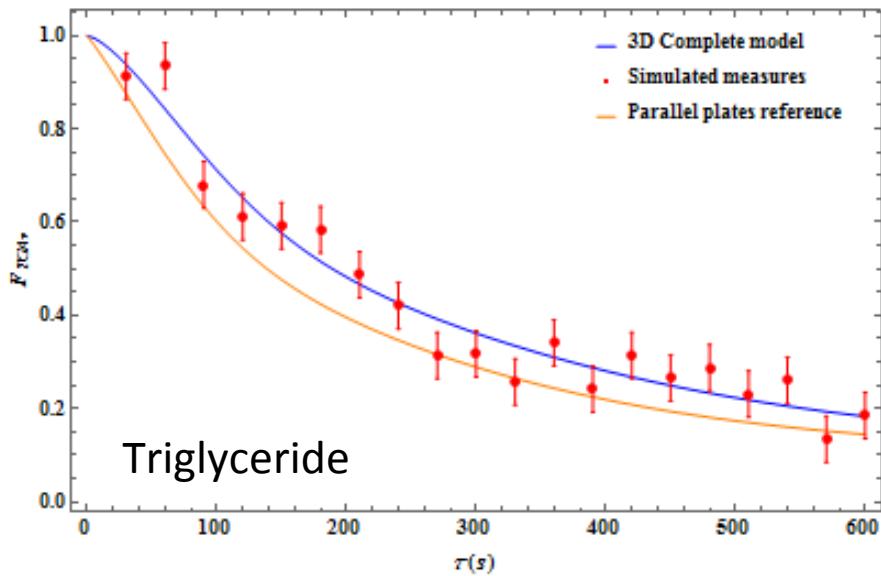
$$\bar{\boldsymbol{\varepsilon}} \approx \bar{\boldsymbol{\varepsilon}}_{\text{reduced model}}$$

$$\tilde{\mathbf{W}} \approx \mathbf{W}_{\text{reduced model}} + \mathbf{W}_{\text{exp}}$$

$$\pi(\mathbf{Y} \mid \mathbf{P}) = (2\pi)^{-I/2} |\tilde{\mathbf{W}}^{-1}|^{-1/2} \exp \left[-\frac{1}{2} \left(\mathbf{Y} - \mathbf{Y}_{\text{reduced model}}(\mathbf{P}) - \bar{\boldsymbol{\varepsilon}} \right)^T \tilde{\mathbf{W}} (\mathbf{Y} - \mathbf{Y}_{\text{reduced model}}(\mathbf{P}) - \bar{\boldsymbol{\varepsilon}}) \right]$$

$$3D \text{ Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad 2D \text{ Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ SIMULATED MEASURES $\sigma = 0.05 \text{Max}(Y_{\text{model}})$

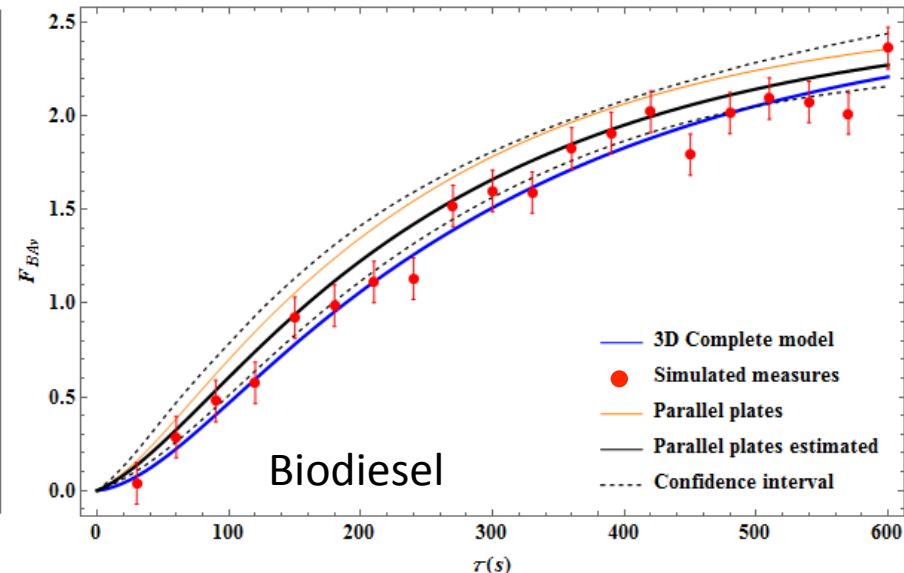
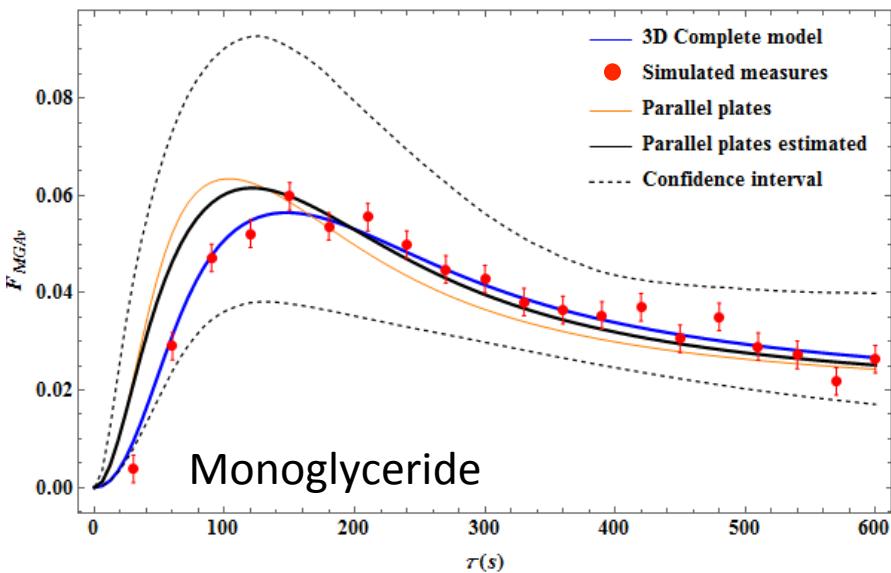
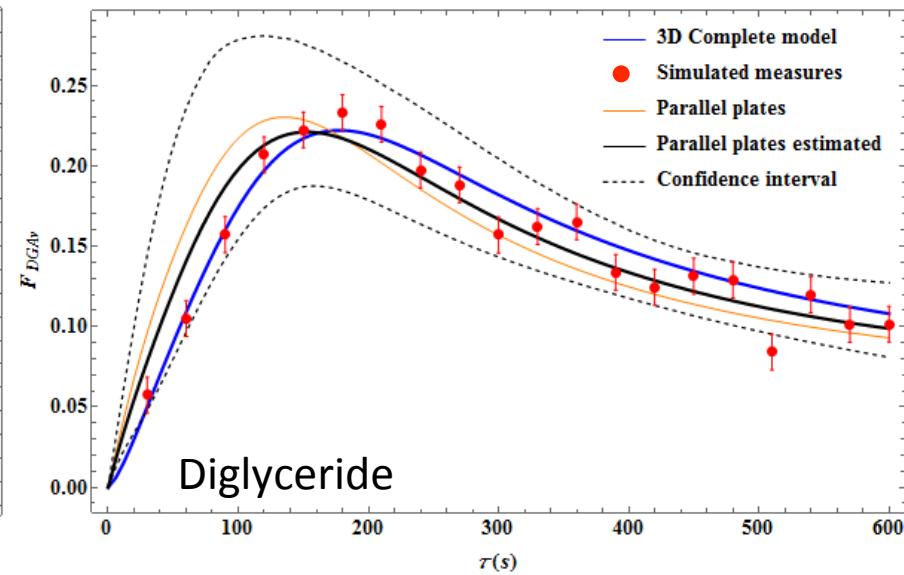
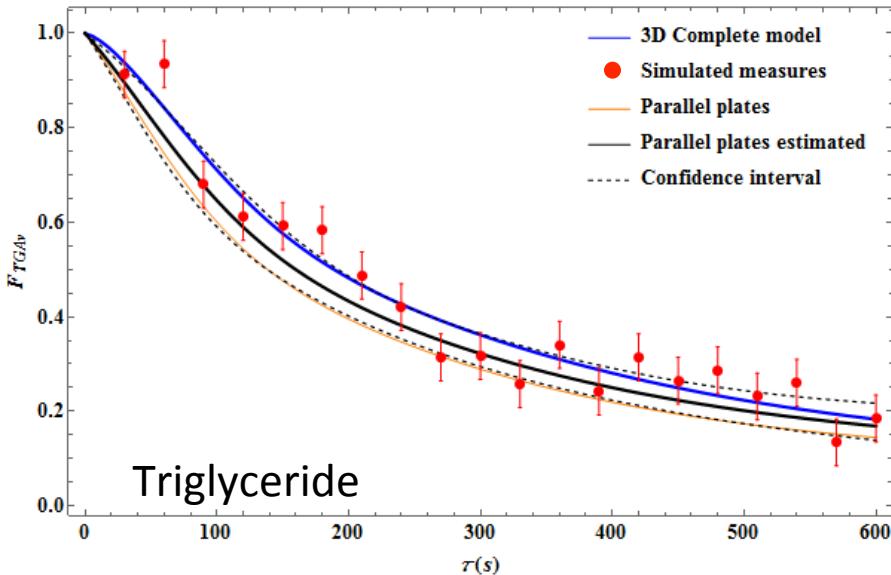


$$3D \text{ Model} \quad \sum_{i=1}^{40} \dots$$

x

$$2D \text{ Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

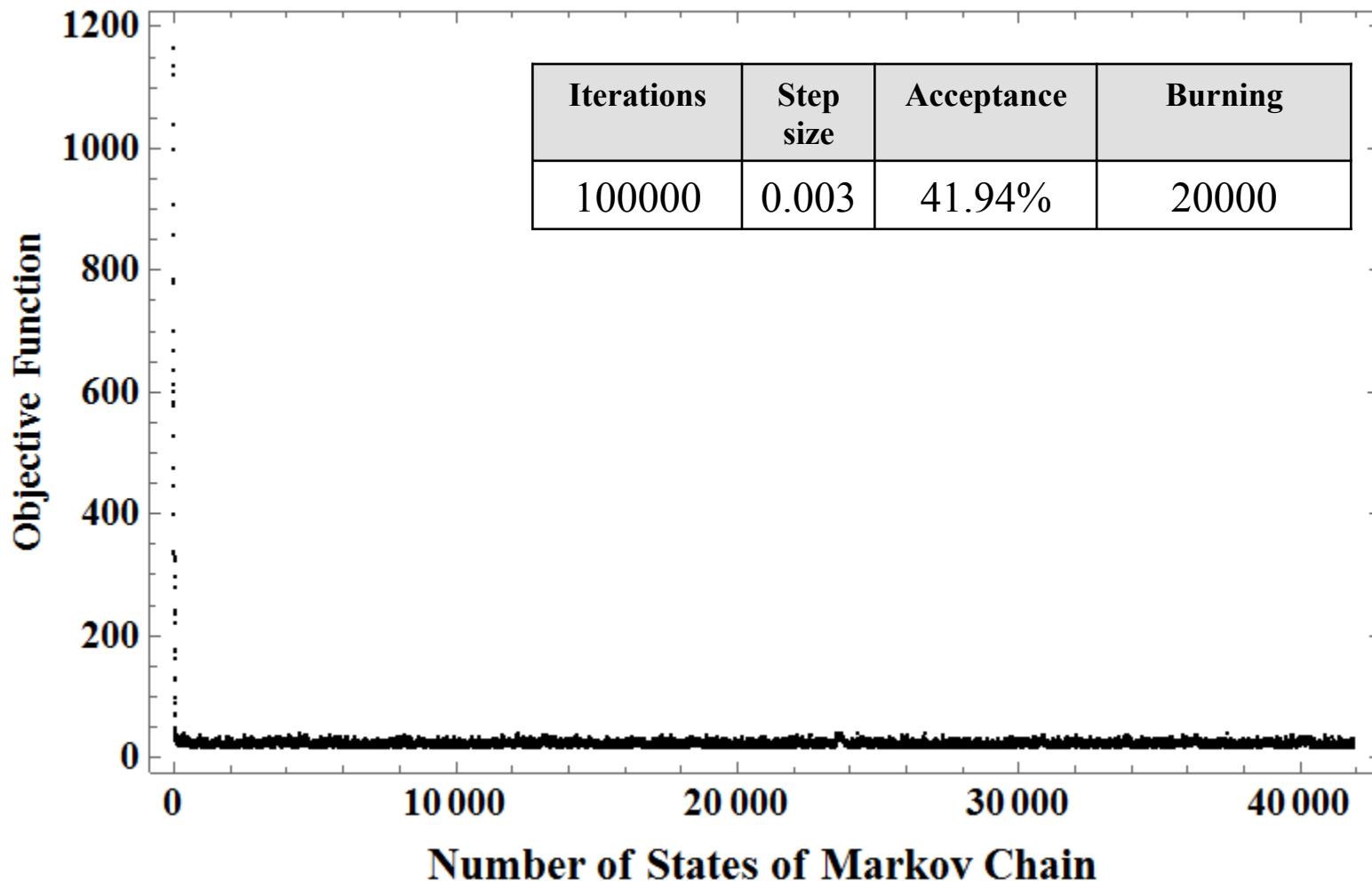
➤ Parameter estimation



$$\text{3D Model } \sum_{i=1}^{40} \dots \quad \times \quad \text{2D Parallel Plates Model } \sum_{i=1}^1 \dots$$

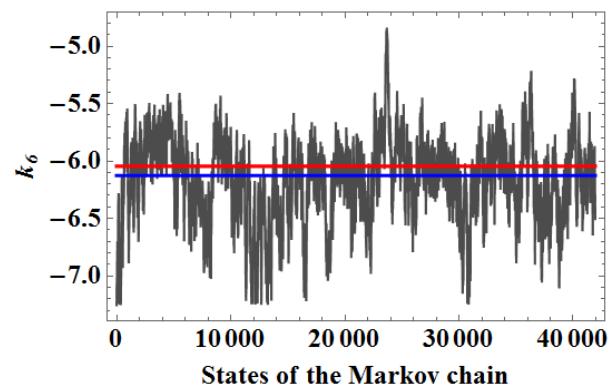
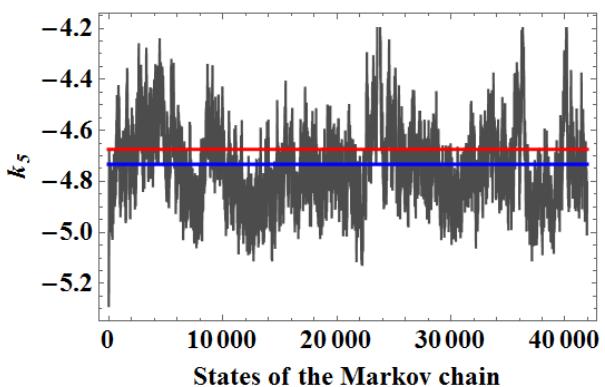
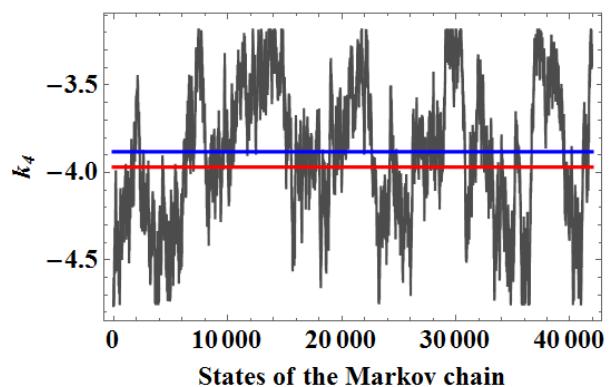
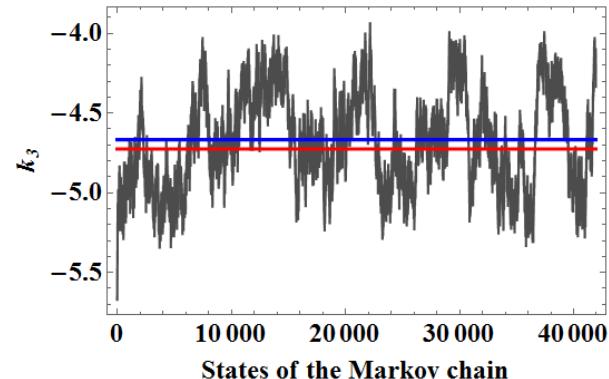
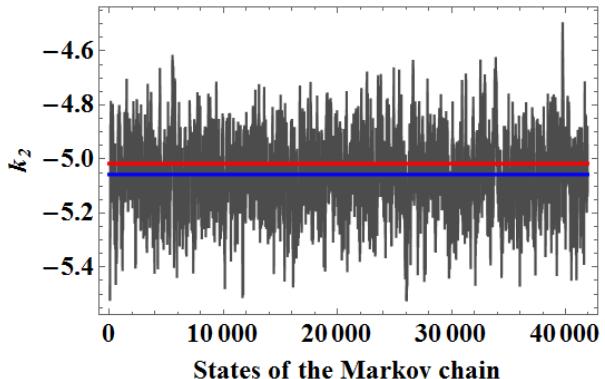
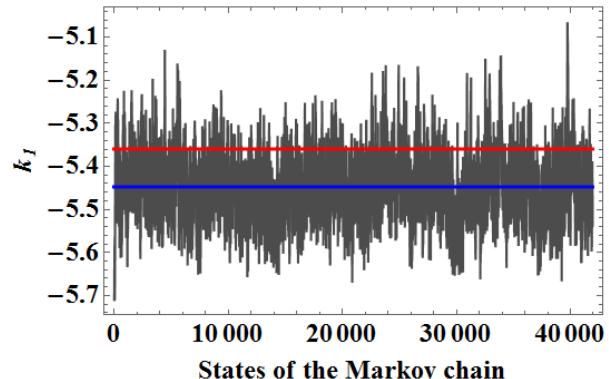
➤ Minimization of objective function

Minimization of objective function with 2D parallel plate model and approximation error model



$$\text{3D Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad \text{2D Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ Markov Chains

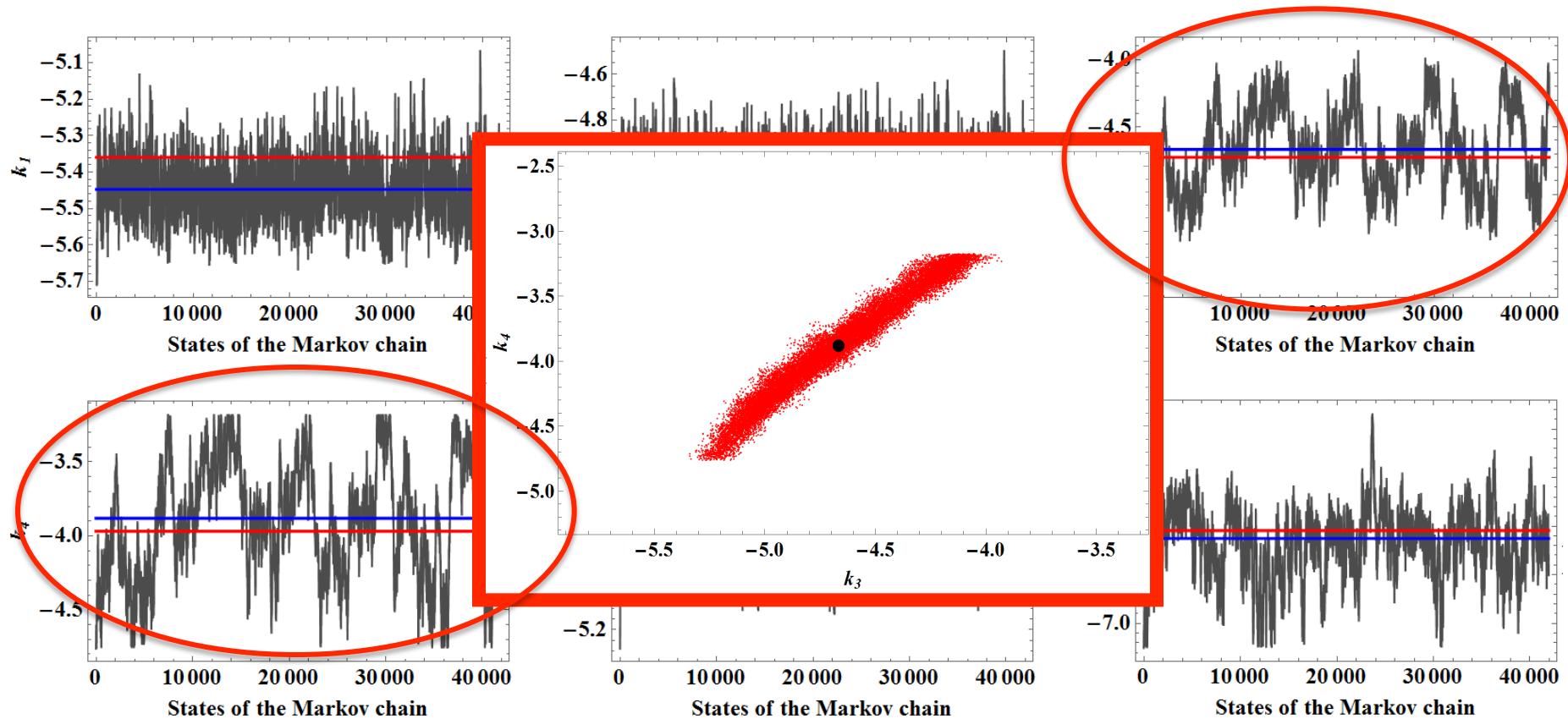


— Estimated parameter

— Reference parameter (Al-Dhubabian, 2005)

$$3D \text{ Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad 2D \text{ Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ Markov Chains



— Estimated parameter

— Reference parameter (Al-Dhubabian, 2005)

$$\text{3D Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad \text{2D Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ ERROR MODEL

Parameters estimated with 2D parallel plate model **WITHOUT** approximation error model

Parameter	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.57254	-5.59546	-5.53751	3.97077
k_2	-6.02003	-5.01669	-5.23631	-5.30769	-5.1436	4.37775
k_3	-5.67101	-4.72584	-5.04866	-5.10333	-4.9534	6.83088
k_4	-4.76279	-3.969	-4.36918	-4.46756	-4.21497	10.0826
k_5	-5.60913	-4.67428	-4.76551	-4.79111	-4.72229	1.95178
k_6	-7.25491	-6.04576	-6.18009	-6.27219	-6.04436	2.22197

Parameters estimated with 2D parallel plate model **WITH** approximation error model

Parameter	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.44772	-5.56511	-5.20121	1.64197
k_2	-6.02003	-5.01669	-5.05721	-5.26888	-4.69399	0.807751
k_3	-5.67101	-4.72584	-4.66665	-5.13613	-4.06344	1.25259
k_4	-4.76279	-3.969	-3.88106	-4.53215	-3.1877	2.2156
k_5	-5.60913	-4.67428	-4.73256	-4.94991	-3.95707	1.24681
k_6	-7.25491	-6.04576	-6.12605	-6.66355	-5.01081	1.3281

$$3D \text{ Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad 2D \text{ Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ ERROR MODEL

$\sum_{i=1}^1 \dots$ Estimated with 2D parallel plate model **WITHOUT** approximation

	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.57254	-5.59546	-5.53751	3.9%
k_2	-6.02003	-5.01669	-5.23631	-5.30769	-5.1436	4.37775
k_3	-5.67101	-4.72584	-5.04866	-5.10333	-4.9534	6.83088
k_4	-4.76279	-3.969	-4.36918	-4.46756	-4.21497	10.0826
k_5	-5.60913	-4.67428	-4.76551	-4.79111	-4.72229	1.95178
k_6	-7.25491	-6.04576	-6.18009	-6.27219	-6.04436	2.22197

$$\bar{\epsilon} \approx \bar{\epsilon}_{\text{model}}$$

$\sum_{i=1}^1 \dots$ Estimated with 2D parallel plate model **WITH** approximation

	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.44772	-5.56511	-5.20121	1.64197
k_2	-6.02003	-5.01669	-5.05721	-5.26888	-4.69399	0.807751
k_3	-5.67101	-4.72584	-4.66665	-5.13613	-4.06344	1.25259
k_4	-4.76279	-3.969	-3.88106	-4.53215	-3.1877	2.2156
k_5	-5.60913	-4.67428	-4.73256	-4.94991	-3.95707	1.24681
k_6	-7.25491	-6.04576	-6.12605	-6.66355	-5.01081	1.3281

$$\bar{\epsilon} \approx \bar{\epsilon}_{\text{reduced model}}$$

$$3D \text{ Model} \quad \sum_{i=1}^{40} \dots \quad \times \quad 2D \text{ Parallel Plates Model} \quad \sum_{i=1}^1 \dots$$

➤ ERROR MODEL

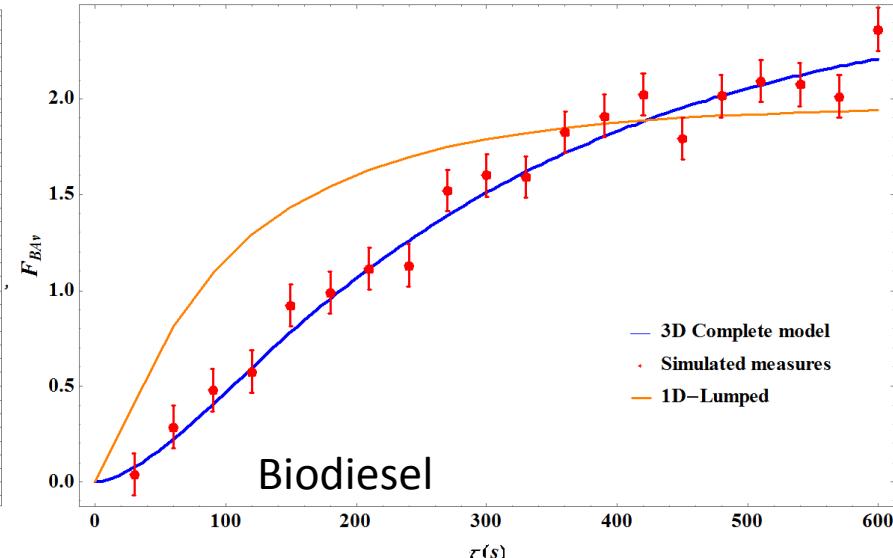
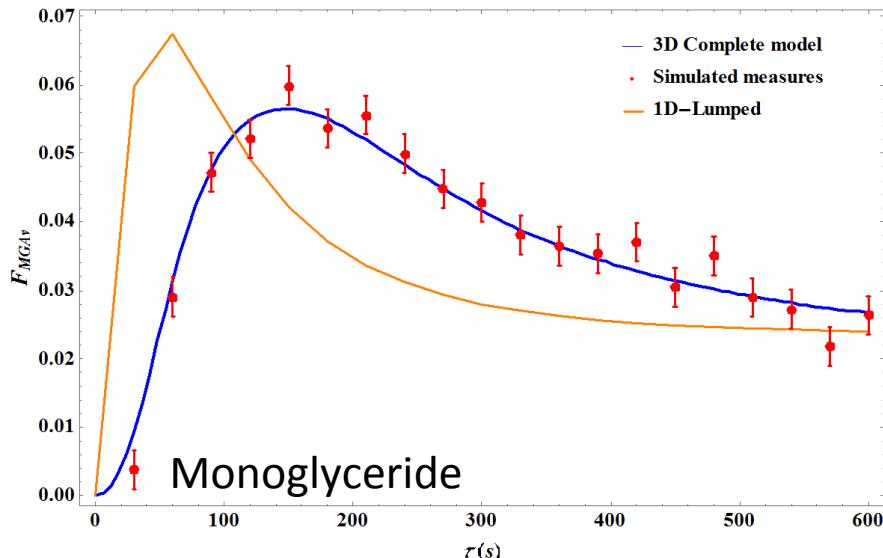
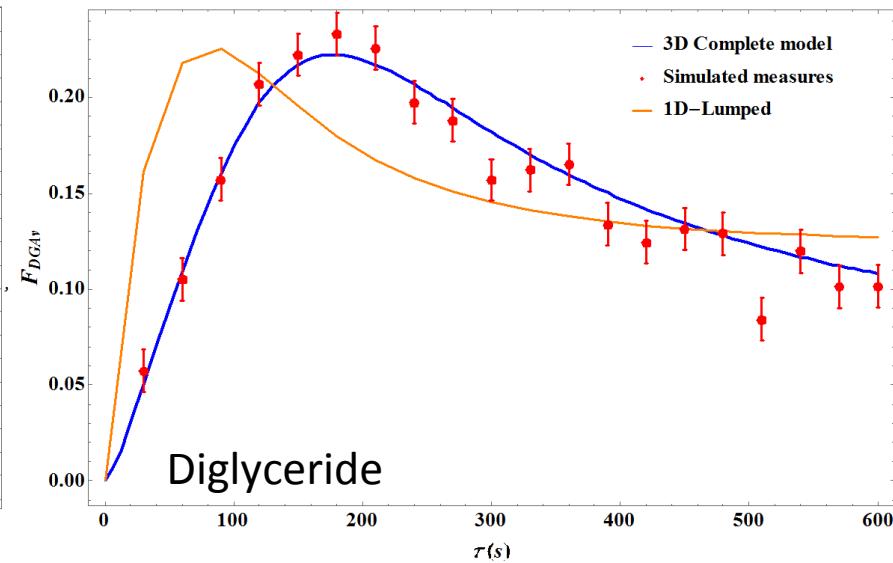
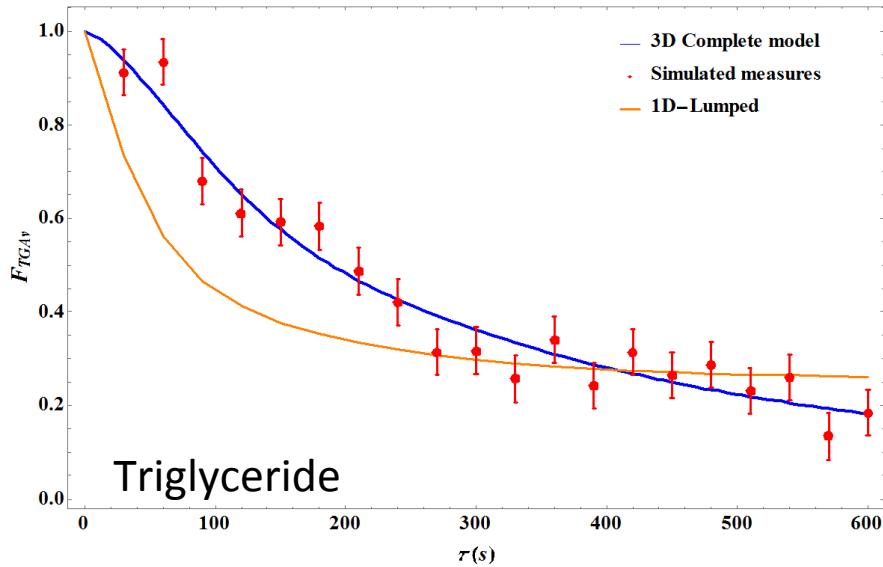
Estimated with 2D parallel plate model **WITHOUT** approximation

	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.57254	-5.59546	-5.53751	3.9%
k_2	-6.02003	-5.01669	-5.23631	-5.30769	-5.1436	4.37775
k_3	model		Comp. time for 1000 states		Comp. time for 200 000 states	
k_4						
k_5	3D with 40 terms		21h		175 days	
k_6	3D with 1 terms		13s		44 min	
	2D with 40 terms		10h		83 days	
	2D with 1 terms		20s		1h	

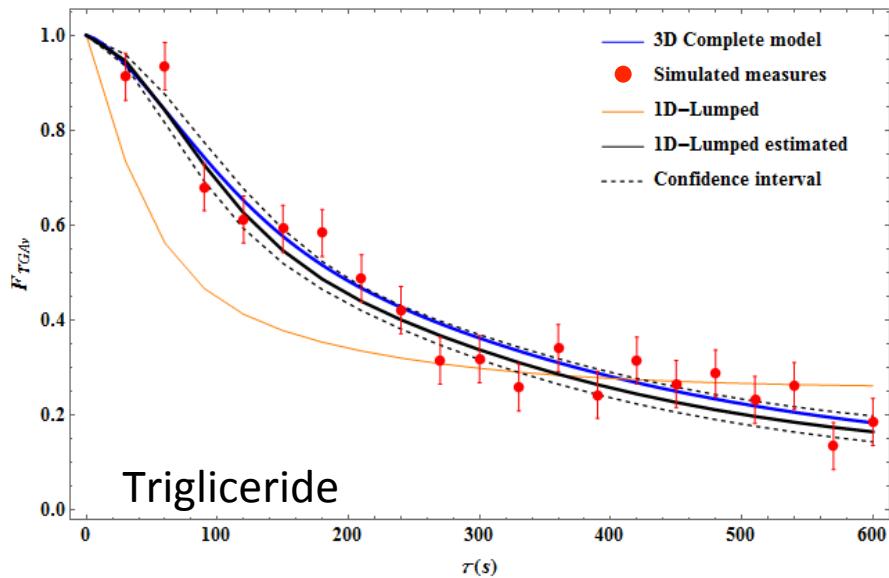
Estimated with 2D parallel plate model **WITH** approximation

	Guess	Reference	Estimated value	Minimum value	Maximum value	Relative error
k_1	-6.43166	-5.35972	-5.44772	-5.56511	-5.20121	1.64197
k_2	-6.02003	-5.01669	-5.05721	-5.26888	-4.69399	0.807751
k_3	-5.67101	-4.72584	-4.66665	-5.13613	-4.06344	1.25259
k_4	-4.76279	-3.969	-3.88106	-4.53215	-3.1877	2.2156
k_5	-5.60913	-4.67428	-4.73256	-4.94991	-3.95707	1.24681
k_6	-7.25491	-6.04576	-6.12605	-6.66355	-5.01081	1.3281

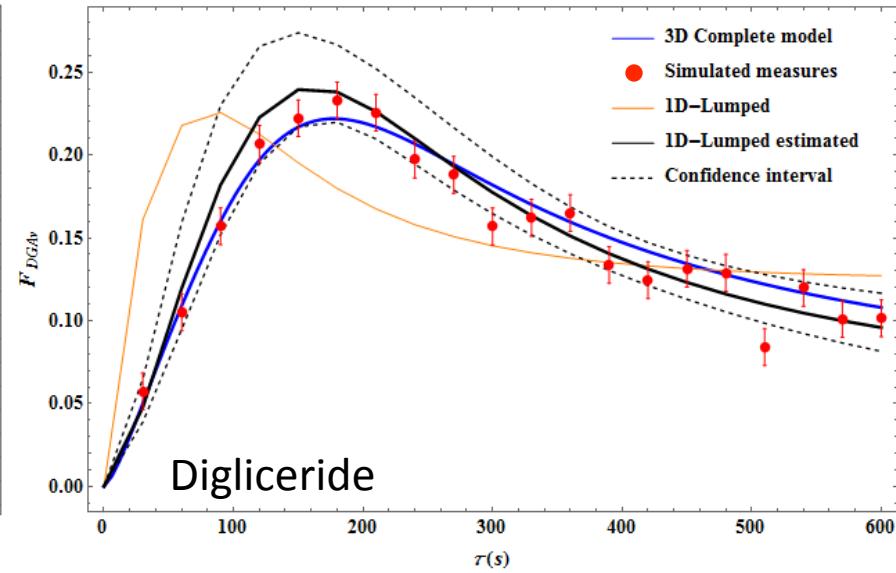
➤ ERROR MODEL



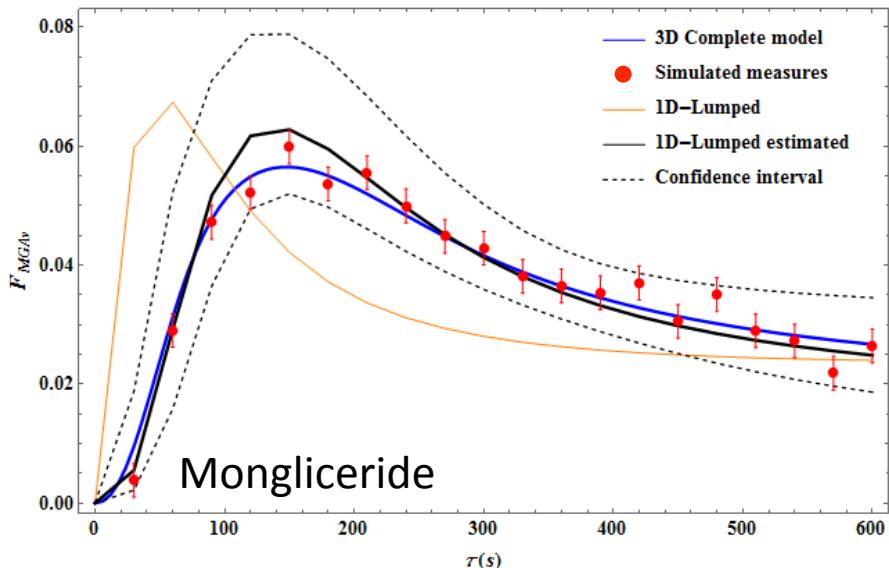
➤ ERROR MODEL



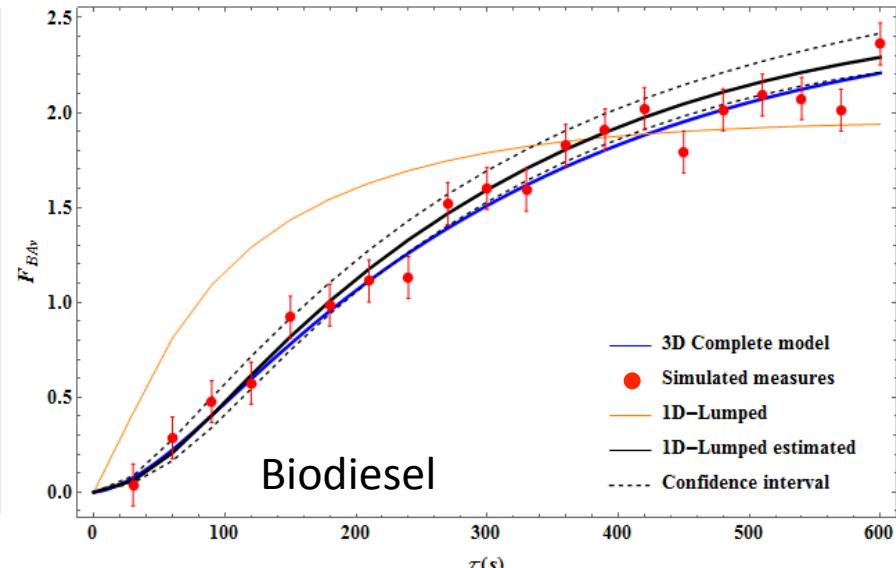
Triglyceride



Diglyceride

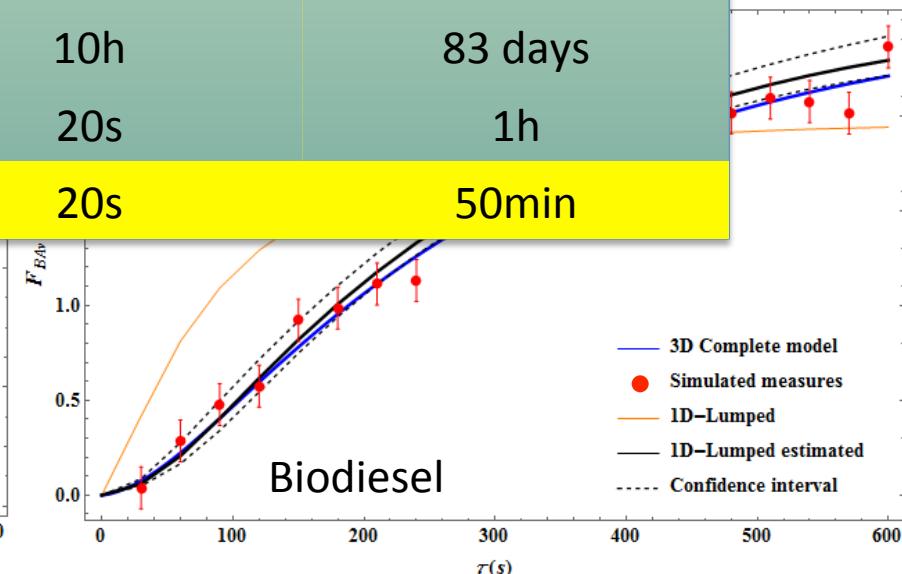
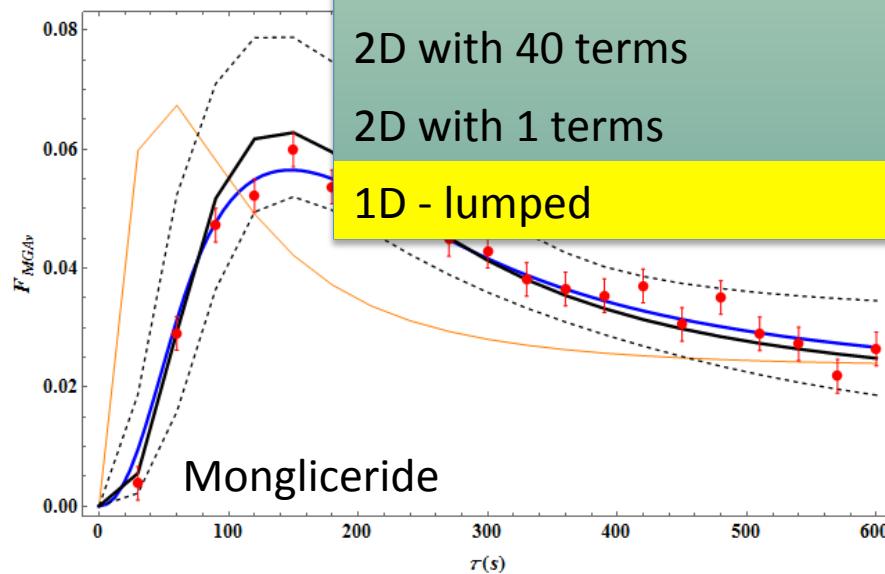
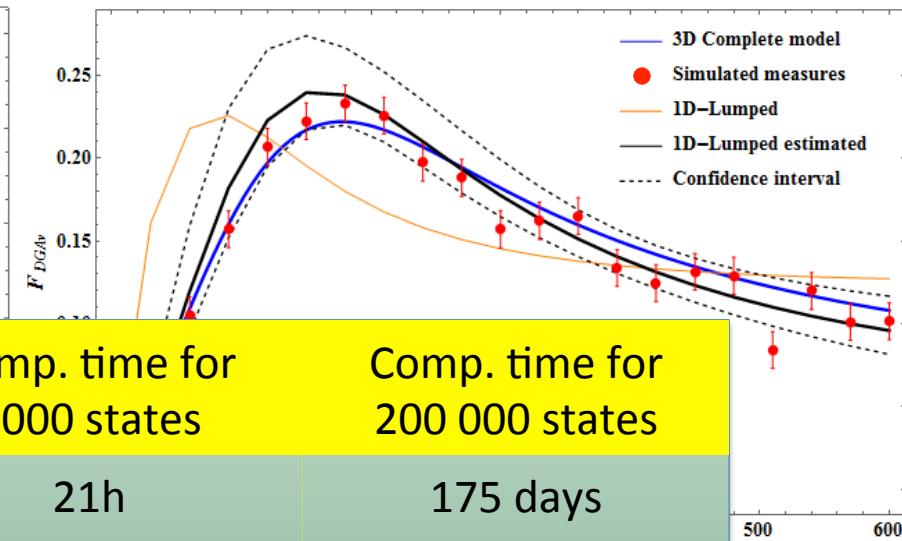
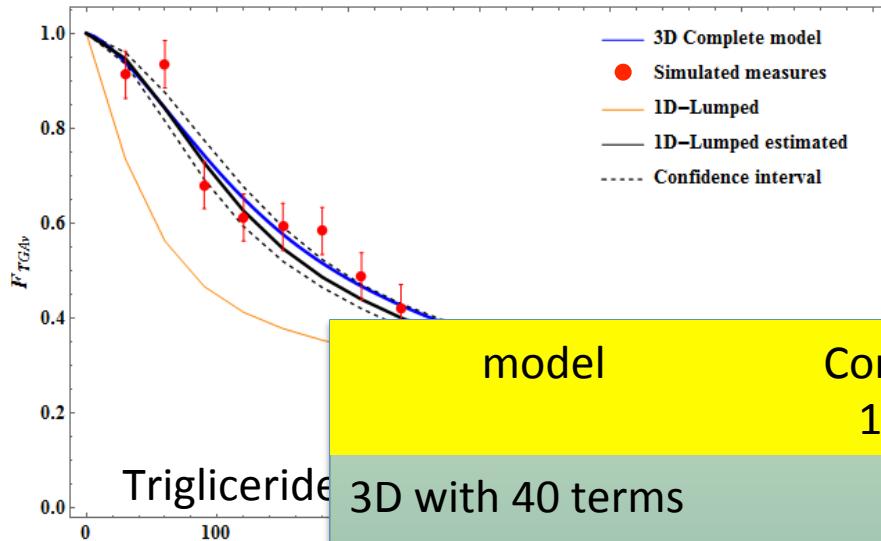


Monglyceride



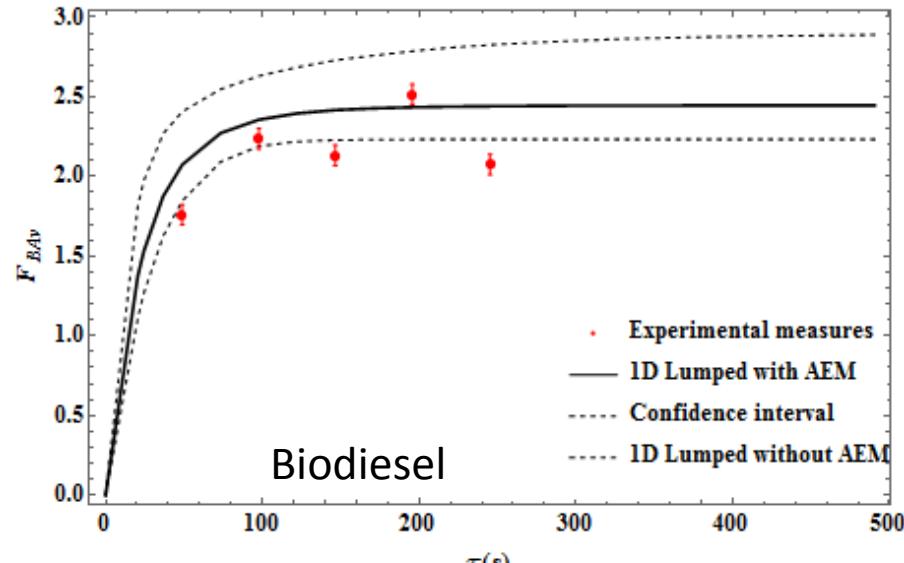
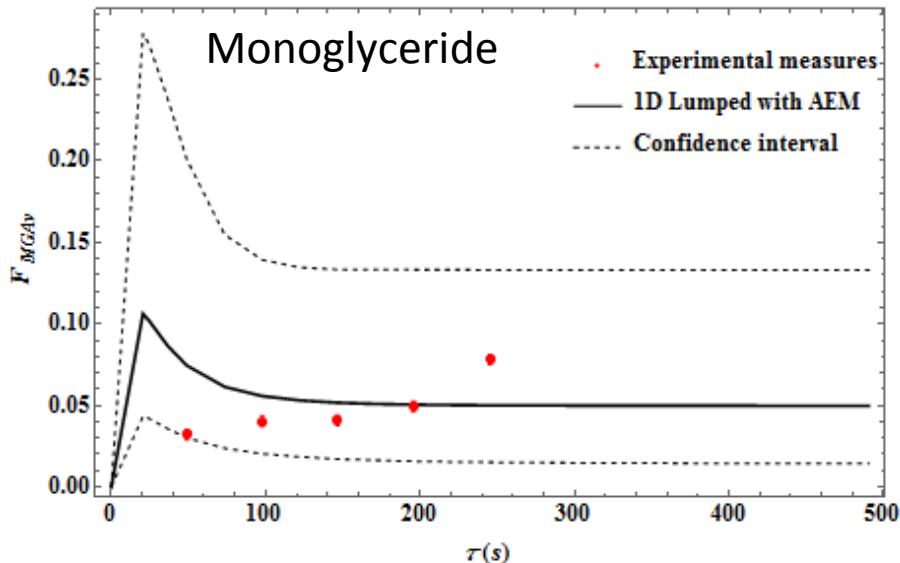
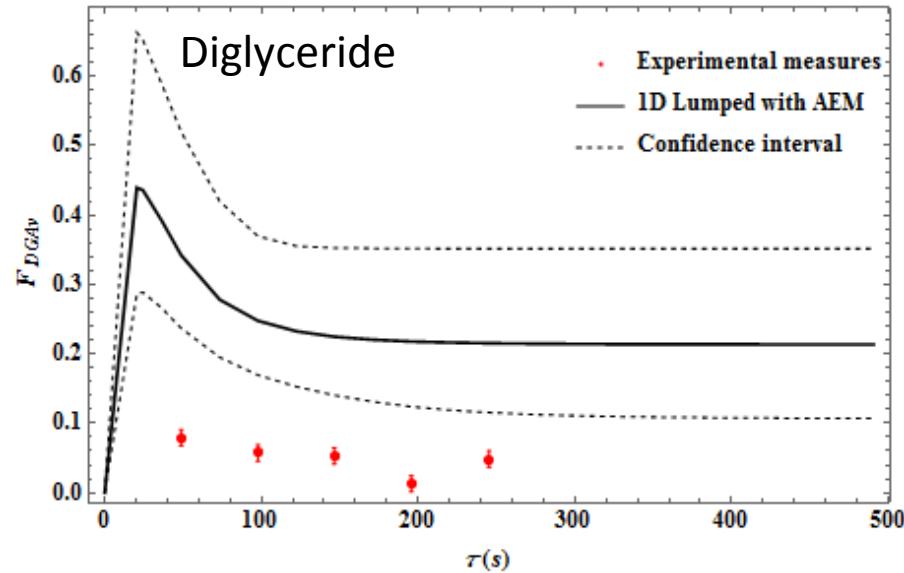
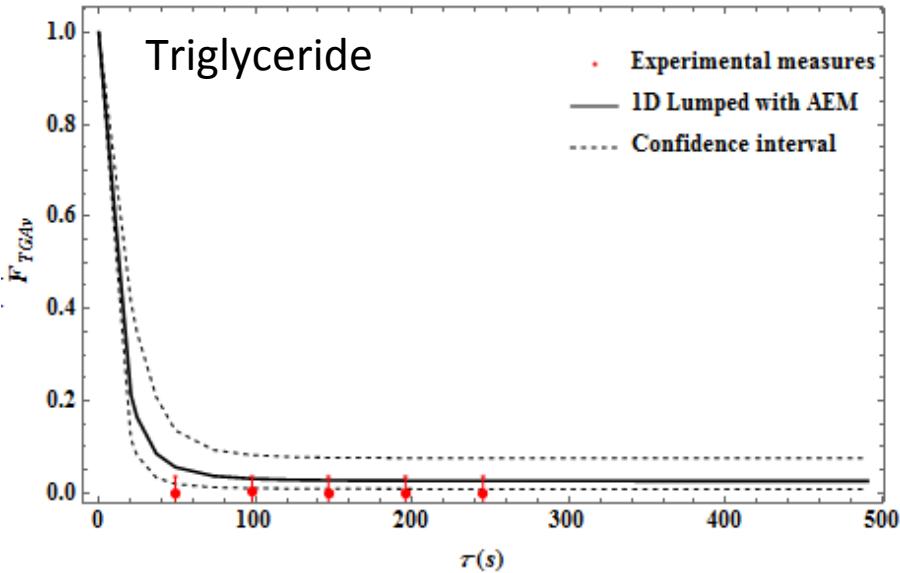
Biodiesel

➤ ERROR MODEL



model	Comp. time for 1000 states	Comp. time for 200 000 states
3D with 40 terms	21h	175 days
3D with 1 terms	13s	44 min
2D with 40 terms	10h	83 days
2D with 1 terms	20s	1h
1D - lumped	20s	50min

➤ ERROR MODEL



R&D Challenges : Biodiesel Production in micro reactors



Validation Experiments

Estimated biodiesel concentration, based on the estimated kinetic constants, in comparison **with two additional cases of residence time.**

Estimated constant	
k_1	0,380
k_2	0,983
k_3	$2,40 \times 10^{-5}$
k_4	$1,62 \times 10^{-5}$
k_5	0,635
k_6	0,038

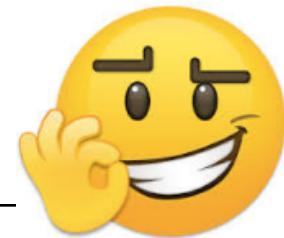
Validation Case	Residence Time
1	0.78 min
2	1.55 min

R&D Challenges : Biodiesel Production in micro reactors



Validation Experiments

Estimated biodiesel concentration, based on the estimated kinetic constants, in comparison **with two additional cases of residence time.**



Estimated constant	
k_1	0,380
k_2	0,983
k_3	$2,40 \times 10^{-5}$
k_4	$1,62 \times 10^{-5}$
k_5	0,635
k_6	0,038

	Validation Case	Residence Time	Biodiesel Conc. Experim. Result [mol/m³]	Biodiesel Conc. Predicted Math. Model [mol/m³]	Percentage error
k_1	1	0.78 min	2.676,96	2.626,26	2,0%
	2	1.55 min	2.646,54	2.623,22	1,1%

R&D Challenges : Biodiesel Production in microreactors



	Biodiesel Production	Device Total weight	Device Total volume
1 module 10 micro-reactors	1,33 L/day	123 g	2,5cm X 4cm X 1,27cm

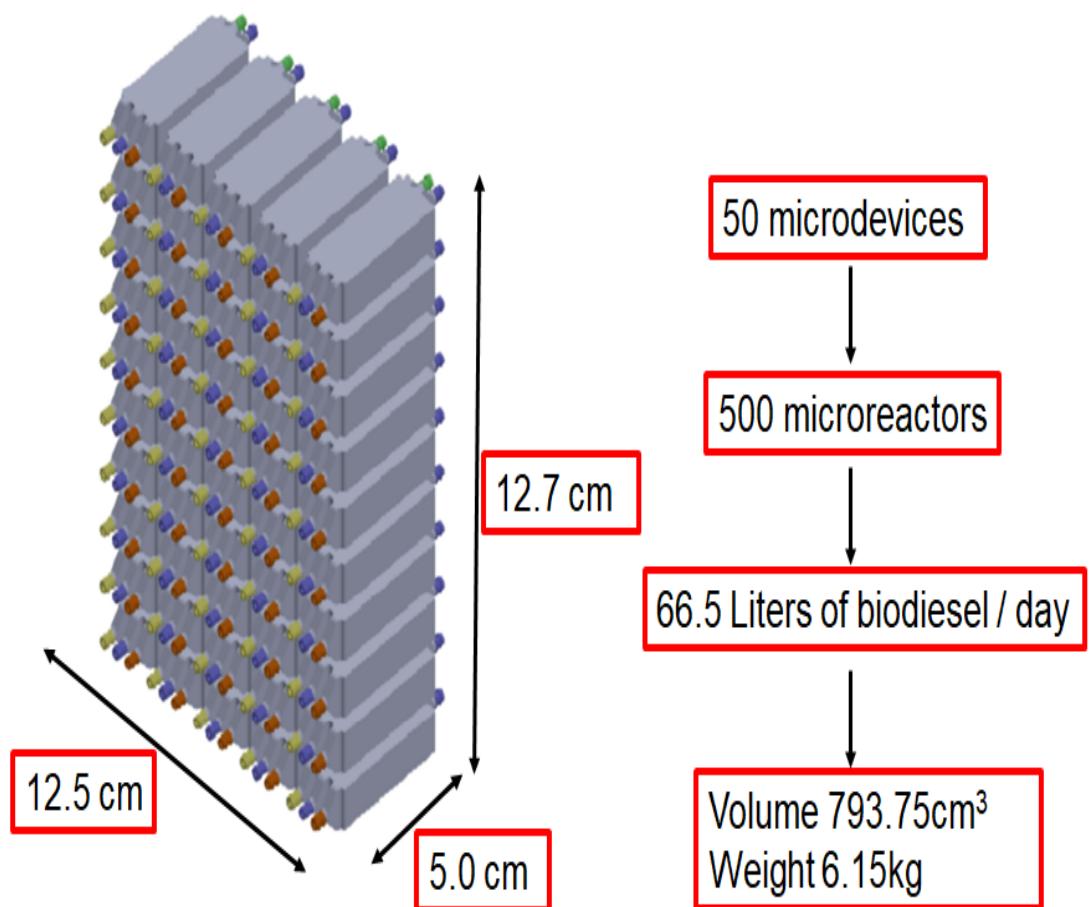
➤ SCALING UP...

R&D Challenges : Biodiesel Production in microreactors



	Biodiesel Production	Device Total weight	Device Total volume
1 module 10 micro-reactors	1,33 L/day	123 g	2,5cm X 4cm X 1,27cm

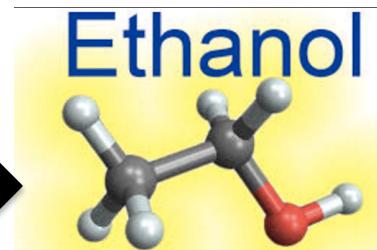
➤ SCALING UP...



R&D Challenges : Biodiesel Production in microreactors



➤ WASTE COOKING OIL (WCO) ...



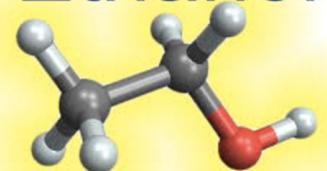
R&D Challenges : Biodiesel Production in microreactors



➤ WASTE COOKING OIL (WCO) ...



Ethanol

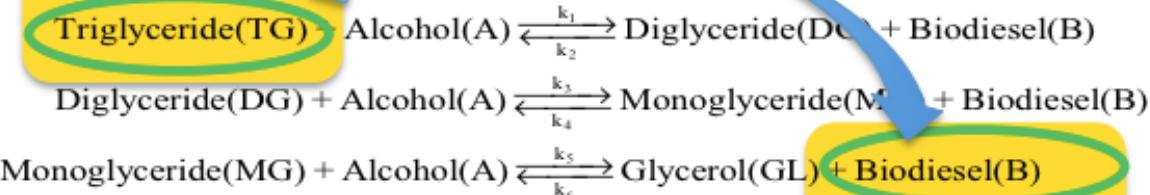


biodiesel



Ethanol/ Oil ratio: 20:1
Catalyst: KOH 1% wt oil
Reaction temperature: 52,3°C
Residence time: 1 min

99.5%



86.2%

R&D Challenges : Biodiesel Production in microreactors

➤ Conclusions

- Complex physical problem can take advantage of both Computational and Experimental Analysis ;
- Successful fabrication of micro reactors – metal/glass and metal/metal 3D printed
- Estimation of kinetic constants from inverse analysis using real experimental data and taking account the error model;
- Demonstration of micro reactors for the synthesis of ethanol based biodiesel with promising results (99,61% of biodiesel production in 35 seconds residence time);

R&D Challenges : Biodiesel Production in microreactors

➤ Conclusions

- Complex physical problem can take advantage of both Computational and Experimental Analysis ;
- Successful fabrication of micro reactors – metal/glass and metal/metal 3D printed
- Estimation of kinetic constants from inverse analysis using real experimental data and taking account the error model;
- Demonstration of micro reactors for the synthesis of ethanol based biodiesel with promising results (99,61% of biodiesel production in 35 seconds residence time);

➤ Future work

- Fabricate a pilot plant with up to 200-500 microrreactors;
- Enhance the conversion of waste cooking oil in the esterification process in microreactor;
- Estimate the kinectic constant for the waste cooking oil esterification;
- Optimize the micro channel structure based on the estimated constant;

ACKNOWLEDGEMENT



Prof. Helcio Orlande



Prof. Marcelo Colaço

**Prof. Antonio Leitao
Prof. Bernd Hofmann**

Our students :

DSc. José Martim Costa Junior Eng. Diego Busson
MSc. Pericles Crisiron Pontes Eng. Saxon Paiz
MSc. Kelvin Chen

UFRJ Collaborators:

**Prof. Luiz Antônio d'Avila
DSc. Cristiane Gimenes de Souza
Prof. Donato Alexandre Aranda
Prof. Yordanka Reyes Cruz**

CTI Collaborators:

**DSc. Jorge Vicente Lopes da Silva
MSc. Paulo Inforçatti
DSc. Izaque Alves Maia**

UCL Collaborators:

**Prof. Stavroula Balabani
Prof. Manish Tiwari**

Sponsoring Agencies:



ACKNOWLEDGEMENT



Prof. Helcio Orlande



Prof. Marcelo Colaço

**Prof. Antonio Leitao
Prof. Bernd Hofmann**

Our students :

DSc. José Martim Costa Junior Eng. Diego Busson
MSc. Pericles Crisiron Pontes Eng. Saxon Paiz
MSc. Kelvin Chen

UFRJ Collaborators:

**Prof. Luiz Antônio d'Avila
DSc. Cristiane Gimenes de Souza
Prof. Donato Alexandre Aranda
Prof. Yordanka Reyes Cruz**

CTI Collaborators:

**DSc. Jorge Vicente Lopes da Silva
MSc. Paulo Inforçatti
DSc. Izaque Alves Maia**

UCL Collaborators:

**Prof. Stavroula Balabani
Prof. Manish Tiwari**

carolina@mecanica.coppe.ufrj.br

LabMEMS – Nano and Microfluidics and Microsystems Laboratory
Mechanical Engineering Dept. (PEM) & Nanoengineering Dept. (PENT)
Universidade Federal do Rio de Janeiro – UFRJ/COPPE
Rio de Janeiro - Brazil