DESIGN AND OPTIMISATION OF STORAGE SYSTEMS BY ADSORPTION FOR NATURAL GAS PROJECT 5

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Research Centre for Gas Innovation
cleaner energy for a sustainable future

University of São Paulo, Brazil
Aug 21 – 22, 2018

Outline

- Introduction;
- Modelling Overview;
- Results for Phase Change Material Optimisation;

Numeric

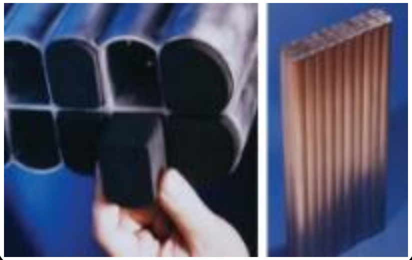
- Differential scanning calorimetry ;
- New cold finger model;
- Comparison of simulation with experiment.

Experimental

Introduction

- **Adsorbed Natural Gas Storage Systems**
  - Adsorption is an exothermic phenomena;
  - As adsorbent temperature rises, adsorption capacity decreases.

ANG System



* Volume of gas at atmospheric conditions per volume of gas at storing conditions (Hirata, 2009)

Method	Temperature (C)	Pressure (MPa)	Density (V/V*)
Compressed	Atmospheric	20	245
Liquefied	-163	Atmospheric	600
Adsorbed	Atmospheric	5	164

- **Phase Change Materials**
  - Significant Phase Change Enthalpy;
    - Can reduce the thermal amplitude of the system where it is

Encapsulated Phase Change Material

Fixed Bed Charge	Butane Working Capacity	Maximum Temperature
Pure AC	66.2 g	85.1 °C
AC + 25 wt-% PCM	77.5 g	65.8 °C

(Zimmermann & Keller 2006)

WORKTRUCKONLINE. Adsorbed Natural Gas Storage Systems. 2016. Avaiable at: <http://www.worktruckonline.com/fc images/articles/madsorbed-natural-gas-storage-systems-1.jpg>

Liquefied Natural Gas. 2016. Avaiable atm: <http://liquidnaturalgasnews.com/wpcontent/uploads/2014/02>.

Hirata, S. C., Couto, P., Lara, L. G., & Cotta, R. M. (2009). Modeling and hybrid simulation of slow discharge process of adsorbed methane tanks. *International Journal of Thermal Sciences*, *48*(6), 1176–1183. https://doi.org/10.1016/j.ijthermalsci.2008.09.001

Introduction

- **Adsorbed Natural Gas Products: Innovation Award (June 06, 2018)**

Modelling Overview

- **Governing Equations Set**

$$q_h(t) = -\rho_l L \lambda \frac{\sqrt{\alpha_l t}}{\sqrt{t}}$$

Heat Transferred to the phase change phenomena.

Energy Balance

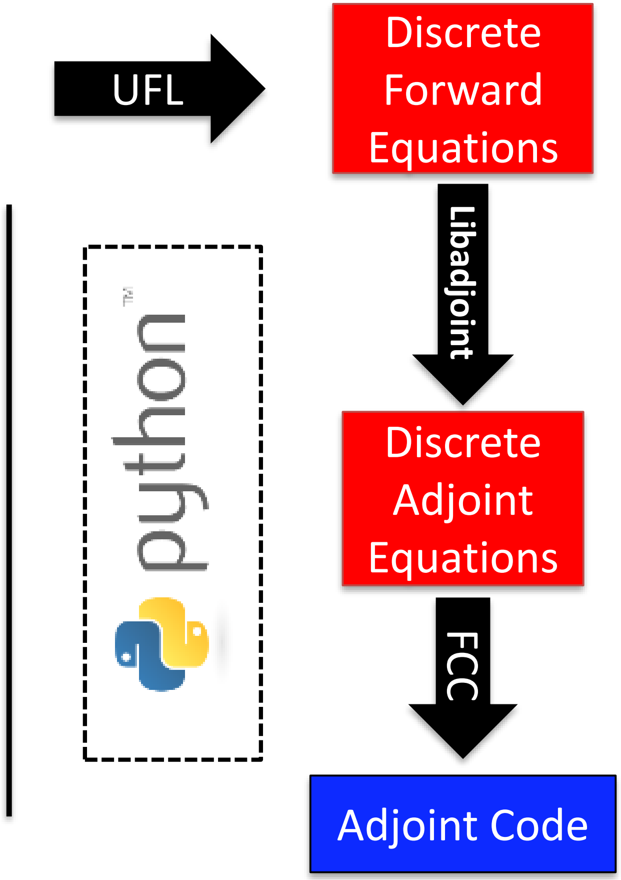
$$\epsilon_t\left(\frac{Cp_g M_g}{R_g}\frac{P}{T}\frac{\partial(T)}{\partial t}-\frac{\partial P}{\partial t}\right)+(1-\epsilon_t)\left(\rho_s Cp_s\frac{\partial(T)}{\partial t}\right)+Cp_g Q\frac{\partial(T)}{\partial t}$$
$$-\frac{Cp_g M_g}{R_g\mu_g}K_s\frac{P}{T}\nabla P\cdot\nabla T-\nabla\cdot\left(k_f\nabla T\right)+q_h=|\Delta H|\frac{\partial(Q)}{\partial t}$$

Mass Balance

$$\frac{\epsilon_t M_g}{R_g}\left(\frac{1}{T}\frac{\partial P}{\partial t}-\frac{P}{T^2}\frac{\partial T}{\partial t}\right)+\frac{\partial Q}{\partial t}-\frac{M_g}{R_g\mu_g}\nabla\cdot\left(K_s\frac{P}{T}\nabla P\right)=0$$

Adsorption

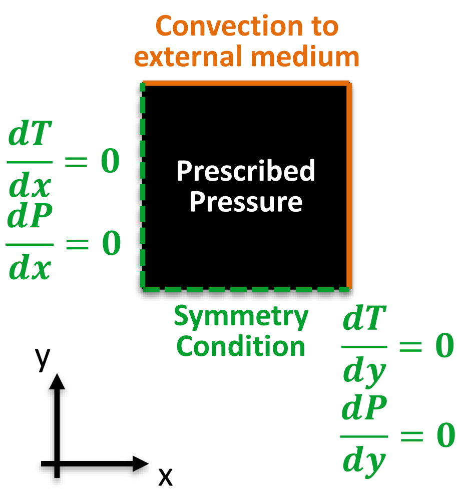
$$\frac{\partial\rho_s}{\partial t}=G_a(\rho_{ss}-\rho_s)$$

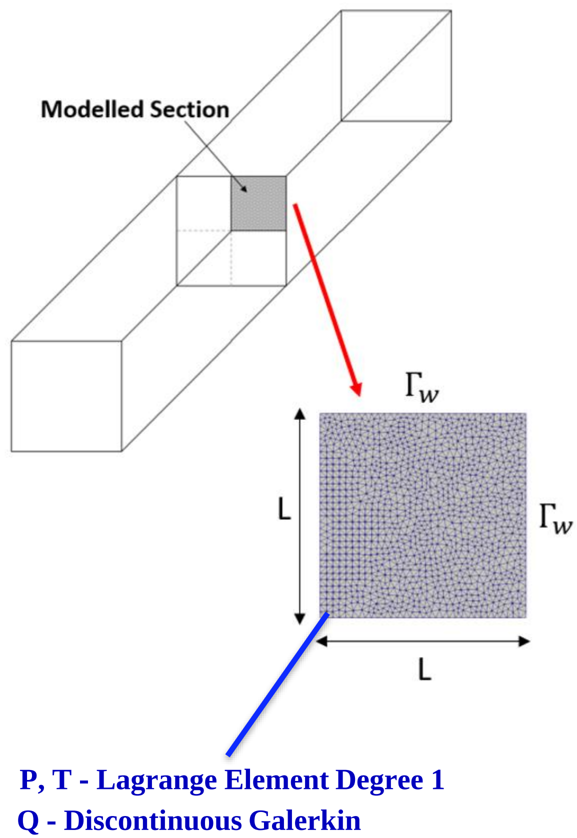


Results for Phase Change Material Optimisation

- **Topology optimisation**
  - **Prismatic Vessel**

Boundary Conditions





Mesh
2D - Triangular
2220 Elements

Dimensions
L = 53.3 mm

Cycle
Temperature: Tini = 293K
Initial Pressure: Pini = 0.1 MPa
Final Pressure: Plet = 3.5 MPa
Heat Convection on Γ_w :700 W/m.K
Total Cycle Time: 300 s
Time Step: 3 s

Optimisation Parameters
Initial Guess: e = 0.0
Iterations : 45
Optimiser: L-BFGS-B

Results for Phase Change Material Optimisation

- **Vessel Section**

Original (Full Carbon) | **Optimised**

Pseudo-Porosity Distribution ε_{pcm} [%]

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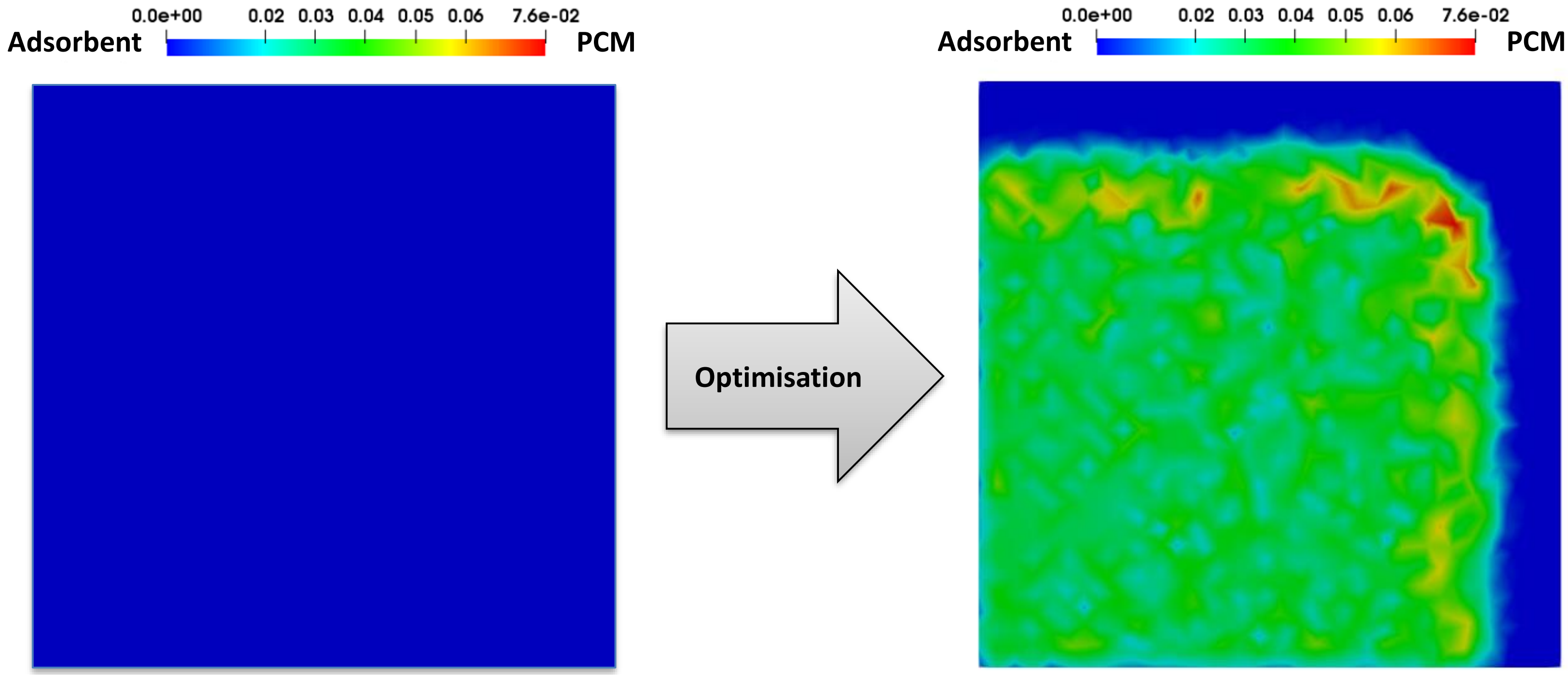
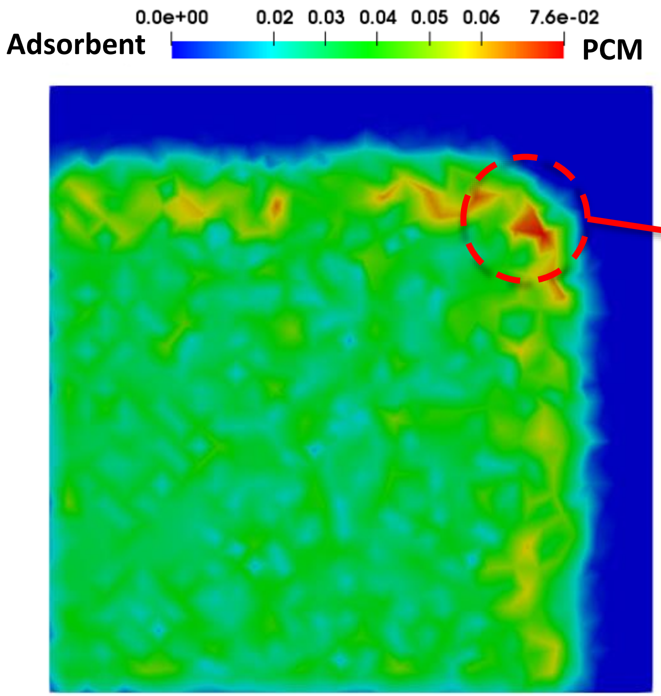
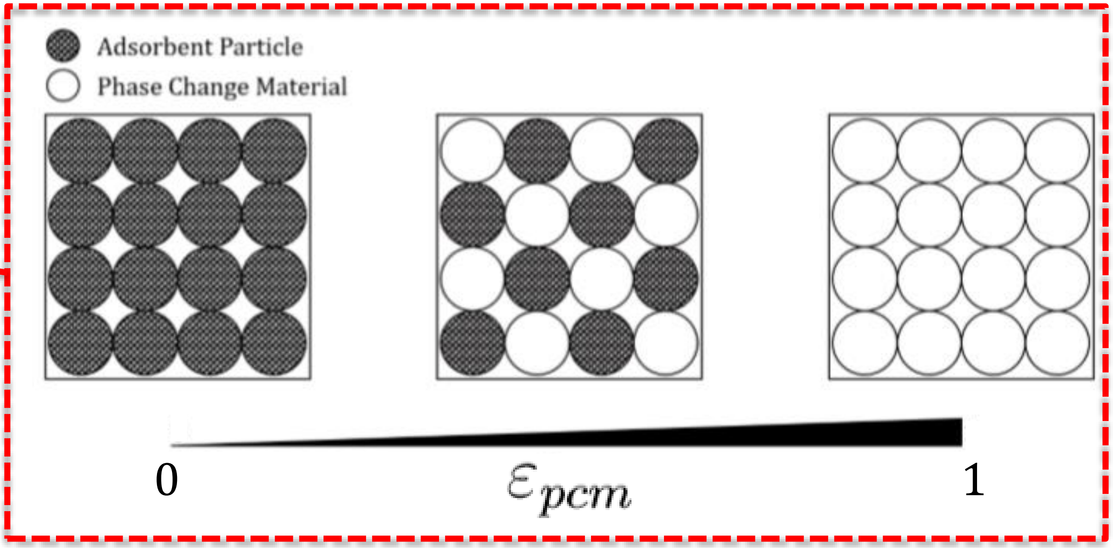


Results for Phase Change Material Optimisation

- **Optimised Design**

Pseudo-Porosity Distribution ε_{pcm} [%]

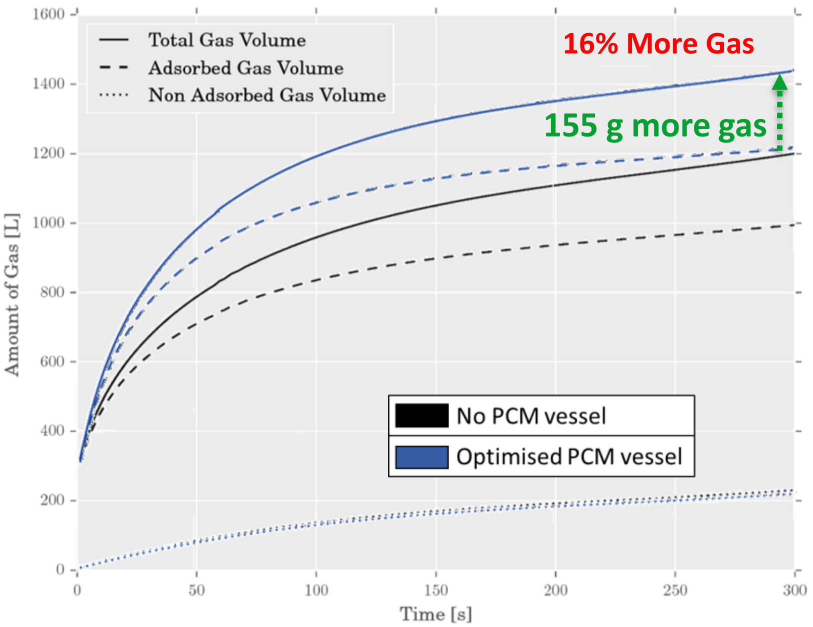




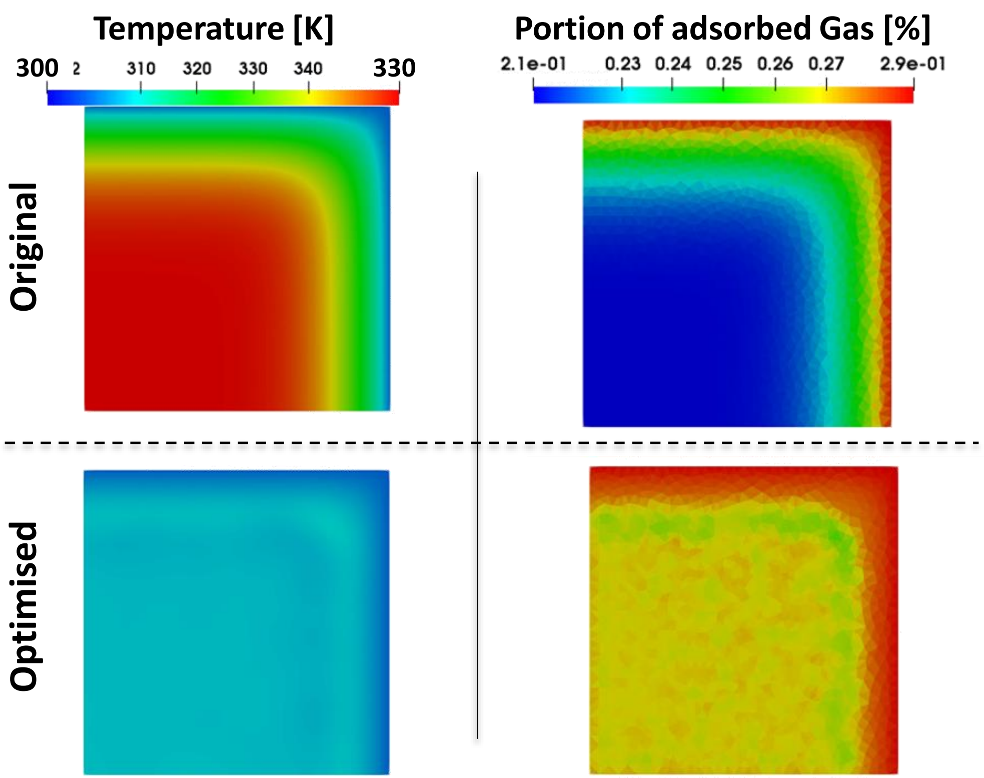
Results for Phase Change Material optimisation

- **Topology Optimisation**

Amount of Gas inside the vessel



By the end of charging cycle



Results for Phase Change Material optimisation

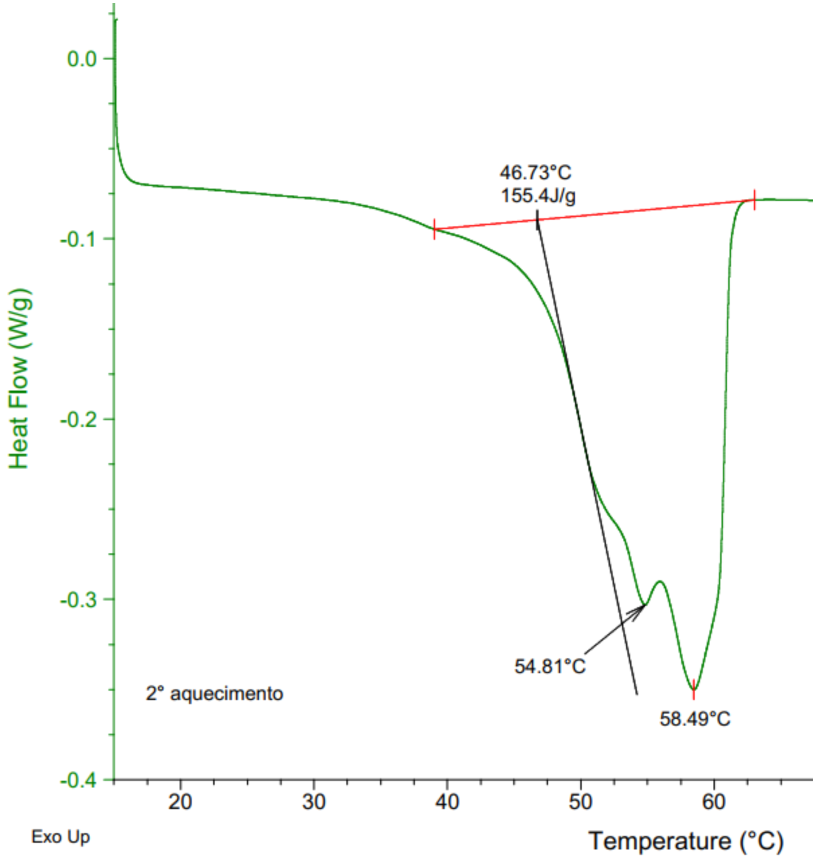
- **Presentations**
  - Workshop Natural Gas & Future Energy Systems. Optimization of an Adsorbed Natural Gas Storage System. 2016;
  - PRADO, D. S.; SILVA, E. C. N. . Topology Optimization Applied to Adsorption Systems with Phase Change Materials. In: 5th International Conference on Engineering Optimization, 2016, Foz do Iguaçu. Book of Abstracts. Rio de Janeiro: E-Papers Serviços Editoriais Ltda, 2016. v. 1. p. 104-104;
  - PRADO, D. S.; SILVA, E. C. N. ; AMIGO, R. C. R. . Optimization of an Adsorbed Natural Gas System with Phase Change Material using the Topology Optimization Method. 2016;
  - Carbon Capture and Storage (CCS) Process & Technologies for Brazilian Market. Optimization Tools for Adsorption Tanks & CCS. 2017;
  - 14th U.S. National Congress on Computational Mechanics. Topology Optimization of an Axisymmetric Adsorbed Natural Gas Vessel with Phase Change Materials. 2017;
  - 13th World Congress in Computational Mechanics. Optimized Phase Change Material Distribution for Adsorption Systems Using Topology Optimization Method in Axisymmetric Model. 2018.

- **Publications**
  - PRADO, D.S.; AMIGO, R.C.R. ; PAIVA, J.L. ; SILVA, E.C.N. . Analysis of Convection Enhancing Complex Shaped Adsorption Vessels. APPLIED THERMAL ENGINEERING, v. 141, p. 352-367, 2018.

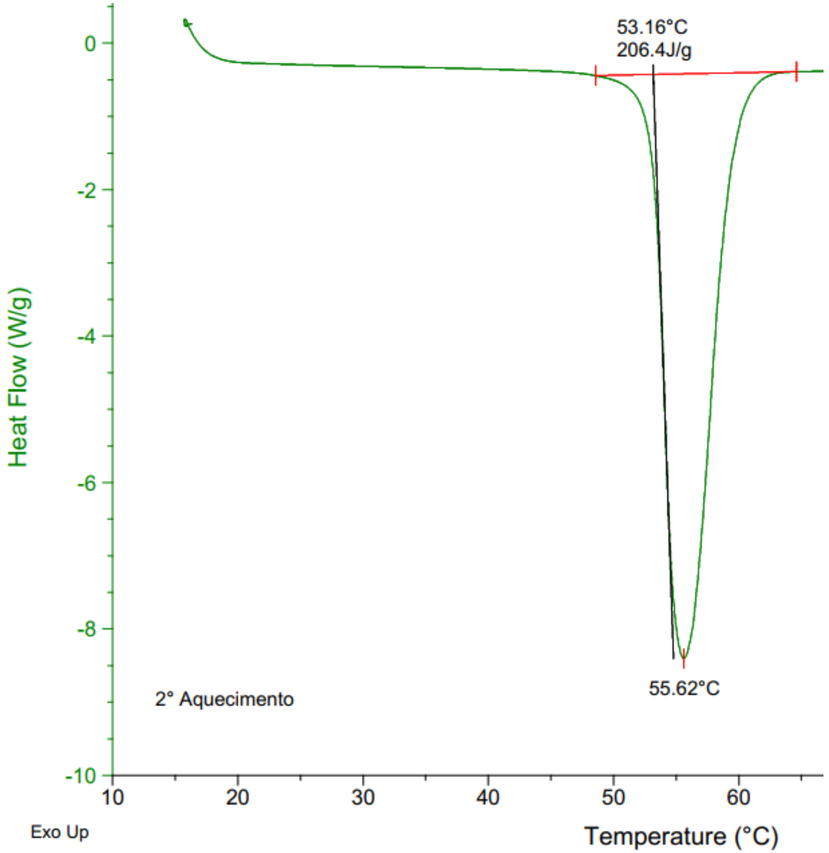
Experimental

Differential scanning calorimetry

Stearic acid

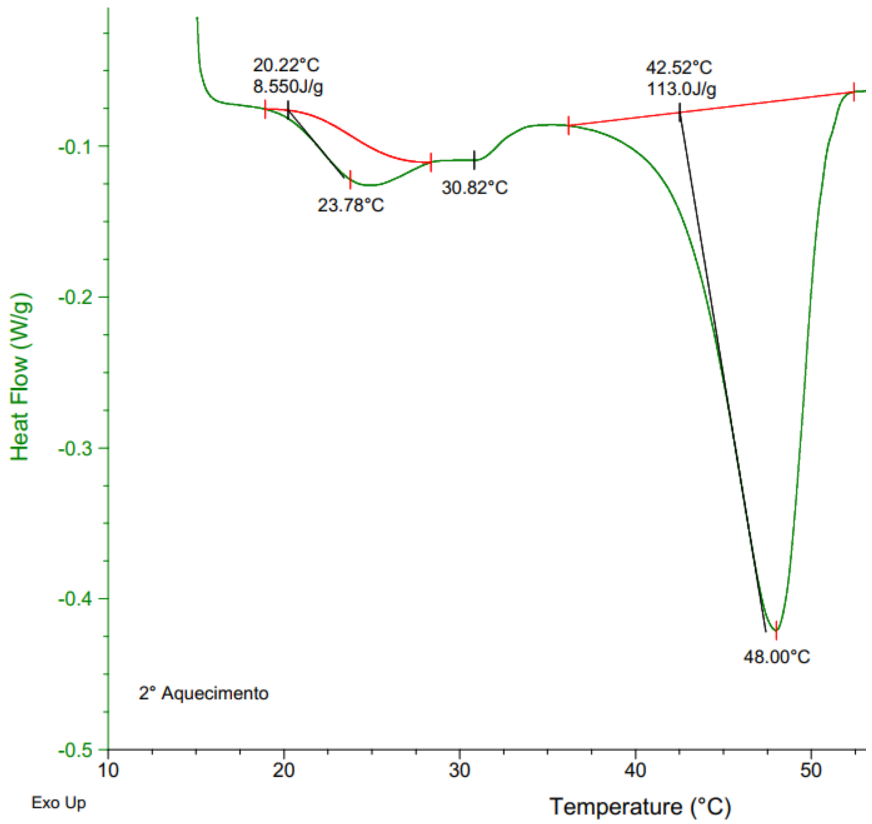


Miristic acid

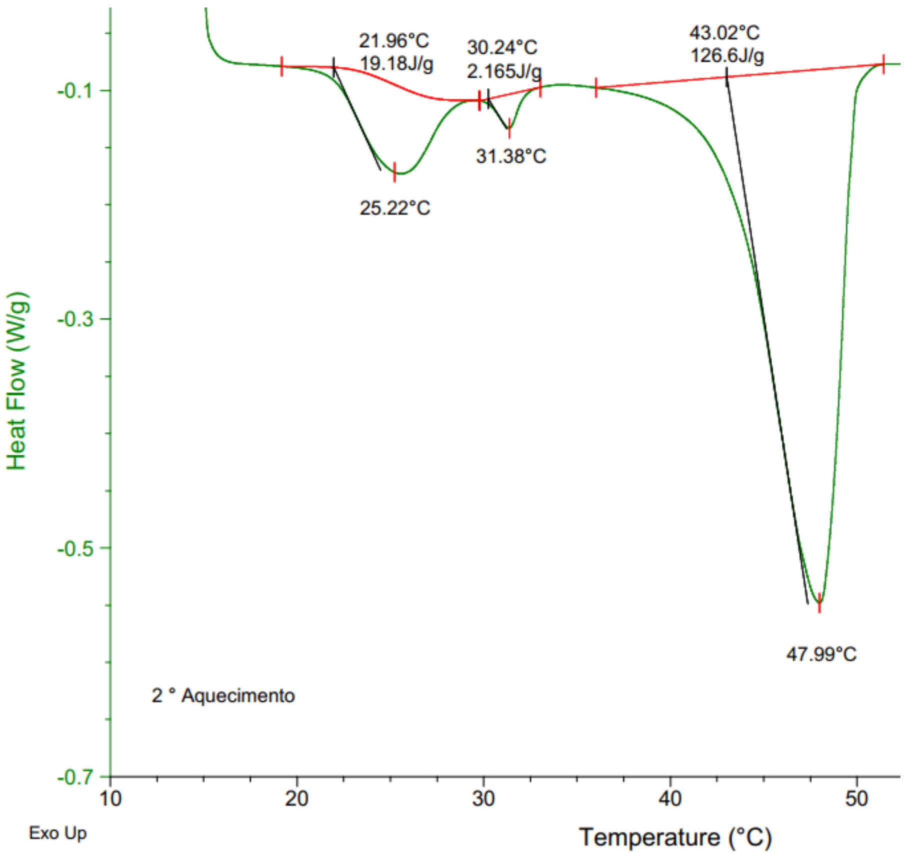


Differential scanning calorimetry

White paraffin

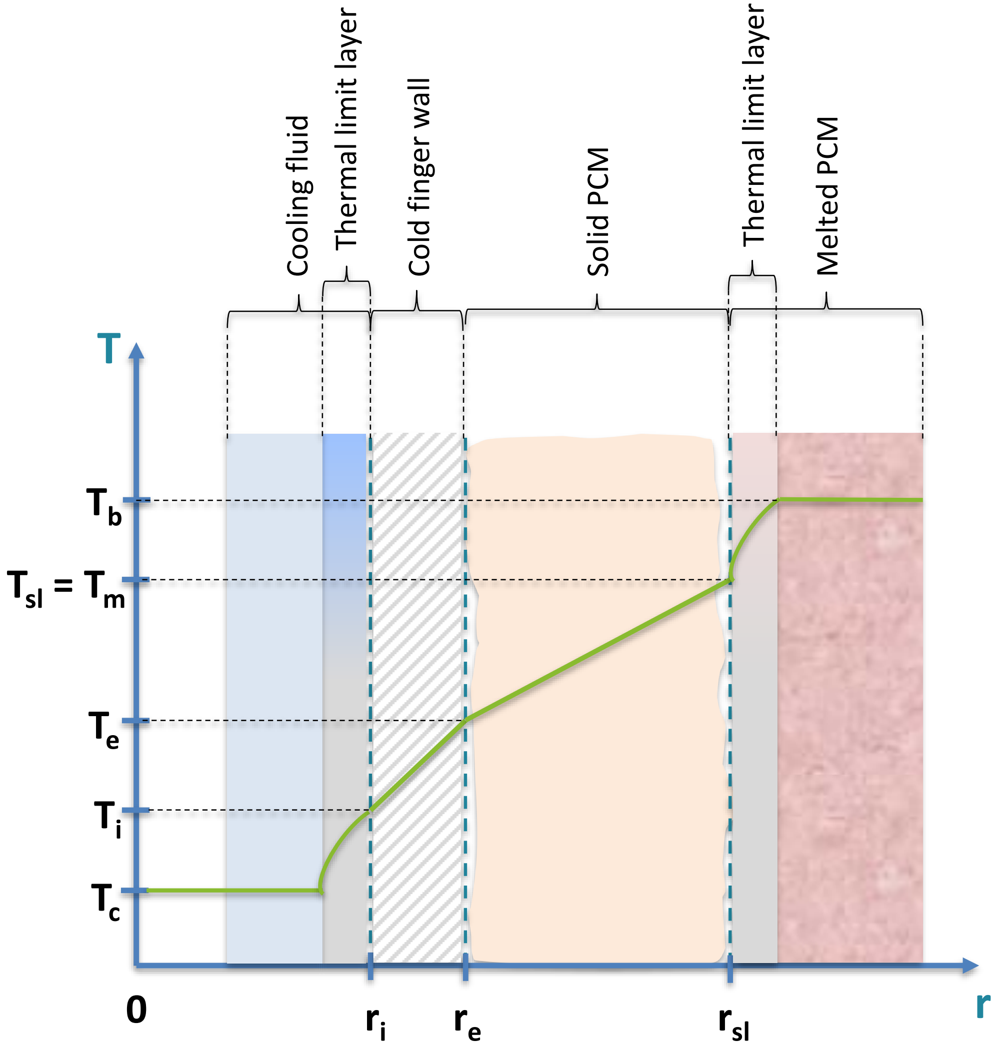


Brown Paraffin



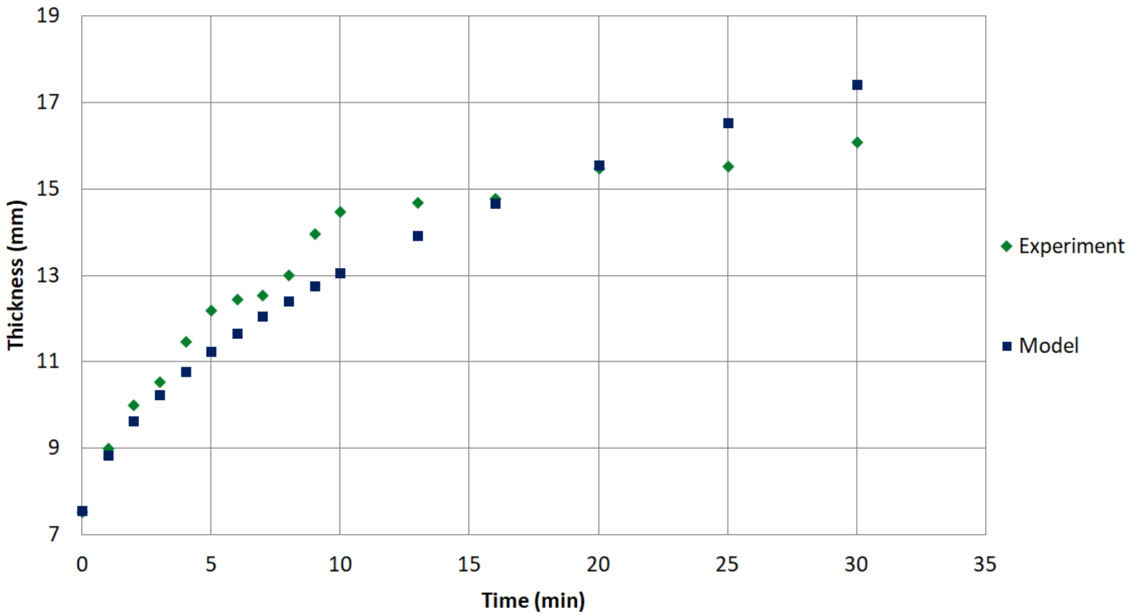
New cold finger model

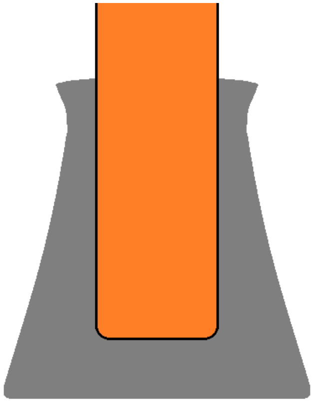
- The new model takes into account the temperature in the molten volume;
- Convection at the solid-liquid interface;
- Physical properties such as density, viscosity, specific heat and thermal conductivity are adjusted by polynomials.



Comparison of simulation with experiment

Crystallization of stearic acid





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