COMPUTATIONAL INVESTIGATION OF THE DYNAMICS OF PHYSICALLY BLOWN POLYURETHANE FOAM

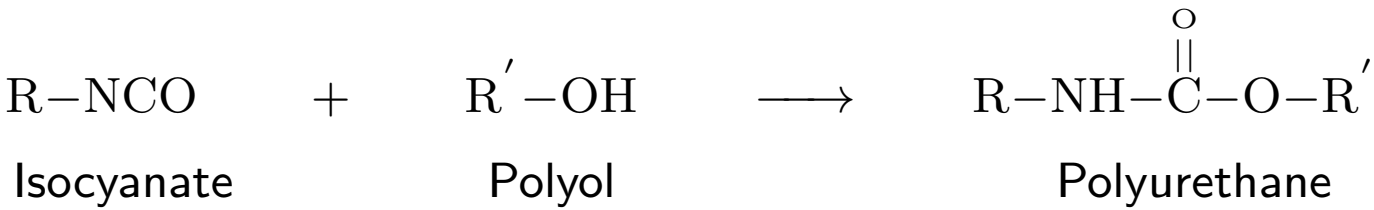
Authors: S. Opadiran [O.A.U], S. Okoya [O.A.U], D. Niedziela [ITWM]

Presented by: S. Opadiran [O.A.U]

INTERNATIONAL CONFERENCE AND ADVANCED WORKSHOP ON MODELLING AND SIMULATION OF COMPLEX SYSTEMS
Date: May 28, 2024.

Introduction

- Polyurethane (PU)



Isocyanate Polyol Polyurethane

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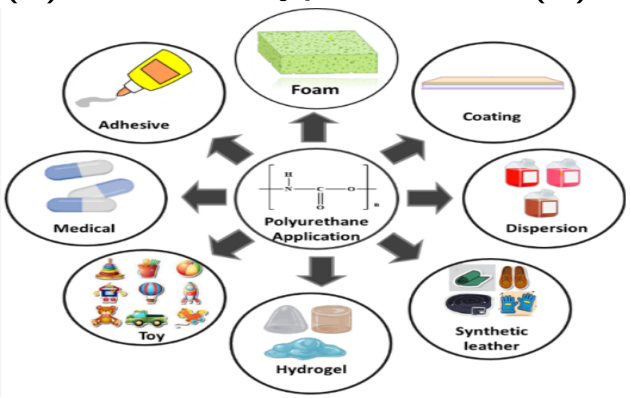

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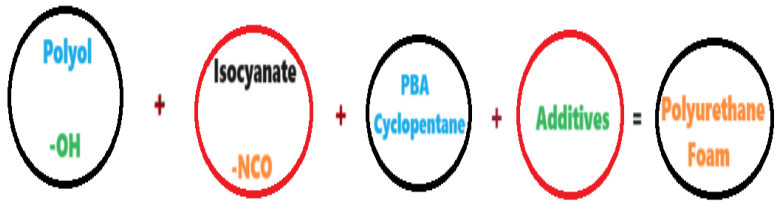

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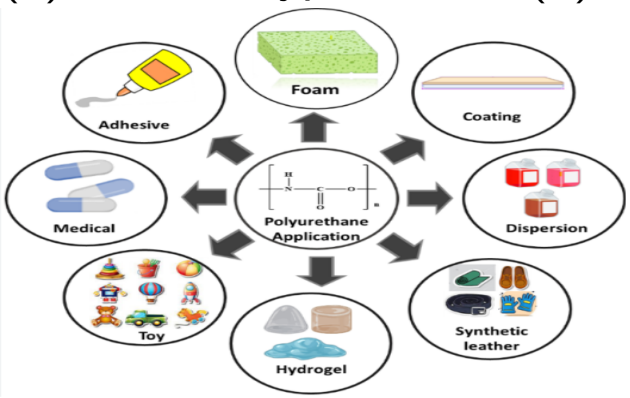

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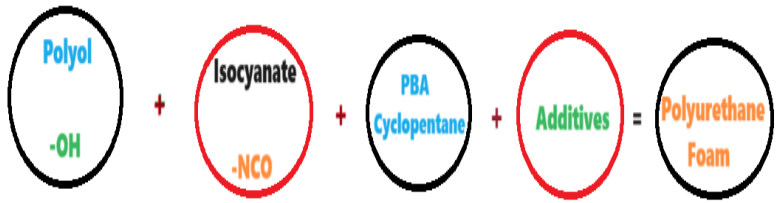

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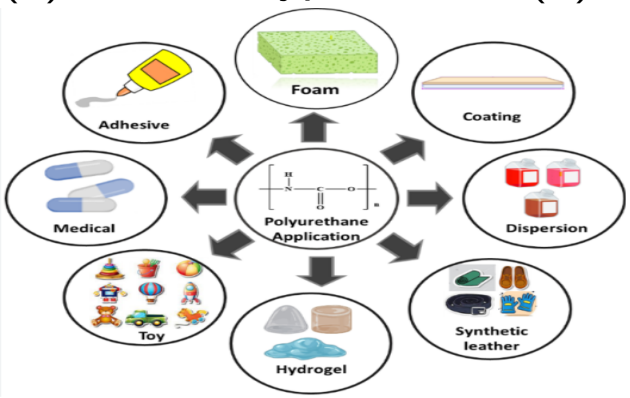

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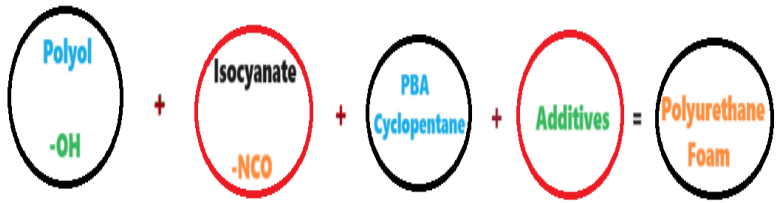

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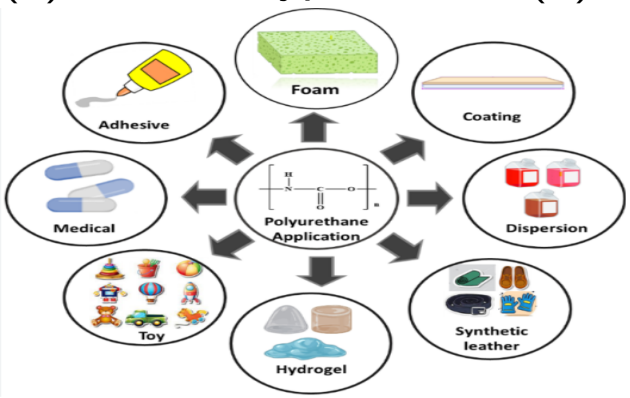

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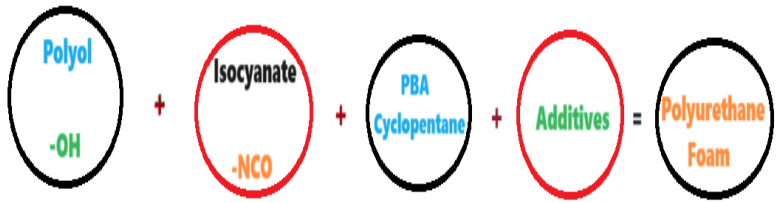

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- The foaming process can be blown: PBA or CBA
  - Physical blowing agents (PBA)
    - Volatile liquid with low boiling poiont
    - Gas introduced under pressure

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- reviewed existing models of physical blown PU foam
- formulated a physical blown PU foam model for FOAM solver (ITWM)
- Validated the model with experimental data in literature

Practical behaviour of the physical blowing agent

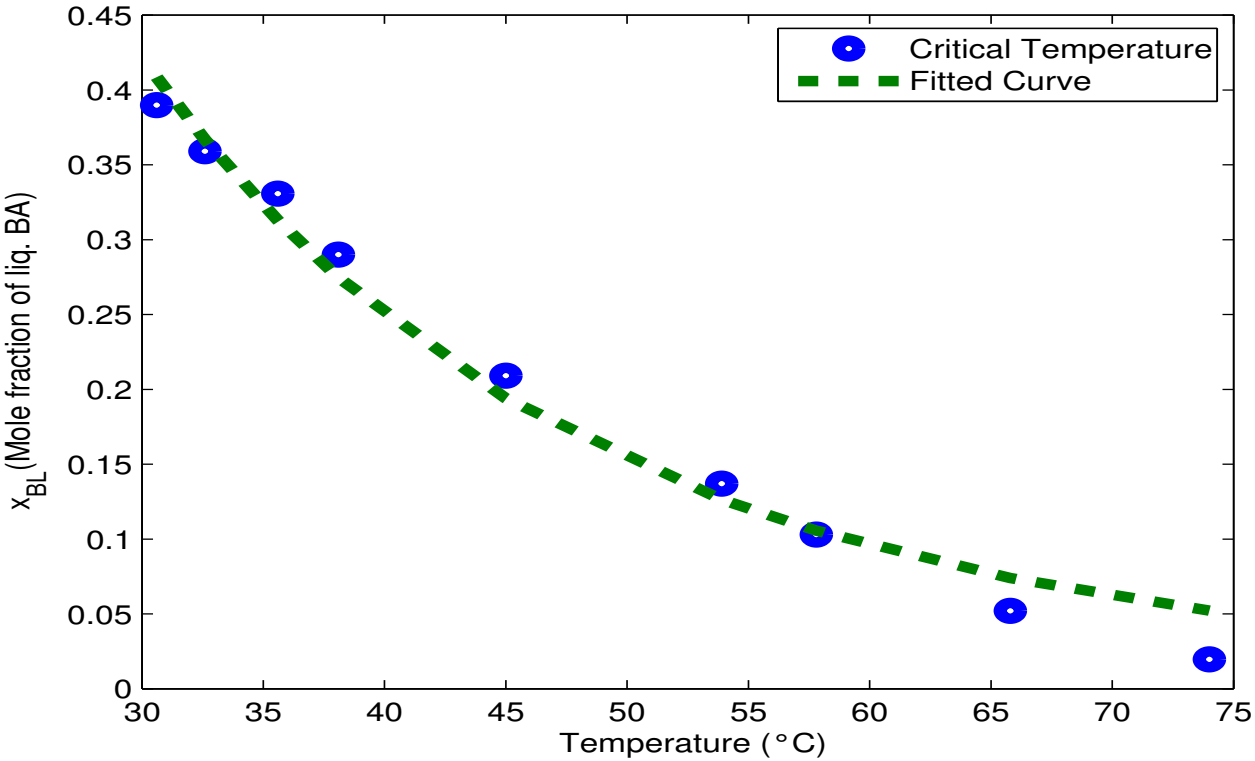

Fig. 1: Illustration of Exp. T_c and Fitted curve of x_{BL}(Tesser et al., 2003).

The behaviour of the BA mole fraction (x_{BL}) is discribed by

$$x_{BL} = f(T_B) = a' \cdot \exp\left(b' \cdot \left(\frac{1}{T_B} - \frac{1}{d'}\right)\right). \quad (1)$$

Mathematical modelling

Firstly, we consider the following equations for the:

PU Polymerization Reaction (Rao et al.,2018)

$$\boxed{\frac{d\xi}{dt} = k\left(b + \xi^m\right)\left(1 - \xi\right)^n,} \tag{2}$$

$$k = \left[\left(0.5 - B\right)\left(1 + \tanh\left(D(t - t_s^{\xi})\right)\right) + 2B\right]\frac{1}{(1 + \omega_c \alpha_T)^{\beta}} k_0 \exp\left(\frac{-E_{\xi}}{RT}\right), \tag{3}$$

$$\log_{10} \alpha_T = -\frac{C_1(T - T_g)}{C_2 + T - T_g}, \tag{4}$$

$$T_g = \frac{T_{go}(1 - \xi) + A\xi T_{g\infty}}{1 - \xi + A\xi}, \tag{5}$$

Energy evolved by the polymerization reaction heats up the Temperature Equation:

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt}, \tag{6}$$

Mathematical modelling

As the temperature of the reacting system increases, the PBA

$$x_{BL}(\text{mol/mol}_{\text{liq. mix.}}) = f(T_B), \tag{7}$$

$$L(\text{g/g}_{\text{poly. mix.}}) = \frac{x_{BL}}{(1 - x_{BL})} \frac{M_B}{M_{no}}, \tag{8}$$

gains heat and evaporate to gas, and it rate of evaporation is

$$\boxed{\begin{aligned} \frac{dL}{dt} &= \frac{M_B}{M_{no}} \frac{1}{(1 - x_{BL})^2} \frac{dx_{BL}}{dT} \frac{dT}{dt} \quad \text{for } T \geq T_c \\ \frac{dL}{dt} &= 0 \quad \text{for } T < T_c \end{aligned}} \tag{9}$$

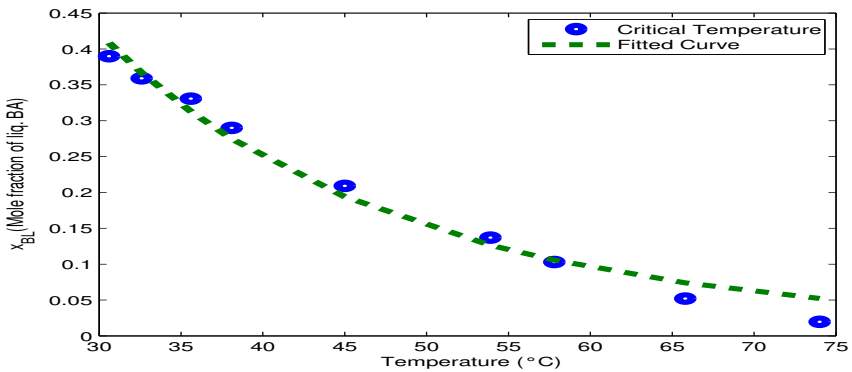

Fig 1: Display of T_c in BA evaporation

Mathematical modelling

Effect of the evaporation leads to a drop in the temperature

$$\boxed{\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} + \lambda' \frac{dL}{dt},} \tag{6*}$$

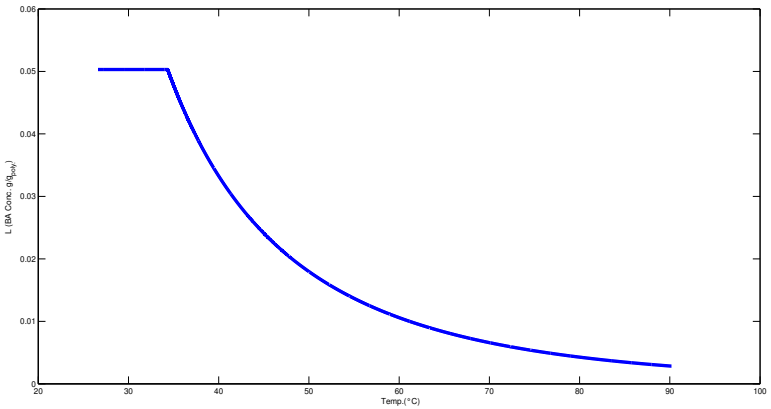

Fig. 2: Plot of Drop in the BA Conc.(L)

$$G(\text{amount of gas generated}) = L_0 - L. \tag{10}$$

The polymer density resulting from gas creation is

$$\rho_F = \frac{1 + L_0}{(G1000RT/PM_B) + (L/\rho_{BL}) + (1/\rho_p)} \tag{11}$$

Method of solution

The collection of all considered equations

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- Initial conditions: T=26.62°C, $\xi = 0, L = 0.0503, 0.0751$

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- Initial conditions: T=26.62°C, $\xi = 0, L = 0.0503, 0.0751$
- Euler method: For the set of ODEs
  - kinetic eqn: $\xi^{k+1} = f_\xi(\xi^k, T^k)$
  - Temp. eqn: $T^{k+1} = f_T(\xi^{k+1}, \xi^k, T^k, L^k)$
  - Evap. eqn: $L^{k+1} = f_L(L^k, T^k, T^{k-1})$

Results & discussion: Adiabatic

In obtaining the polymerization parameters an adiabatic condition was first considered and the temperature increase

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt},$$

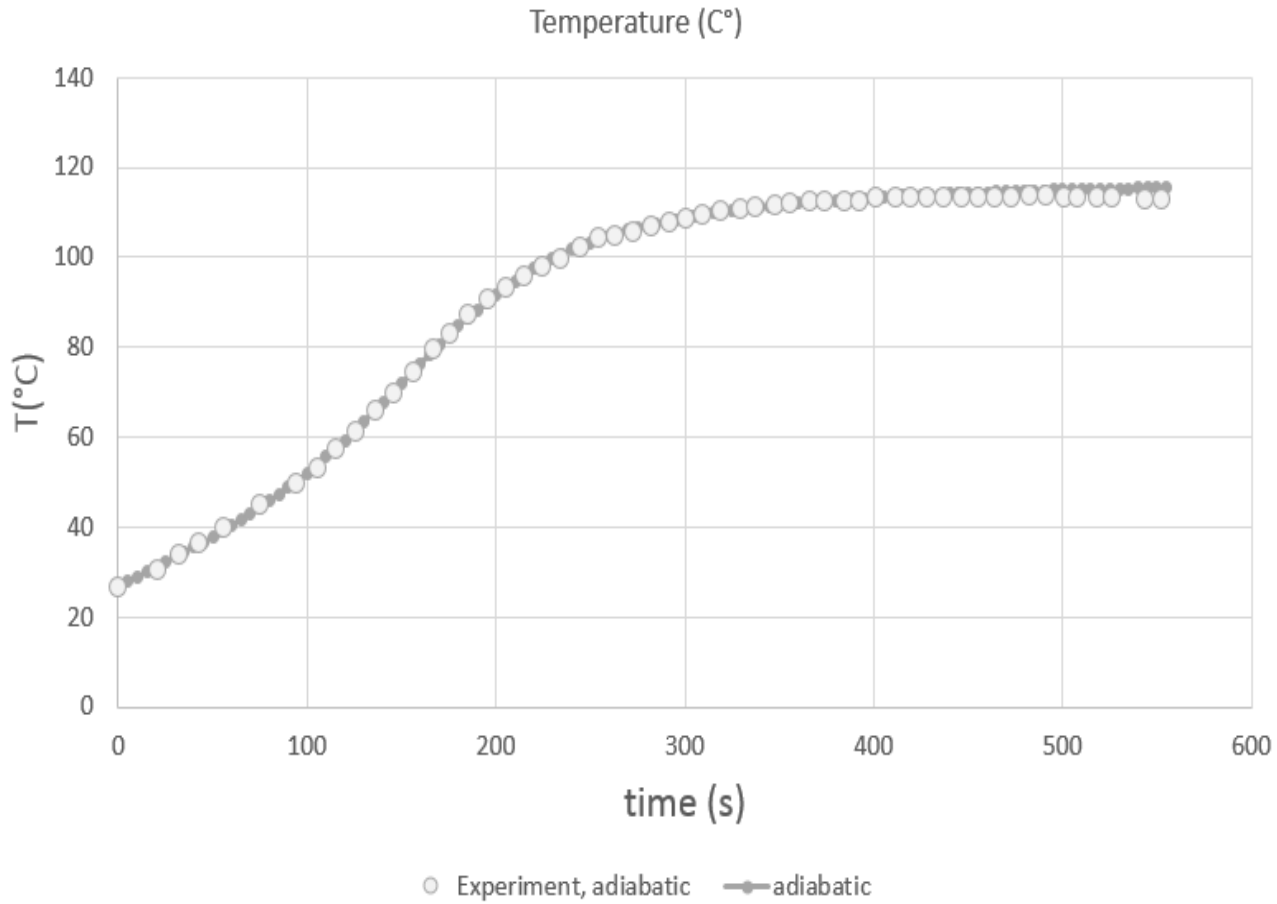


Fig. 3: Temperature of polymerization react. (Adiabatic) Tesser et al. (2003)

Results & discussion: Non-adiabatic

For the non-adiabatic case with effect of diffusion,we introduced term in (12) to calibrate U

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} - U(T - T_0). \tag{12}$$

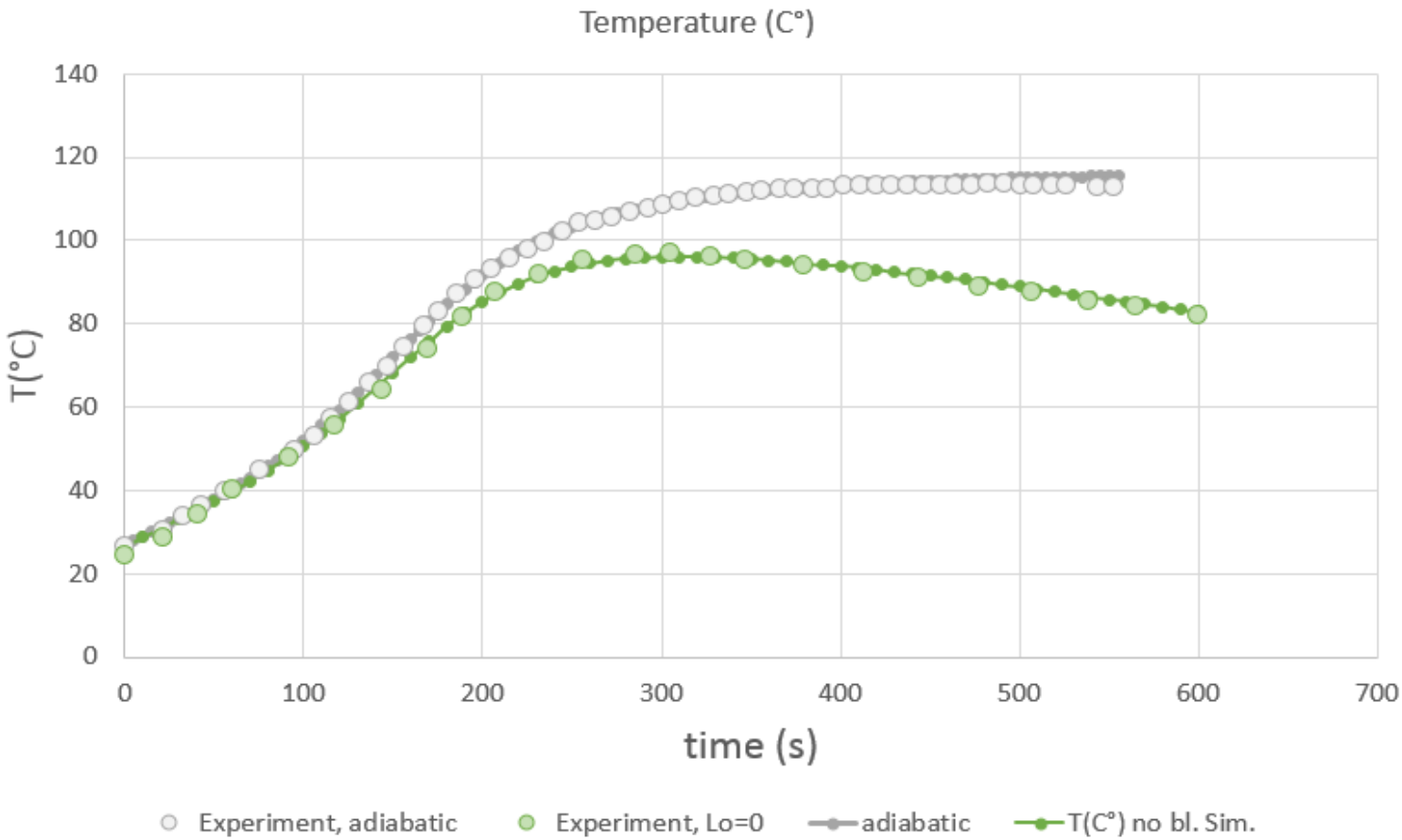
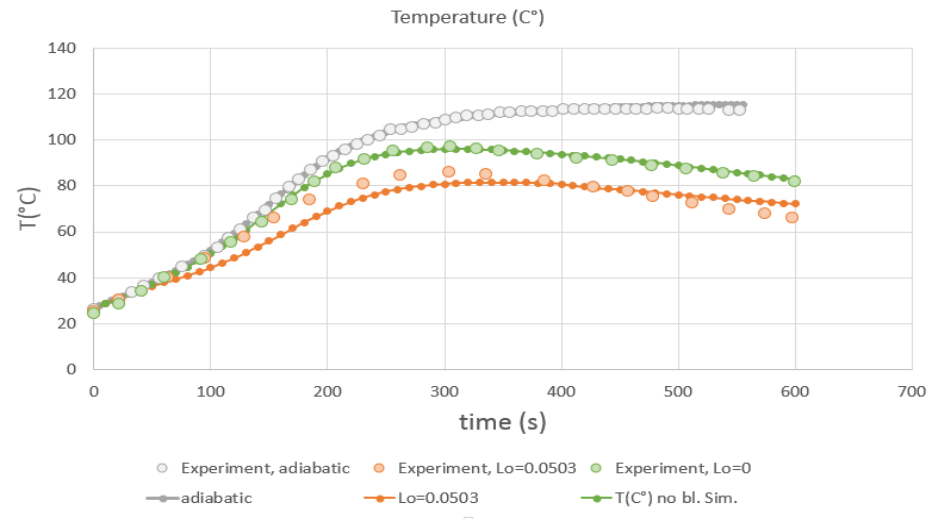


Fig. 4: Temperature drop due to diffusion (non-adiabatic)

Results & discussion: Characteristics of PU Foam with $L_0 = 0.0503$



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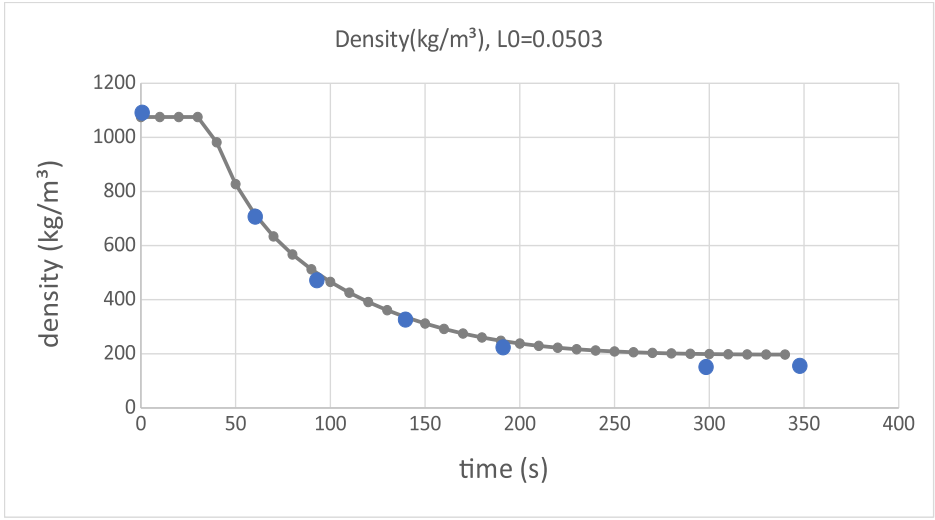

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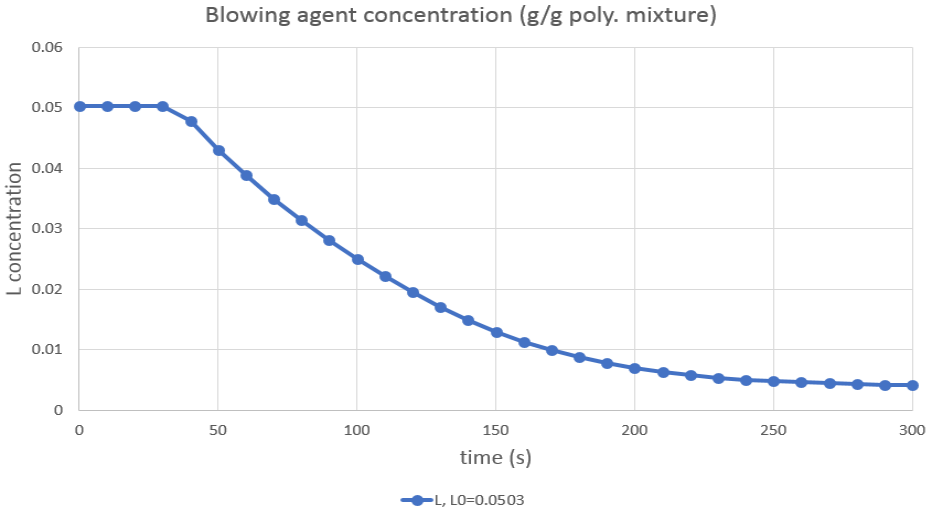

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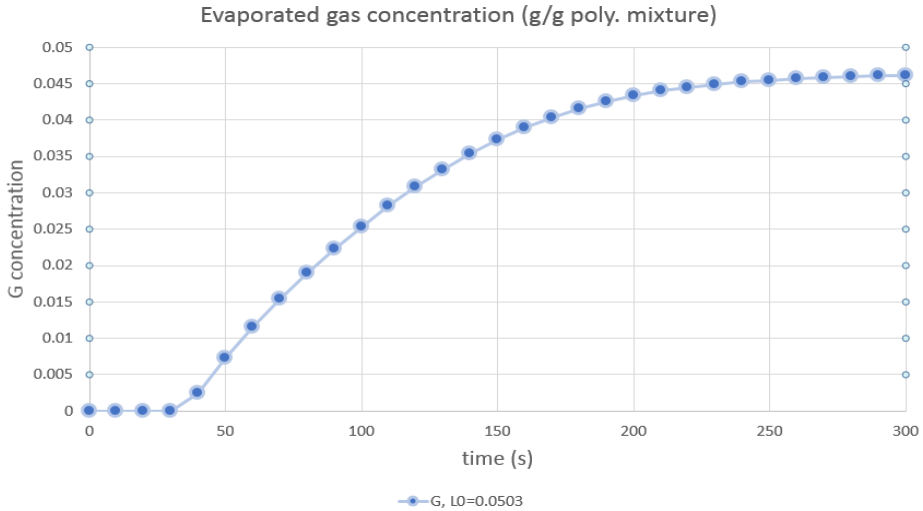
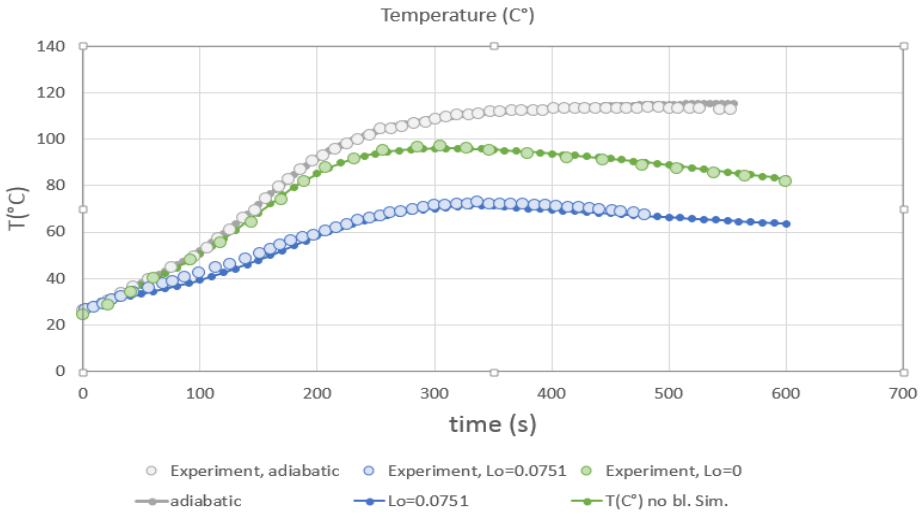


(d)

Fig. 5: Plots of (a) Tempterature (b) density (c) L (d) G for $L_0 = 0.0503$.

Results & discussion : Attributes of PU Foam with $L_0 = 0.0751$



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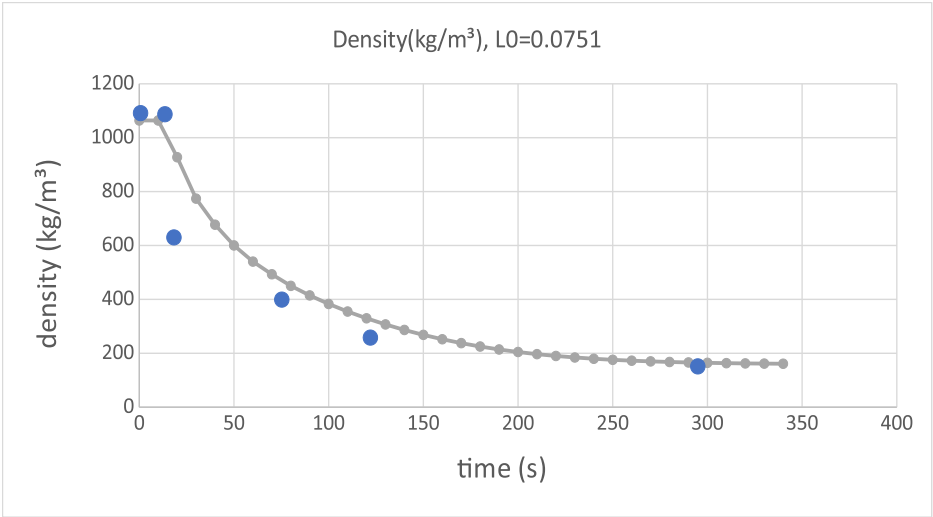

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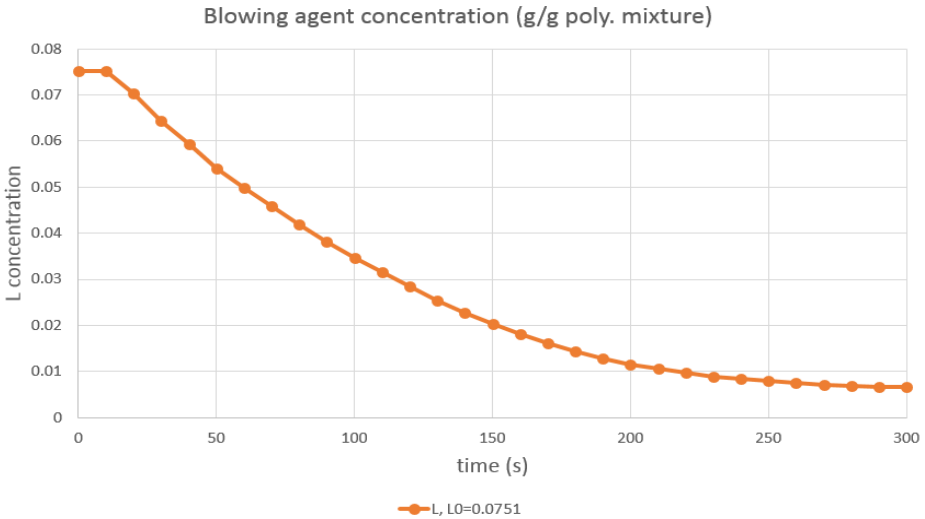

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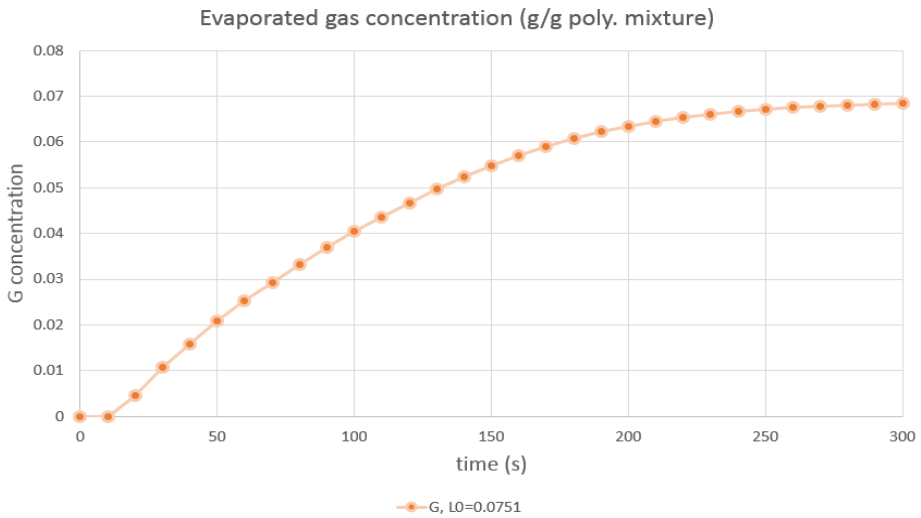

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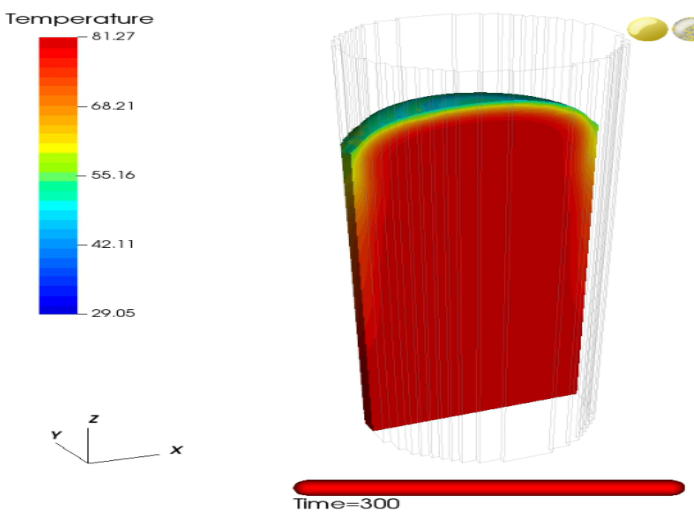
Fig. 6: Plots of (a) Temperature (b) density (c) L (d) G for $L_0 = 0.0751$.

Results & discussion : 3D PU foam growth

The considered system of ODEs was transfered to the existing foam solver in the instistitute, FOAM, and this allowed us to perform full 3D simulation.

Video 1: Growth of the PU foam in the cylinder cup (300secs)

Results & discussion : 3D results of the PU foam T, L and density



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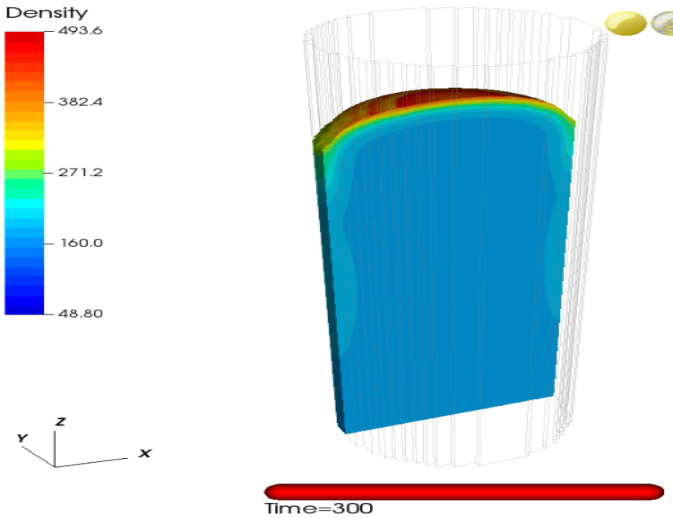

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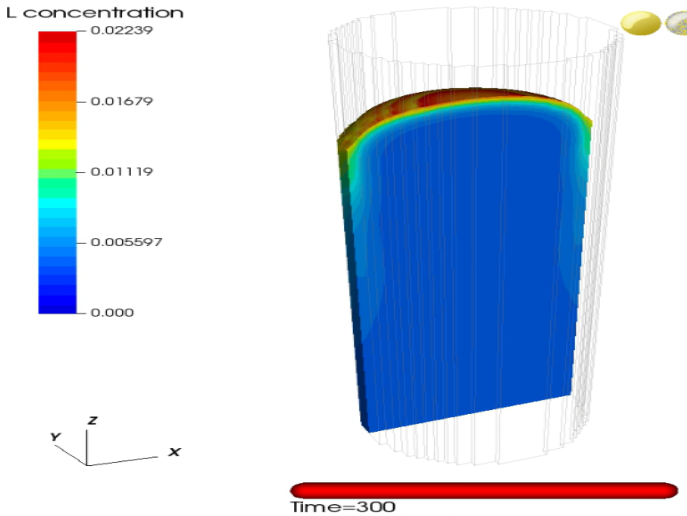

(c)

Fig. 7: Plots of (a) Temperature (b) Density (c) Blowing agent conc. (L)

Results & discussion : 3D and ODE density compared

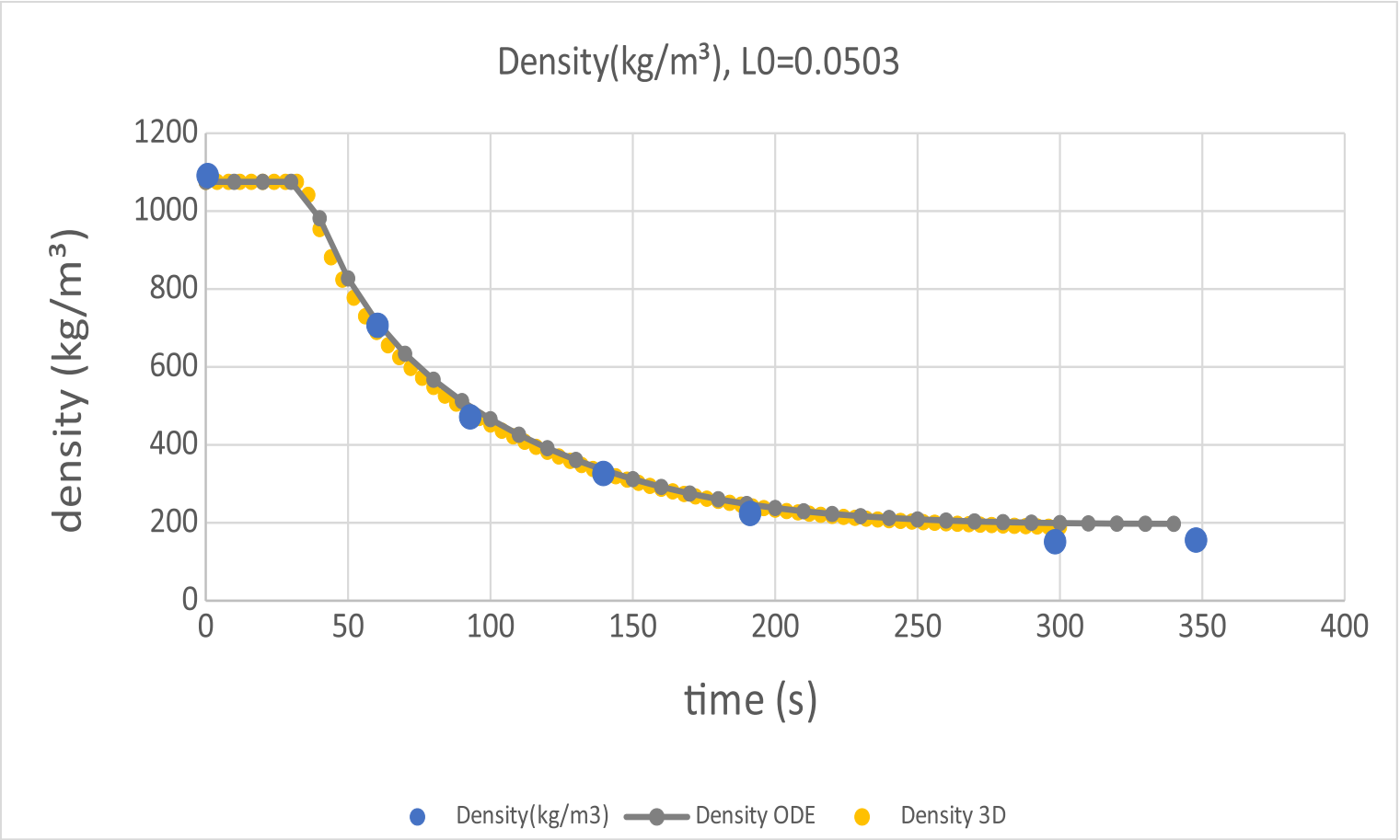

Fig. 8: Plots of ODE and 3D densities for $L_0 = 0.0503$.

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- Transfer of the ODE system to full 3D system implemented in the foam simulation software, FOAM, was achieved.
- From our observation the model is satisfactory for a rough description of the main occuring foam phenomena.

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THANKS FOR LISTENING!!!