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International Conference and Advanced Workshop
on Modelling and Simulation of Complex Systems

Presents

The ICAWMSCS Seminar Series

February 2026 (Every month on the first Monday)

Title:

Unsteady 3D modelling of the polyurethane foam expansion process

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Virtual Zoom Meeting

Zoom Link:
https://zoom.us/j/97592772965?pwd=i5N0uHHUa5qKWodS8g4ASLrKNviwHJ.1

Meeting ID: 975 9277 2965
Passcode: 359799

2nd Feb, 2026
12:00 pm WAT

UNSTEADY 3D MODELLING OF THE POLYURETHANE FOAM EXPANSION PROCESS

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

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

ICAWMSCS 2026 SEMINAR SERIES

Date: February 2, 2026.

Outline

- Introduction
- Statement of research problem
- Motivation
- Specific objectives of research
- Research methodology
- Model formulation
- Literature review
- Method of solution
- Results and discusion
- Conclusion
- Contribution to knowledge
- References

Introduction

- What are polymer foams?

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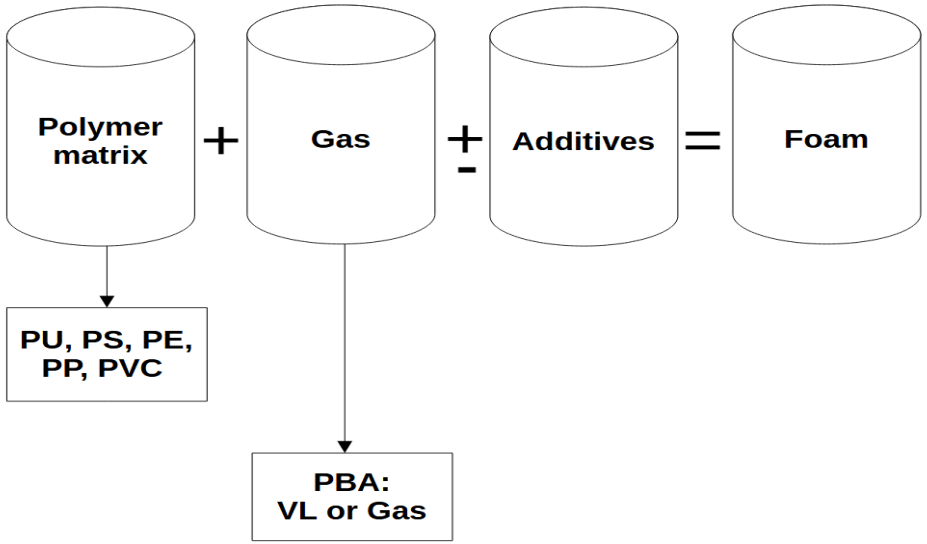

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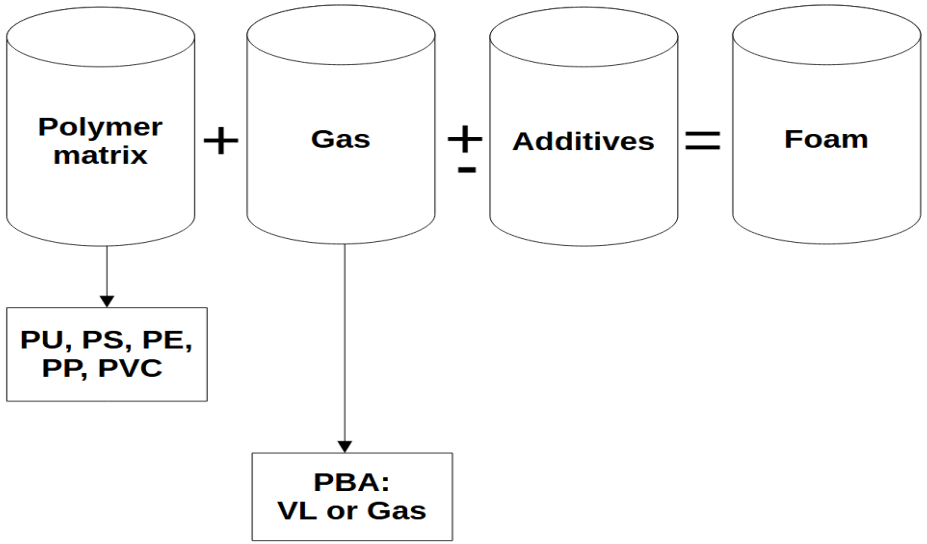

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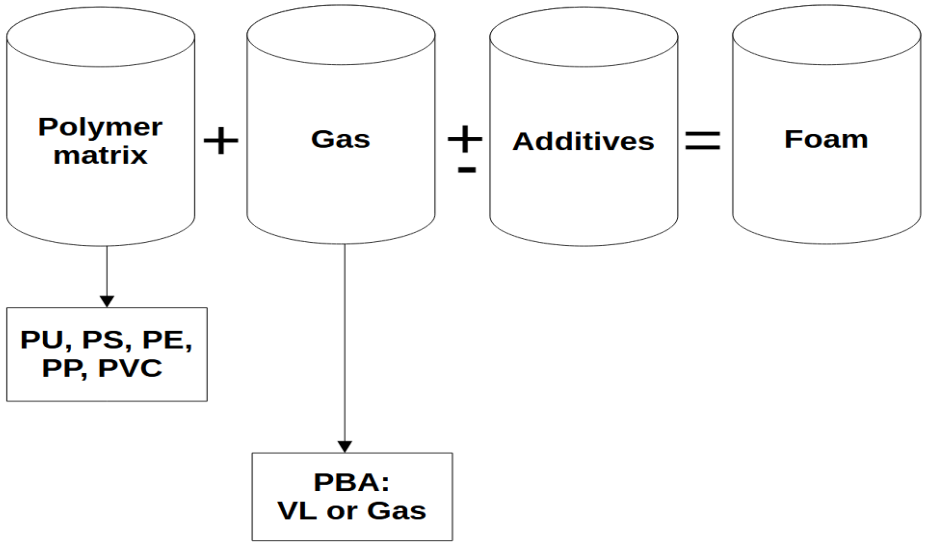

- Dynamics of PUF formation: Polymerization reaction & Blowing agent evaporation

- Polym. rxtn: $\underset{\text{Isocyanate}}{R-NCO} + \underset{\text{Polyol}}{R'-OH} \longrightarrow \underset{\text{Polyurethane}}{R-NH-\overset{\overset{O}{\|}}{C}-O-R'} + \Delta H_{Heat}$

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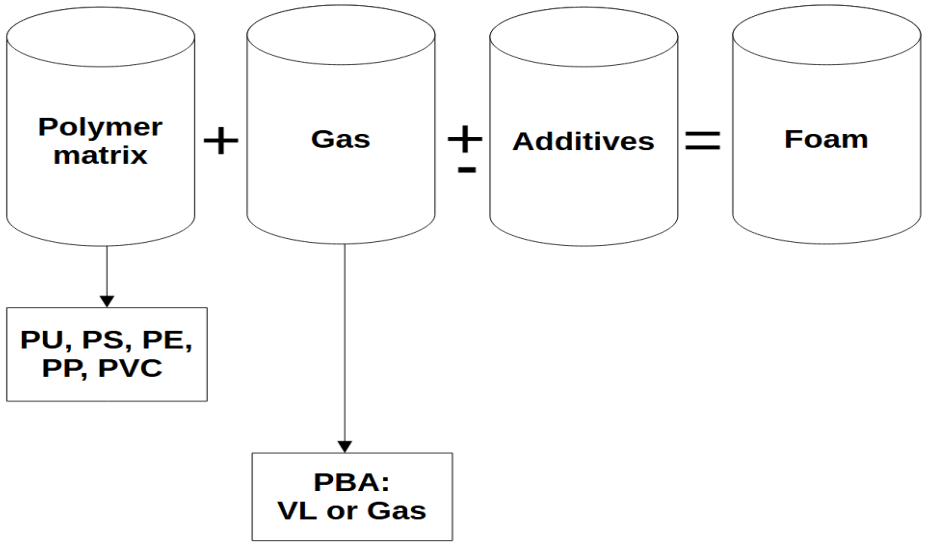

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- Chem. rxn.(poly.)→Heat gen.→BA evap.→Bubb. nucl.→Gas diff.→ Visc.→Foam

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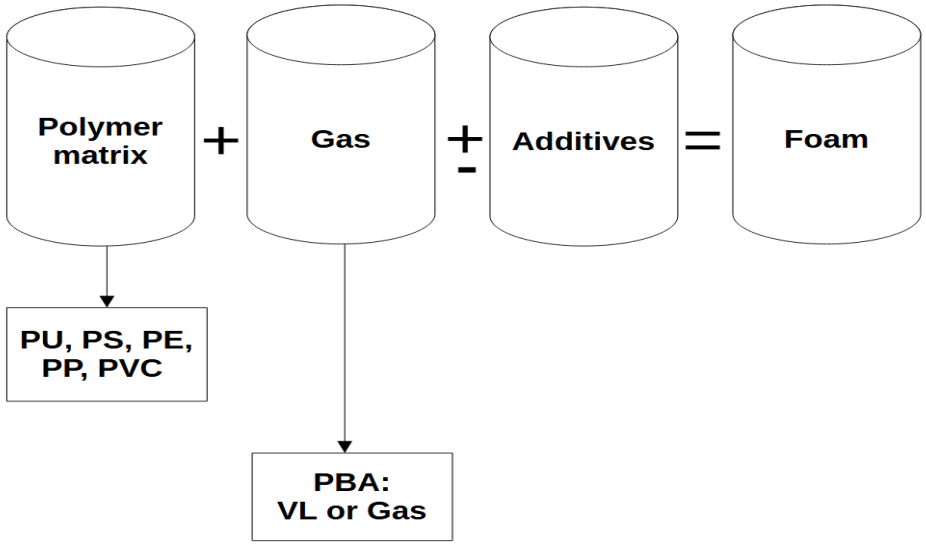

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- Chem. rxn.(poly.)→Heat gen.→BA evap.→Bubb. nucl.→Gas diff.→ Visc.→Foam
- To study & model the dynamics:
  Fittn exp. data(foam TR & BA mol frac)→vap rate of BA mass frac→polymer conv→density & tempt variation→full 3D model (via fund. laws of FM)

Statement of research problem

Despite the numerous researches on the physical foaming process of polyurethane (PU), there is still a gap in understanding how process conditions (such as system pressure and temperature as well as the blowing agent concentration) influences the foaming properties. More-so, there is dearth of comprehensive mathematical 3D models in the literature for controlling and predicting PU foaming properties optimally. Therefore, this research seeks to contribute to existing knowledge by developing a robust 3D mathematical models for controlling the physical foaming process and predicting the foaming properties of PU foam.

Motivation

Polymeric foams such as PUF play an essential role across various industries (such as the automobile industry, aerospace industry, and construction industry). However, producing foams with customized properties can be very challenging due to the complex dynamics of the foaming process. Existing studies in this regard, such as Ireka et. al. (2015), considered the chemically blown polyurethane foaming process, but not the physical foaming process, and the investigations such as Rojas et al (1972) and Baser khaker (1994) that considered the physical foaming process were inappropriately modelled while Tesser et. al. (2004) incorporated effect of water and the study was based on experiment. These gaps motivates the need for the present study.

Objectives of the research

The specific objectives of the research are to

(i) formulate the equations governing the unsteady expansion and dynamics of polyurethabe foam under non-isothermal condition;

(ii) obtain model parameters from existing data via parameter fitting;

(iii) solve the resulting system of equations numerically and validate the models with existing data from literature; and

(iv) determine the effects of the process conditions on the final foam density profiles using the models obtained.

Research methodoloy

(i) The mathememetical model of the polyurethane foam expansion will be formulated from the conservation laws of mass, momentum, energy, and the transport of gas concentration, evolution of density, ideal gas law and appropriate rheological equations.

(ii) The emerging model parameters will be obtained via fittn. of our developed temporal evol. model (non-linear ODEs) to exp. data.

(iii) The resulting system of the coupled nonlinear PDE of the unsteady 3D model will be solved using the finite volume method & the result will be compared with lit.

(iv) The impact of process conditions (temperature, pressure and gas concentrations) will be examined on the foam density profiles and shown through graphical plots.

Polyurethane foam: Geometry of reaction system

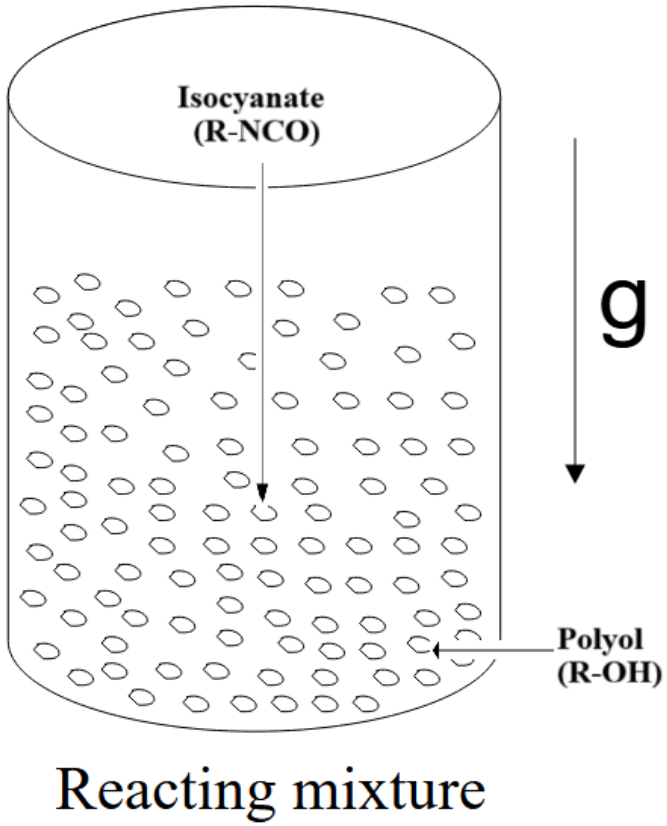

Fig. 1: Physical geometry of the PU reacting system

Model formulation

General equations of flow

Continuity equation:

$$\nabla \cdot \vec{v} = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho\right) \tag{1}$$

Momentum equation:

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \nabla \cdot \left(\mu[\nabla \vec{v} + \nabla \vec{v}^{T}]\right) + \vec{F} \tag{2}$$

Energy equation:

$$\rho C_p \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T) + Q_{source} - Q_{sink} \tag{3}$$

Polymeriz./Concen. eqn.:

$$\frac{D\xi}{Dt} = D\nabla^2 \xi + F(\xi) \tag{4}$$

$$NB : \mu \implies \quad \mu_{PU} = f(T, \xi, \dot{\gamma})$$

PUF: Model 1−Unsteady state reaction system

Model 1: Assumptions

- a) A point inside the cylinder is considered
- b) Impact of flow is negligible (i.e conv. terms are negligible)
- c) The system is unsteady and spatially homogeneous i.e $\nabla T = \nabla \xi = \nabla \vec{v} = \nabla p = 0$
- d) The model focuses on the conservation law (3) i.e $\rho C_p \frac{dT}{dt} = Q_{source} - Q_{sink}$
- e) & (4) Polymerization reaction follows Rao et al. (2018) cure model i.e $\frac{d\xi}{dt} = f(\xi) = k(b + \xi^m)(1 - \xi)^n$

Model 1 reduced equations: PU foaming process

Following assumption (e), the polymerization equation (4) becomes

$$\frac{d\xi}{dt} = k\left(b + \xi^m\right)\left(1 - \xi\right)^n, \tag{5}$$

where the parameters

$$k = \left[\left(0.5 - B\right)\left(1 + \tanh\left(D(t - t_s^{\xi})\right)\right) + 2B\right]\frac{1}{(1 + \omega_c \alpha_T)^{\beta}} k_0 \exp\left(\frac{-E_{\xi}}{RT}\right), \tag{6}$$

$$\log_{10} \alpha_T = -\frac{C_1(T - T_g)}{C_2 + T - T_g}, \tag{7}$$

$$T_g = \frac{T_{go}(1 - \xi) + A\xi T_{g\infty}}{1 - \xi + A\xi}. \tag{8}$$

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While the energy equation (3) becomes

$$\rho_p C_p \frac{dT}{dt} = \left(\rho_p H_R \frac{d\xi}{dt}\right)_{Heat\ \ Source}$$

Tempt. change **Heat due to polymerization**

Model 1 reduced equations: PU foaming process

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While the energy equation (3) becomes

$$\rho_p C_p \frac{dT}{dt} = \left(\rho_p H_R \frac{d\xi}{dt}\right)_{Heat\ \ Source} - \left(h(T - T_0)\right)_{Heat\ \ Sink}$$

Tempt. change **Heat due to polymerization** **Heat transfer to surrounding**

Model 1 reduced equations: PU foaming process

Following assumption (e), the polymerization equation (4) becomes

$$\frac{d\xi}{dt} = k\left(b + \xi^m\right)\left(1 - \xi\right)^n, \tag{5}$$

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Tempt. change **Heat due to polymerization** **Heat transfer to surrounding** **Heat due to evaporation**

Model 1 reduced eqns: Mass frac. (L) of BA & foam density (ρ_f)

From the mass fraction of the PBA expressed as

$$L = \frac{x_{BL}}{(1 - x_{BL})} \frac{M_B}{M_{no}}, \tag{10}$$

The rate of evaporation of the PBA is described by the piecewise function

$$\frac{dL}{dt} = \begin{cases} \frac{M_B}{M_{no}} \frac{1}{(1-x_{BL})^2} \frac{dx_{BL}}{dT} \frac{dT}{dt} & \text{for } T \geq T_B \\ 0 & \text{for } T < T_B \end{cases} \tag{11}$$

The final foam density ρ_f, is computed according to

$$\rho = \frac{m}{v}, \quad \rho_f = \frac{m_{\mathrm{p}} + m_{\mathrm{BL}}}{v_{\mathrm{BG}} + v_{\mathrm{BL}} + v_{\mathrm{p}}} = \frac{1 + L_0}{(G1000RT/PM_B) + (L/\rho_{BL}) + (1/\rho_p)} \tag{12}$$

And the associated initial conditions for Equations (5) - (12) are:
$T = 26.62^{\circ}\mathrm{C},\ \xi = 0, L = 0.0751$

NB: $\lambda' = \lambda \cdot \rho_{bl}$ & $h = h'\rho_p$

Comparison of experimental & sim. mole frac. at diff. tempt.

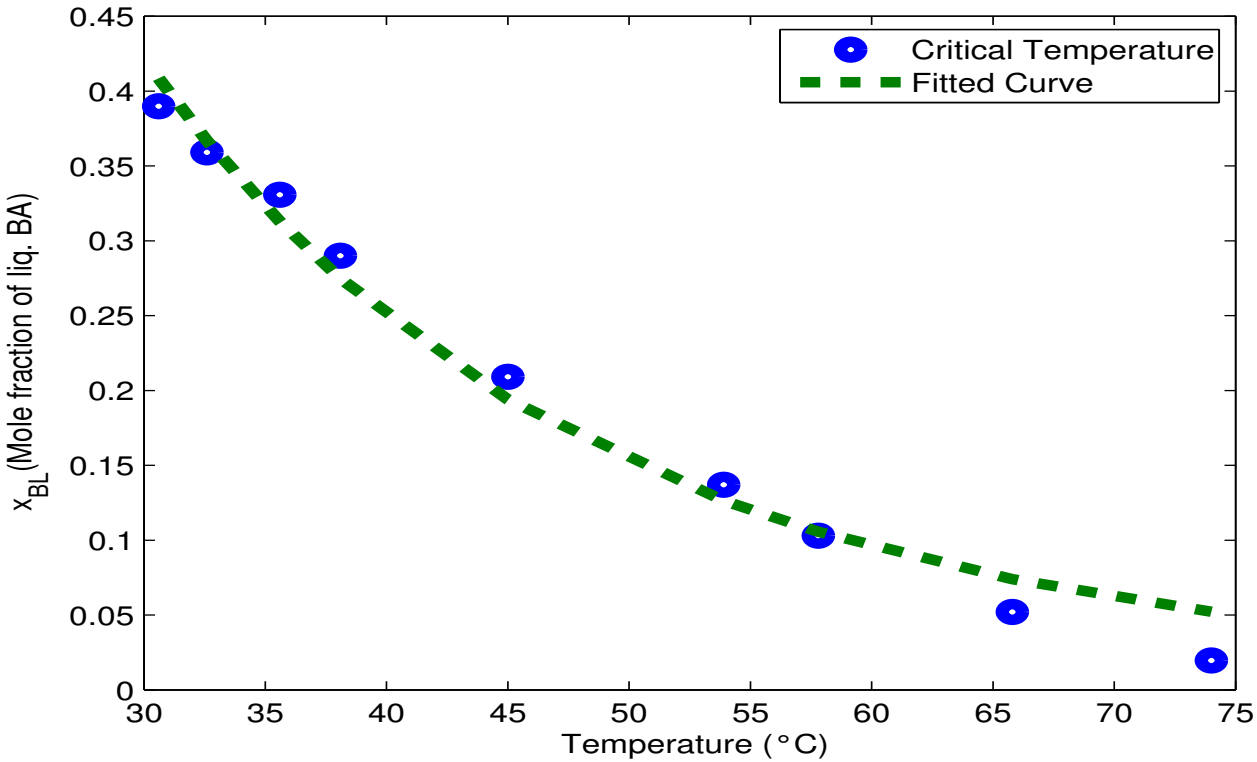


Fig. 2: Illustration of exp. x_{BL} (Tesser et al., 2004) and model curve

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

$$x_{BL} = f(T) = a' \cdot \exp\left(b' \cdot \left(\frac{1}{T} - \frac{1}{d'}\right)\right). \tag{13}$$

Comparison btw exp. & sim. adiabatic experiment

The polymerization parameters were obtained by considering an adiabatic condition

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} - \cancel{h(T - T_0)} + \cancel{\left(-\lambda' \frac{dL}{dt}\right)}$$

$$\frac{d\xi}{dt} = k(b + \xi^m)(1 - \xi)^n$$

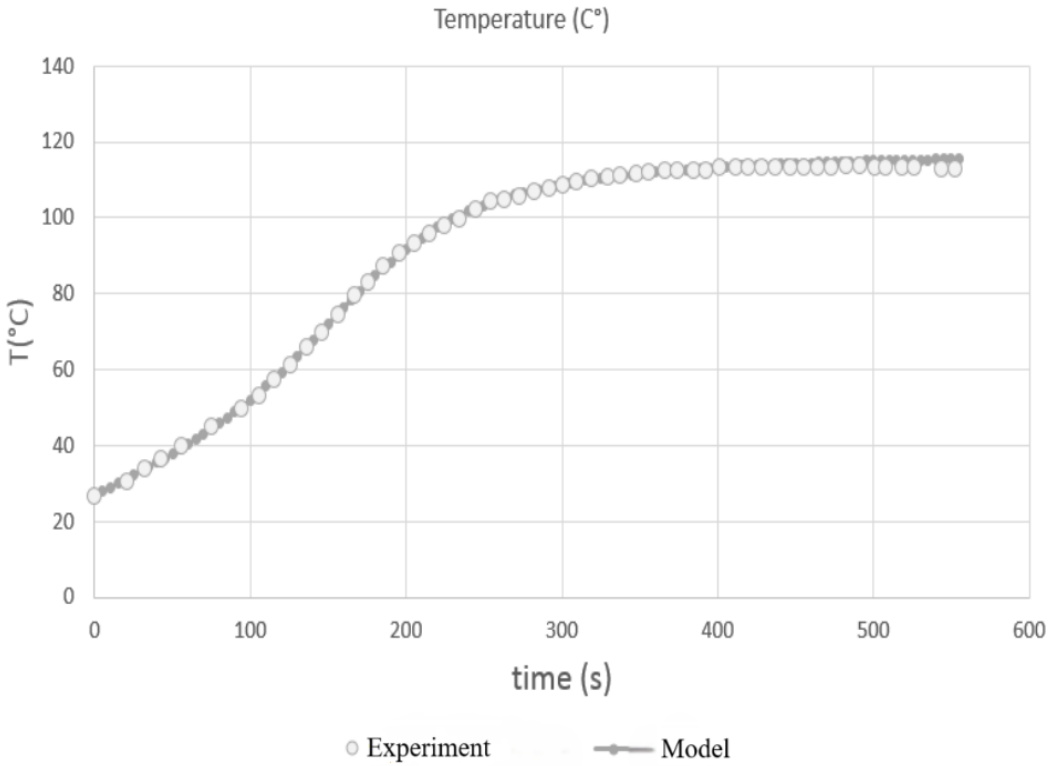


Fig. 3: Temperature of polymerization react. (Adiabatic) Tesser et al. (2004)

Comparison btw. exp. & sim. non-adiabatic experiment

For the non-adiabatic case with effect of HTS,the term below is introduced to calibrate h

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} - h(T - T_0) + \cancel{\left(-\lambda' \frac{dL}{dt}\right)}$$

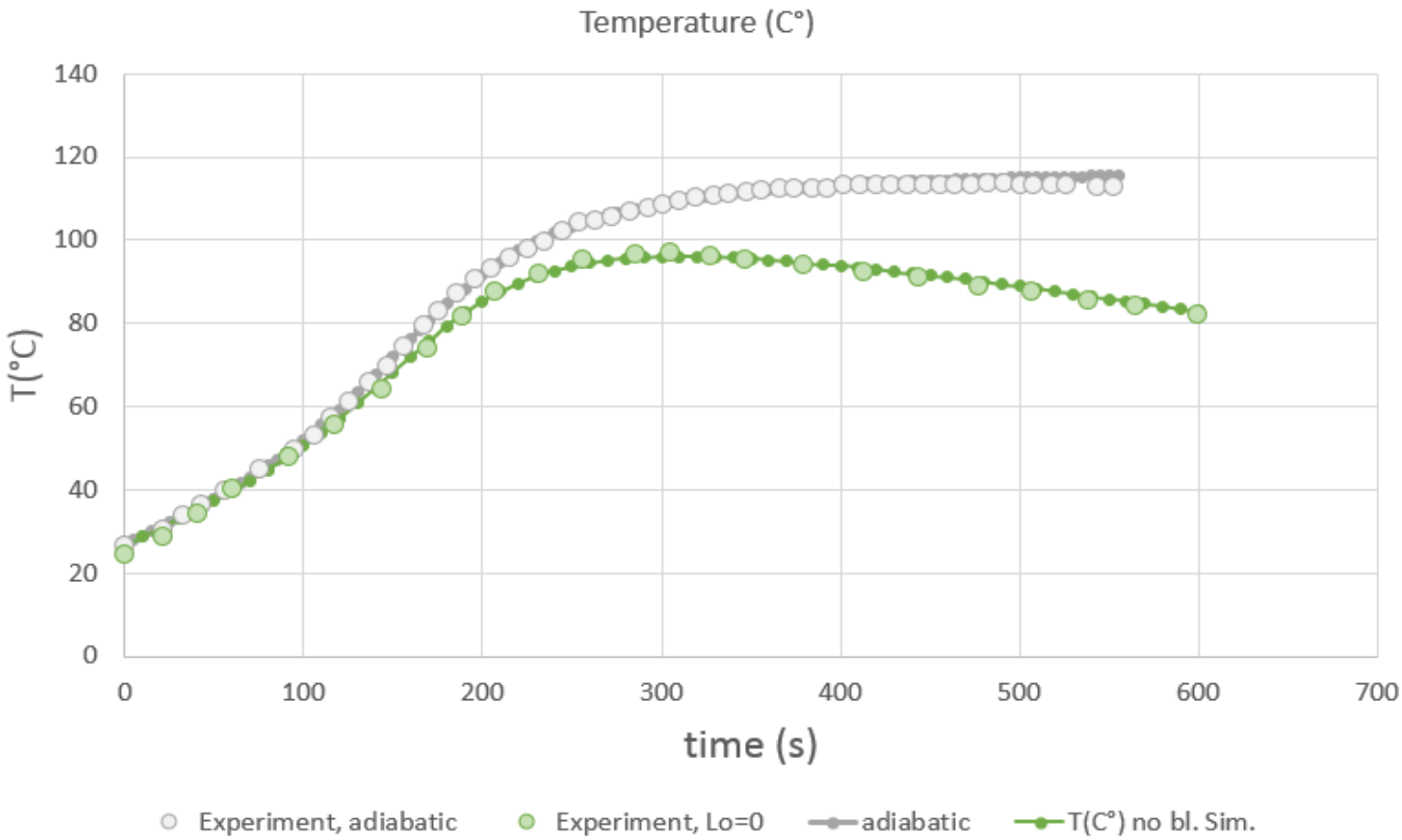


Fig. 4: Temperature drop due to HTS (non-adiabatic)

Comparison btw. exp. & sim. impact of BA evap. with $L_0 = 0.0751$

The rate of evaporation is introduced to calibrate λ'

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} - h(T - T_0) + \left(- \lambda' \frac{dL}{dt} \right)$$

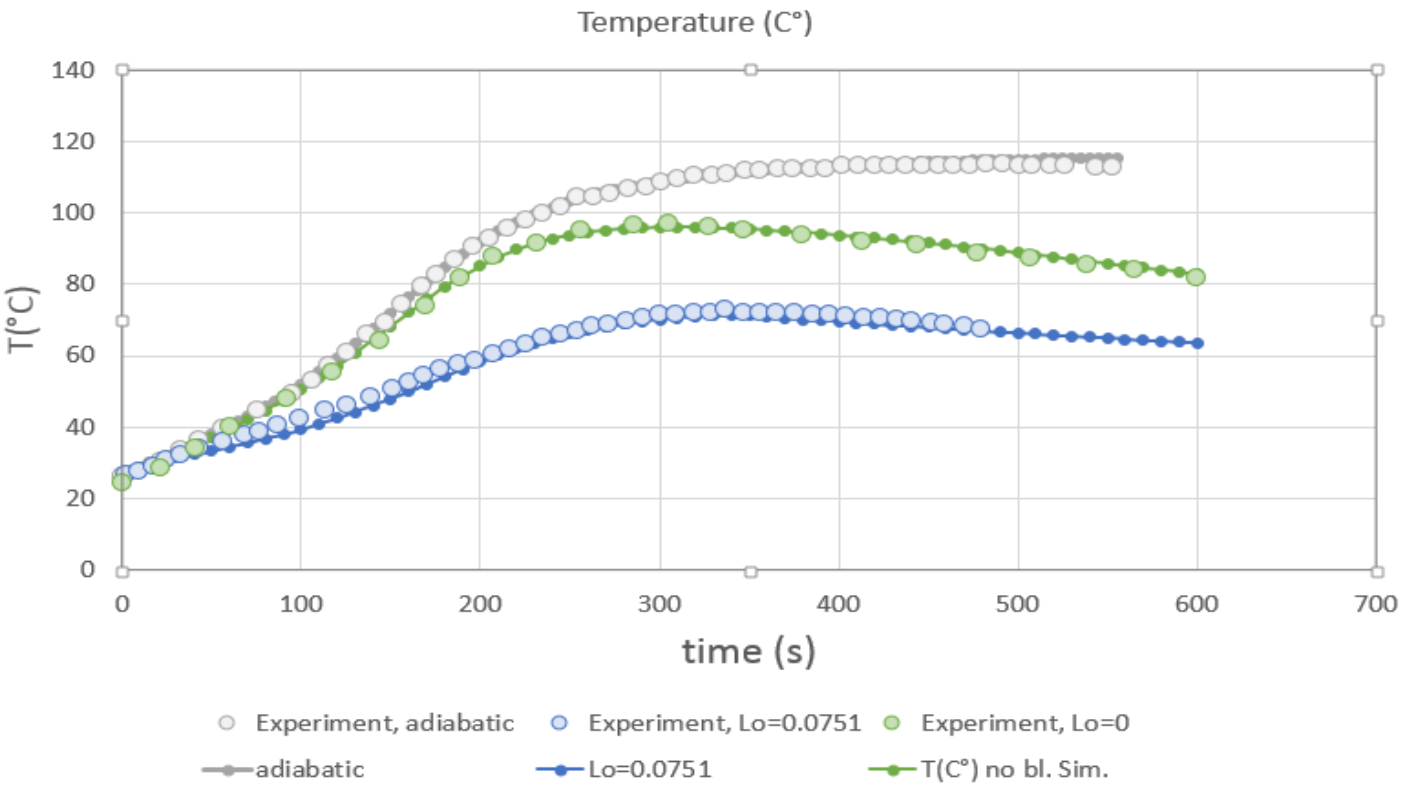


Fig. 5: Temperature drop due to evaporation for $L_0 = 0.0751$.

Comparison btw. exp. & sim. impact of BA evap. with $L_0 = 0.0503$

$$\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} - h(T - T_0) + \left(- \lambda' \frac{dL}{dt} \right)$$

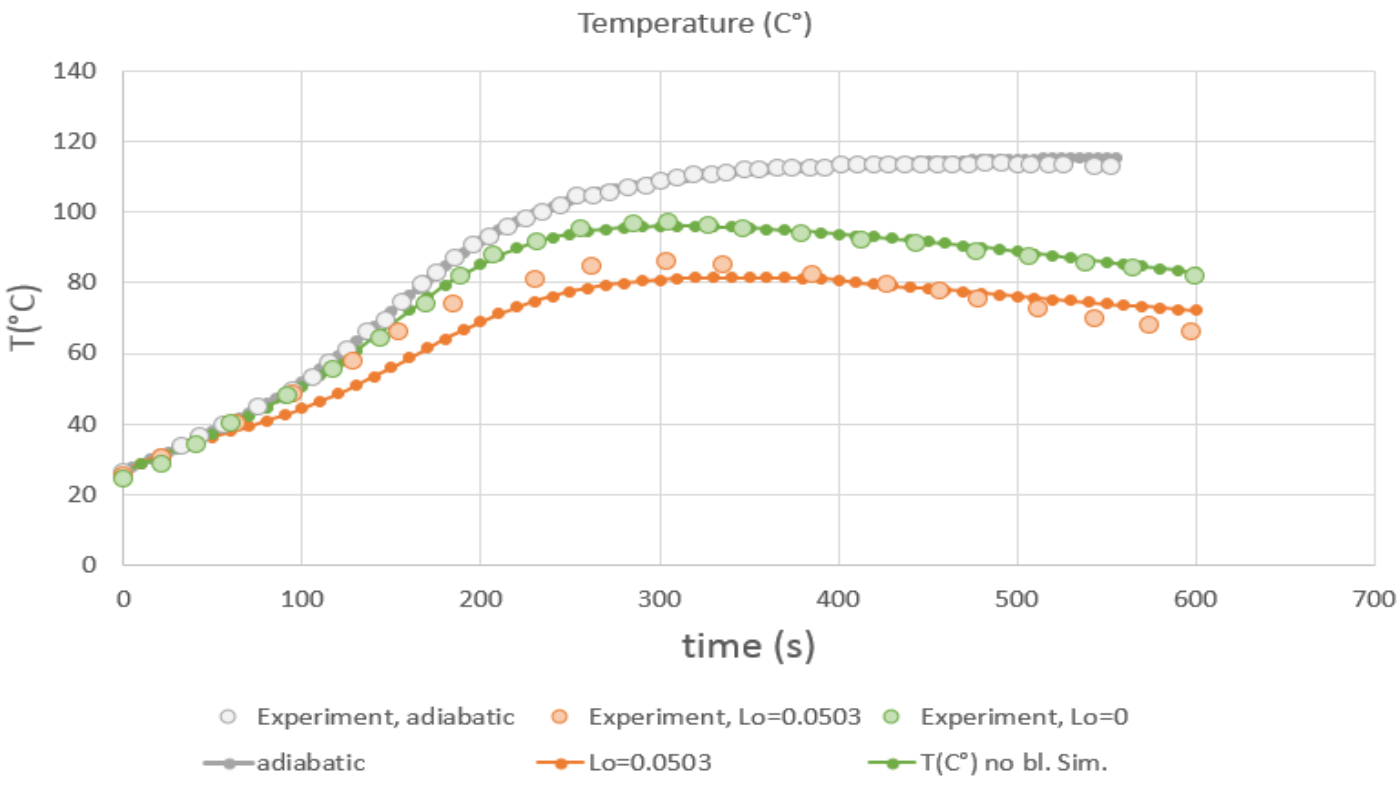


Fig. 6: Temperature drop due to evaporation for $L_0 = 0.0503$.

Hence, the unsteady state model equations for the physical blown PU foam is

$$
\left.
\begin{aligned}
&\frac{d\xi}{dt} = k\left(b + \xi^m\right)\left(1 - \xi\right)^n, \\
&k = \left[\left(0.5 - B\right)\left(1 + \tanh\left(D(t - t_s^{\xi})\right)\right) + 2B\right] \frac{1}{(1+\omega_c \alpha_T)^{\beta}} k_0 \exp\left(\frac{-E_{\xi}}{RT}\right), \\
&\log_{10} \alpha_T = -\frac{C_1(T - T_g)}{C_2 + T - T_g}, \\
&T_g = \frac{T_{go}(1-\xi) + A\xi T_{g\infty}}{1 - \xi + A\xi}, \\
&\rho_p C_p \frac{dT}{dt} = \rho_p H_R \frac{d\xi}{dt} + \left(-\lambda' \frac{dL}{dt}\right) - h(T - T_0), \\
&\frac{dL}{dt} = \begin{cases} \frac{M_B}{M_{no}} \frac{1}{(1-x_{BL})^2} \frac{dx_{BL}}{dT} \frac{dT}{dt} & \text{for } T \geq T_c \\ 0 & \text{for } T < T_c \end{cases} \\
&\rho_f = \frac{1 + L_0}{(G1000RT/PM_B) + (L/\rho_{BL}) + (1/\rho_p)}
\end{aligned}
\right\} \quad (14)
$$

And the associated initial conditions are: $T = 26.62^{\circ}\text{C},\ \xi = 0, L = 0.0751$

PUF: Model 2 formulation (Unsteasy 3D system)

Model 2: Assumptions

- a) A half open cylinder is considered
- b) Impact of flow is significant: convective term
- c) The flow is driven by the volume expansion, S_p
- d) The system is unsteady and spatially inhomogeneous in 3D (x, y, z)
- e) Variable κ & μ
- f) The model considers all the conservation laws 1 & 2, 3 & 4
- g) Polymerization reaction follows Rao et al. (2018) cure model

The unsteady 3D model for the physical blown PU foam is

$$
\left.
\begin{aligned}
&\text{Continuity equation:} \quad \nabla\cdot\vec{v} = S_p \quad \text{where} \quad S_p = \frac{1}{V(t)}\frac{dV(t)}{dt},\\
&\text{Mom. equation:} \quad \rho\left(\frac{\partial\vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v}\right) = -\nabla p + \nabla\cdot\left(\mu[\nabla\vec{v} + \nabla\vec{v}^{\,T}]\right) + \rho\vec{g},\\
&\text{Energy equation:} \quad \rho C_p\left(\frac{\partial T}{\partial t} + \vec{v}\cdot\nabla T\right) = \nabla\cdot(\kappa\nabla T) + \rho H_R\frac{d\xi}{dt} + \left(-\lambda'\frac{dL}{dt}\right),\\
&\text{Concentration equation:} \quad \frac{\partial\xi}{\partial t} + \vec{v}\cdot\nabla\xi = k\left(b + \xi^m\right)\left(1-\xi\right)^n,\\
&\text{Evaporation rate equation:} \quad \frac{dL}{dt} = \begin{cases} \frac{M_B}{M_{no}}\frac{1}{(1-x_{BL})^2}\frac{dx_{BL}}{dT}\frac{dT}{dt} & \text{for } T \geq T_c \\ 0 & \text{for } T < T_c \end{cases}\\
&\text{Foam density equation:} \quad \rho_f = \frac{1+L_0}{(G1000RT/PM_B)+(L/\rho_{BL})+(1/\rho_p)}
\end{aligned}
\right\} \quad (15)
$$

Literature review: PU foaming process

Author(s) /(Year)	Title	Model	Quantity Studied/Methodology
Tesser et. al., (2004)	Modeling of Polyurethane Foam Formation	**Unsteady:**✓ **Dimension:** 0 **Evapor. Eqn:**✓* **Foam Density:**✓* **Conv. Term:** × **Heat S/S:**✓	L_0 Numerical integration (Livermore Solver for ODE) LSODE
Seo and Youn (2005)	Numerical analysis on reaction injection molding of polyurethane foam by using a finite volume method	**Unsteady:**✓ **Dimension:** 3 **Evapor. Eqn:**✓* **Foam Density:**✓* **Conv. Term:** ✓* **Heat S/S:**✓	T, ρ_f Finite volume method
Niyogi et. al., (2014)	Modeling of Bubble-Size Distribution in Water and Freon Co-Blown Free Rise Polyurethane Foams	**Unsteady:**✓ **Dimension:** 0 **Evapor. Eqn:**× **Foam Density:**✓ **Conv. Term:** × **Heat S/S:**✓	T, P, ρ_f Adams–Moulton method

Literature review: PU foaming process

Author(s) /(Year)	Title	Model	Quantity Studied/Methodology
Ireka et. al., (2015)	Computational modelling of dependent properties on the complex dynamics of chemically blown polyurethane fom	**Unsteady:**✓ **Dimension:** 3 **Evapor. Eqn:**× **Foam Density:**✓* **Conv. Term:** ✓ **Heat S/S:**✓	$H(t), T$ Finite volume method
Rao et. al., (2018)	Density predictions using a finite element/level set model of polyurethane foam expansion and polymerization	**Unsteady:**✓ **Dimension:** 3 **Evapor. Eqn:**× **Foam Density:**✓ **Conv. Term:** ✓ **Heat S/S:**✓	T, ρ_f Finite element method
Opadiran & Okoya (2021)	Importance of convective boundary layer flows with inhomogeneous material properties under linear and quadratic Boussinesq app around a horizontal cylinder	**Unsteady:**× **Dimension:** 2 **Evapor. Eqn:**× **Foam Density:**× **Conv. Term:** ✓ **Heat S/S:**✓	T, μ Mid-Point method

Literature review: PU foaming process

Author(s) /(Year)	Title	Model	Quantity Studied/Methodology
Salawu & Okoya (2024)	Exothermic diffusion-reaction and explosion branch chain of an asymmetrical heating channel with convective heating	**Unsteady:**✓ **Dimension:** 1 **Evapor. Eqn:**× **Foam Density:**× **Conv. Term:** ✓ **Heat S/S:**✓	T Finite difference technique
Opadiran & Okoya (2025)	Mathematical modelling of the dynamics of polymeric foams formation	**Unsteady:**✓ **Dimension:** 3 **Evapor. Eqn:**✓ **Foam Density:**✓ **Conv. Term:** ✓ **Heat S/S:**✓	L_0, T, ρ_f Finite volume method

Method of solution: PU foaming process

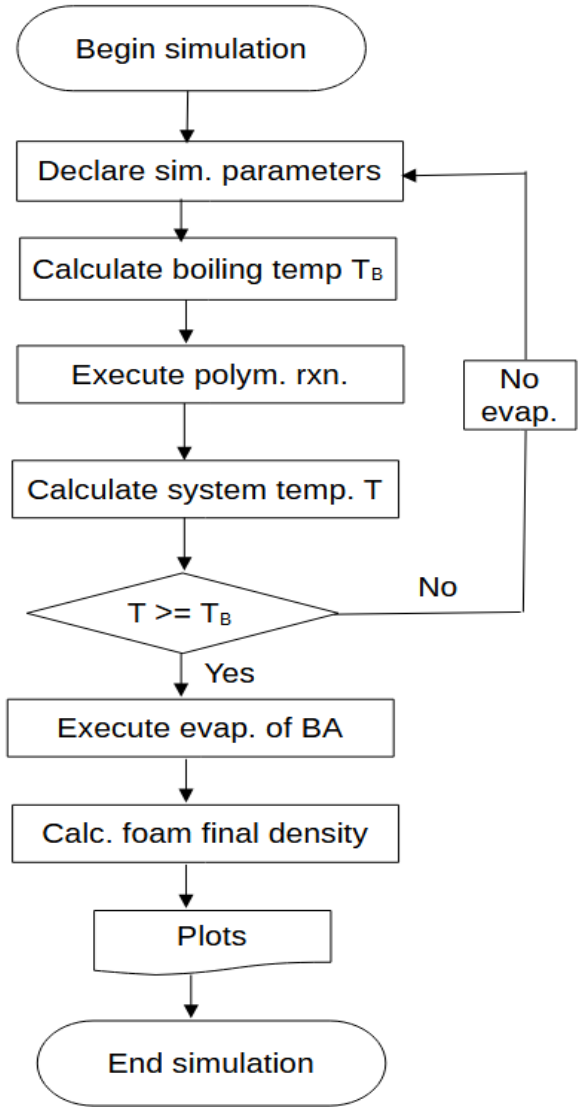
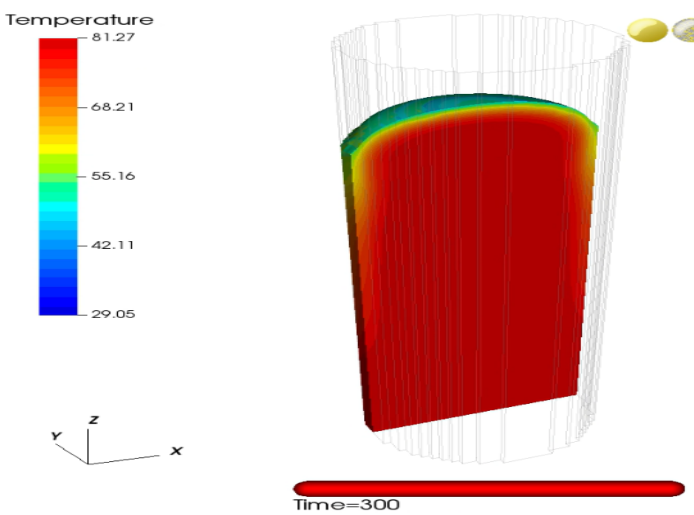


Fig. 7 Flow chart of the model implementation

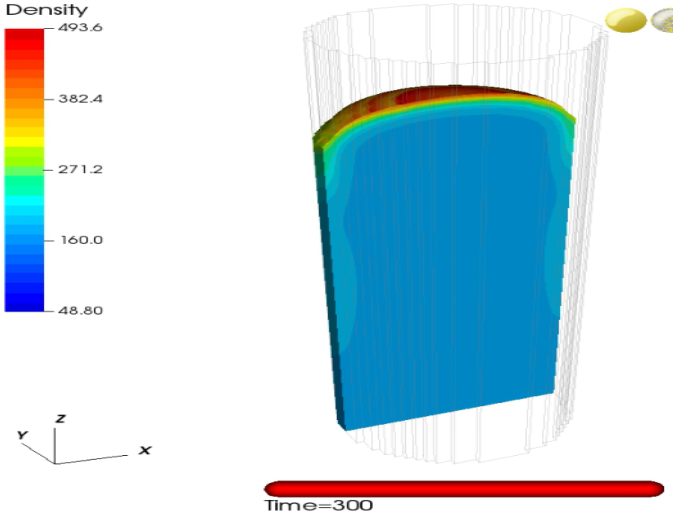
Results & discussion : Polyurethane foam expansion

Video clip: Foam expansion and growth in 3D simulation (300secs)

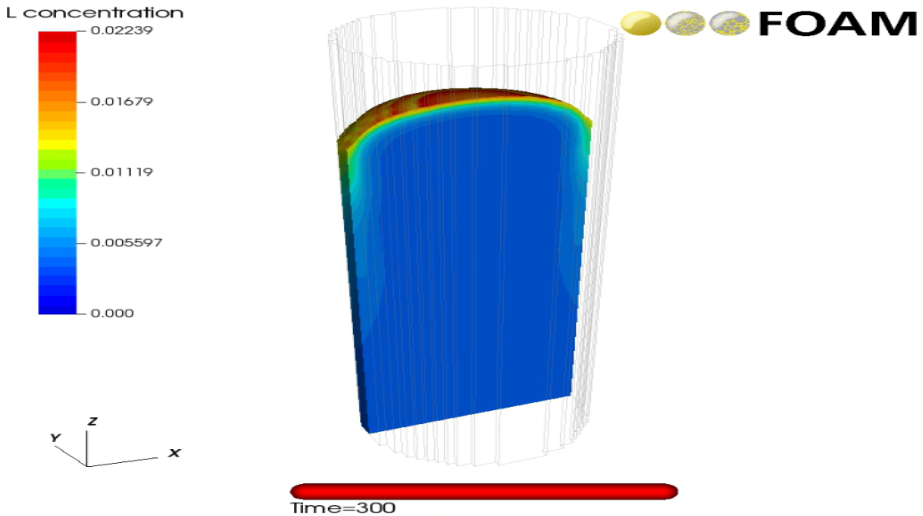
Results & discussion : 3D Polyurethane foaming cross-sections



(a)



(b)



(c)

Fig. 8: 3D plots of foam (a) Temperature (b) Density (c) Blowing agent conc.

Conclusion

The vital conclusions of the present study include:

- The theoretical predictions of the blowing agent mole fraction showed excellent agreement with experimental report.
- Furthermore, the model predictions for temperature rise fits well the experimental data.
- The predicted final foam density of the foamed product matches well the experiment.
- Results of the 3D model showed realistic prediction of the foaming properties.
- The model of the dynamics for physically blown PUF formation presented, would thus be useful for the development of new foam formulations.

Contribution to knowledge

This research work will make available mathematical models to pedict the final foam densities of polymeric foams. Results of the foam densities reported in this study will enrich the body of literature and stimulate further research on polymeric foams and also help industrialists in their design and safety assessment of foams in cushioning and structural applications.

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Danke furs Zuhoren—Question! Question!! Question!!!

Nomenclature & Units

- ρ=density (kg/m^3); h'= (J/kg.k.s)
- $\vec{v}$=velocity (m/s); $H_R = \lambda$= (J/kg.k)
- t=time (s); $K_H = mol/m^3/Pa$; $R = (J/mol.k)$
- p=pressure (N/m^2 *or* $kg/m.s^2$); $D_f = m^2/s$
- μ=viscosity (kg/m.s); $D = (1/s)$
- $\vec{F} = \rho g = body\ force\ (gravity)\ (kg/m^2.s^2)$
- c_p=specific heat at constant pressure (J/kg.k)
- κ=thermal conductivity (W/m.k)
- T=temperature (k); $\gamma = J/m^2$; $R_g = J/mol.K$
- Q=heat generation constant ($W/m^3.k$); $J = 1/s.m^3$
- $m, n, \omega_c, \beta, A, D, B =$ fitting parameters
- g=acceleration due to gravity (m/s^2)
- E_ξ, xi=activation energy (J/mol), extent of polymerization
- α_T= shift factor for time-temp. superposition
- κ_0; C_1, C_2= rate coefficient (1/s);WLF constants
- T_g, T_{go}=glass transition temperature (K);of the unreacted material
- k = Arrhenius-type rate equation (1/s)