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Simulation the Performance of Blowing Agents for Polyurethane Polymerization Reaction

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ABSTRACT

The objective of the current study is to determine the accuracy of a computational model that has been developed to simulate polyurethane foaming reactions by comparing its results with experimental findings on the system using both physical and chemical blowing agents. There was high concordance between the model outputs and the laboratory results in regard to the temporal development of reaction temperature as well as the resulting foam density, both of which were highly faithful recreations. The discussion provided further information about the optimization of the performance of cyclohexane, particularly when used in synergy with chemically active blowing agents, which speed up foaming. Besides, the polymerization dynamics were contained in the simulation, thus providing rich information on the structural changes that occur during the foaming process. Taken together, the results present a strong basis for the process performance optimization, as well as the predictive modeling of the blowing agent behavior. In the future, it will involve expanding the simulation model to include a wider range of agents, reaction mechanisms, and kinetics.

1. Introduction

The demand in the polyurethane (PU) market has been growing every year due to the wide choice of usage. The growth rates per year are about 5-10, and the international use of raw material is over 12 million metric tons. PU has found use in building and refrigeration rigid insulation, cushioning furniture, and elastomeric furniture and tires. Polyurethane foams are prepared by reacting polyol(s) and isocyanate (in the presence of catalysts, surfactants, fire retardants, and physical and/or chemical blowing agents). [1]

Foam morphology is obtained through the use of a blowing agent that forms a cellular, gas-filled structure. In most cases, liquid blowing agents are combined with liquid polyol monomers before they are combined with isocyanate monomers. The blowing agent plays the role of transforming a solid plastic or elastomeric precursor into a foam. In the case of the physical blowing agents, the exothermic reactions cause the heat to evaporate the agent. To achieve the successful formation of foam, a coordination of temperature rise, which induces the evaporation of the blowing agent, with the corresponding rise in viscosity, which is necessary in foaming the gas cells, is required. The blowing agent controls the density of the foam, cellular microstructure, and morphology; all these factors are essential in the end-use performance. [2-4]

Waters are normally used as chemical blowing agents, as they react with isocyanate to create carbon dioxide. This exothermic reaction yields heat that is used together with the exothermic polymerization reaction to evaporate a secondary physical blowing agent (PBA), further

providing more gas to foam and giving desired foam properties. [5, 6]

Inert liquids that have low boiling points are referred to as physical blowing agents. These agents evaporate in the place of heat and temperature increase due to reactions that are exothermic in nature. The amount and the nature of the physical blowing agent determine the foam density by forming and filling in gas cells. The higher the content of the blowing agent, the less dense the foam tends to be, and thereby, it influences the foam's resistance to compressing forces and thermal conductivity. [7]

The choice of a suitable blowing agent depends on a sweet combination of interdependent performance indicators:

1. Cell Size and Distribution: Uniform small cells tend to provide better mechanical characteristics and thermal insulation. Diffusivity and solubility of the blowing agent have a direct effect on the density of the cell nucleation.
2. Foam Density: Density is used to measure the amount of mass divided by the volume of 1 unit and is negatively proportional to the amount of gas added. The low-density foams used have the benefit of being used as an insulator, though at the cost of being mechanically weak.
3. Thermal Conductivity: The transfer of heat in the foam is mainly controlled by the gas phase that fills the cells. thermal conductivity Gases with low thermal conductivity (carbon dioxide, nitrogen) offer better insulating properties; gases with hydrogen or methane can unintentionally increase conductivity.
4. Mechanical Strength: The cell wall is fabricated by using a polymer matrix and needs to have enough thickness to support mechanical loads. The blowing agent controls the thickness of the walls through the control of the rate of gas discharge and the viscosity of the melt.
5. Acoustic Absorption: In acoustic absorbing foams, the damping of acoustic waves depends on the size of the cells, the thickness of the walls, and the density of the gas.
6. Environmental Impact: Global Warming Potential (GWP) and Ozone Depletion Potential (ODP) are very important environmental indicators. HFC-134a and other common fluorinated agents have a GWP of about 1,430, and emerging agents, including HFO-1234yf and carbon dioxide, have GWPs of less than 1.
7. Processability: The blowing agent has to be chemically compatible with polyurethane systems, should not hinder the kinetics of curing, and should be worked safely in the conditions of industrial manufacturing.

Practically, such measures are often incompatible. A blowing agent that forms incredibly small cells can give rise to a foam that is too dense, and one that forms larger cells can cause loss of structural integrity. Therefore, the use of an appropriate blowing agent is a multi-dimensional optimization problem. [7, 8]

The global climate goals and the local regulatory frameworks have greatly contributed to the push of developing low-GWP blowing agents. The Kigali Amendment to the Montreal Protocol, for example, aims at the phase-down of high-GWP hydrofluorocarbons (HFCs), and this directly impacts the polyurethane industry. Moreover, the European Union REACH regulation, which is being augmented by the Eco-Label Directive, forces manufacturers to resort to the use of chemicals that would have minimal environmental and health risks. In that regard, less harmful blowing agents like CO_2, HFOs, and bio-derived gases are under systematic consideration. However, replacement of traditional agents is not simple; the new agents should match or even surpass the performance of old chemicals besides fitting perfectly well on the existing production lines, which may also necessitate changes in mixing, curing, and ventilation systems. [9, 10]

The experimental research on blowing agents is costly and time consuming. Each new agent will be subjected to a specific series of characterization tests, which include decomposition temperatures under the assistance of the differential scanning calorimetry, rheometry to determine the change in the viscosity, rate of gas evolution under the assistance of the gravimetric analysis and the thermal conductivity tests to determine the insulating properties. Besides, when the blowing agents and other additives, such as surfactants, flame retardants, or fillers, are combined, the

parameter space increases exponentially [11-13]. A simulation framework has a number of benefits:

- Parametric Exploration: It is possible to rapidly test the performance trends by changing the concentration of blowing agent, temperature, pressure and the content of catalysts without any laboratory experiment.
- Mechanistic Insight: Simulations can be used to identify transient temperature fields, local gas concentrations and cell nucleation processes that are hard to measure experimentally.
- Optimization: Predictive models may assist in the process of selection of blowing agents which satisfy a number of performance criteria in a single experiment, minimizing the amount of experimental trials.
- Safety and Compliance: The manufactures can preempt issues regarding safety by modeling the potential of thermal runaway of the new blowing agents.
- Economic Analysis: The business can be informed by the addition of cost models to the blowing agent and process modifications.

Despite this encouraging fact, the simulation of polyurethane foams using blowing agents is a complex undertaking that consists of a series of difficulties [14-16]:

1. Multiphysics Coupling: The system encompasses chemical kinetics, heat transfer, mass diffusion, and fluid dynamics, and all these work on different timescales. These processes require advanced numerical solving software and a thorough stability test to couple.
2. Phase Change and Compressibility: The gas that is produced by blowing agents expands, pushing the fluid flow in the melt. The proper description needs the addition of gas compressibility and the interfacial behavior between gas and polymer melt.
3. Computational Expense: Time-dependent, fully coupled simulations are computationally expensive and can often require high-performance computing equipment, particularly when three-dimensional geometries are taken into account.
4. Non-Newtonian Rheology: This is the shear-thinning, viscoelastic fluid behavior of the polymer melt, mostly at later stages of the reaction and when the viscosity rises significantly. Constitutive models like the Carreau model or the Cross model need to be included.
5. Cell Nucleation and Growth: The foaming initiation is associated with the nucleation—a stochastic process that is sensitive to nucleation sites, supersaturation, and interfacial tension. These phenomena are normally captured using phase-field or level-set methods.
6. Scale Bridging Experiments: Typically, study macroscopic foams (cm to m), and simulations are often studied at micro- or nanoscale to elucidate the cell dynamics. Adaptation to these scales needs homogenization or up-scaling procedures.
7. Parameters Identification: There are many kinetic and transport parameters that cannot be directly measured but have to be deduced based on the data collected in the experiments, and this leads to uncertainties propagating through the simulation.

In light of these challenges and the pressing need for environmentally benign blowing agents, the present simulation study seeks to [13, 17]:

1. Develop a Unified Multiphysics Model that integrates chemical reaction kinetics, heat and mass transfer, viscoelastic rheology, and phase change dynamics specific to polyurethane foams.
2. Validate the model against experimental benchmarks such as foam density, cell size distribution, and thermal conductivity for a set of canonical polyurethane formulations.
3. This simulation aims in determining the failure of cyclohexane physical blowing agent and how adding a chemical blowing agent enhance its performance.
4. Extended to determine the polymer degree of polymerization. The results presented here suggest that the simulation framework still has room to grow.
5. Provide decision-support outputs such as contour maps of foam density versus blowing agent concentration and

temperature, or Pareto fronts balancing mechanical strength and GWP.

6. include additional side reactions that occur during foaming, introduce refined or newly measured kinetic parameters, and eventually predict physical properties of the final foam structure.

The creation of a strict simulation system of polyurethane foams with a combination of various blowing agents promises to significantly improve the efficiency and work of industries due to the reduction of the time and financial expenses involved in the creation of the product. The method can be used by manufacturers to conduct a rapid screening of candidate blowing agents, to design specifically for a given application, e.g., high-performance automotive insulation or low-density packaging foams, and to maintain compliance with the emerging regulatory environments. [18]

Also, the knowledge gained via such simulations can be used to guide the rational design of new blowing agents that can simultaneously have low global warming potential, high gas yield, and the optimal rheological properties, and, thus far, this combination has eluded researchers. In a larger-scale context, the modeling approach can be generalized to other polymer foams such as epoxies and polyesters and can also be generalized to composite foams that contain fillers or fibers. It also can be used as a source of life-cycle assessment tools, and thus a comprehensive analysis of the environmental impact of foam products from cradle to grave would be made. In the end, the developments contribute to the shift towards a circular economy, in which materials are designed to perform well, be sustainable, and be recyclable.

The integrated simulation model designed in the research can effectively recreate the temperature profile, the kinetics of foam density, and polymerization of the system with the use of both chemical and physical blowing agents. Unlike the previous models, it can sufficiently explain the initial difference that is found in the foaming of cyclohexane by taking advantage of its thermal properties. As the cyclohexane is co contaminated with water, the predictive power of the model is also improved. The use of a measure of the extent of the polymerization has produced new mechanistic information regarding the development of foam patterns. All of these qualities provide a more complete and experimentally verified system of evaluating and optimizing the functioning of blowing-agents. This will in turn form the basis of future extensions that will incorporate more agents, secondary reactions and optimized kinetic pathways.

2. Experimental Procedure

Table 1 provides a description of foaming compositions that have an isocyanate index of 110. The several stiff polyurethane foams were all made using the same amounts of polyol, catalyst, surfactant, fire retardant, and isocyanate. The Huntsman Corporation was responsible for the production of the isocyanate known as Rubinate M, whereas Dow Chemical developed Voranol 360. Experiments were conducted to evaluate the effectiveness of several blowing agents while keeping the amount of each constant. The properties of Voranol 360 and PMDI, which were utilized in the gel and foaming formulation, are presented in Table 2. Using the formulations shown in Table 1, foaming experiments were conducted to produce polyurethane gels and foams with a variety of physical blowing agents. The following procedures were followed during the course of the experiments:

- The plastic cap is first filled with the B-side mixture, and then the A-side component is added on top.
- The mixture was combined for a total of 10 seconds using a mixer set to 2000 revolutions per minute.
- The foaming blend is allowed to grow until the temperature of the foam starts to drop.

A type-K thermocouple was implemented in conjunction with a data recorder to determine the temperature of the foam reaction. The chemicals were mixed with the use of a floor-model drill press that had a high-speed blender connected to it. All the experiments were conducted under the same environmental conditions. Each experiment was repeated three times and the average value was considered.

Table 1. Recipes used in the experiments.

Materials	Formulation (g)
PMDI (Polymeric Methylene Diphenyl Diisocyanate)	77
Voranol 360	70
Cat 1	0.44
Surfactant	0.6
Fire retardant	2
Blowing agent	Different amount as shown in figures

3. Simulation Software

The simulation code is based on a simple algorithm that links the chemical behavior of the polyurethane system to numerical integration in MATLAB. The beginning is made by defining the input conditions, such as the formulation recipe and the values of initial state variables. Further, all these inputs are provided to the MATLAB environment, where the core model is solved by the ODE45 solver. At each step, ODE45 continuously interacts with the reaction-kinetics module which has stored the chemical data and the rate expressions governing the polyurethane reactions. In this way, while the system evolves in time, the solver continuously updates the concentrations, reaction heat, gas generation, and related variables. After the calculations have been completed, the code returns an output of the predicted reaction temperature, foam density, and DP, representing a complete dynamic picture of the foaming process. The simulated reactions are listed in Table 2.

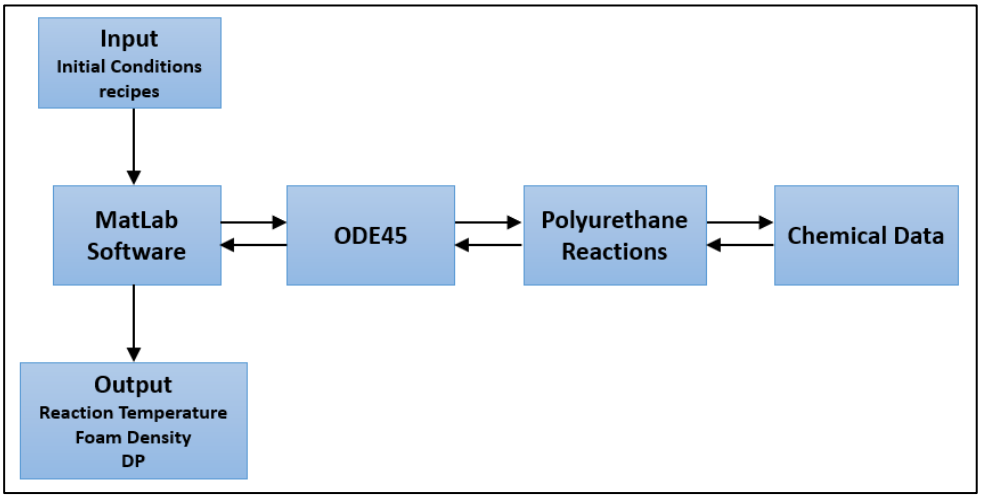


Figure 1. Algorithm for simulating polyurethane foaming reaction.

Table 2. Polyurethane foaming reactions.

No.	Reaction
1	$A + B \rightarrow P$
2	$A + P_B \rightarrow P$
3	$P_A + B \rightarrow P$
4	$P_A + P_B \rightarrow P$

4. Physical System and Assumptions.

To simplify the process of presenting the representation of foaming process in the simulation framework, a set of simplifying assumptions were made.

- The bubbles created in the foam are considered to continue with a perfectly spherical shape in the course of their development, and any effect of gravity on their development is not taken into consideration.
- It is assumed that a steady thermodynamic equilibrium will exist at the gasliquid interface of the whole foaming process.
- The ideal gas that is in the bubble interior is an ideal gas in all the modeled conditions.

- The simulation excludes any phenomenon of bubble collapse, deformation, or distortion, even those caused by collision.
- The heat emitted in the chemical reactions is assumed to be the same all along the temperature range that is being studied, which is assumed to be between about 25 0 C and 130 0 C.
- It is assumed that the process of homogeneous nucleation occurs and no effort is made to model the nucleation process; rather a predefined density of sites already included in the computational program defines the initial population of bubbles [9].
- The entire system is deemed so that none of the portion of the blowing agent is lost during foaming action [10, 11].
- The model has imposed adiabatic behavior, and thus, all variables are uniformly distributed spatially, and therefore, gelation is supposed to take place concomitantly across the entire mold and hence all bubbles everywhere are presumed to be stopped expanding at the same moment.
- The aspect of interaction between the growing bubble and the adjacent bubbles or the liquid resin boundaries are excluded, due to the assumption that the next growth process becomes dominated by diffusion inside the thin liquid layer, which is confined around each bubble [8].
- Motion of bubbles through the reacting medium in a transitional manner is not taken into account.
- The changes in volume that occur due to mixing in the liquid phase are not considered.

5. Results and Discussion

5.1 Software verification

Figure 2 offers a broader look at how the polyurethane system evolves when different blowing routes are used. Although both the chemical and physical blowing agents ultimately push the material through the familiar stages of heating, expansion, and stabilization, each pathway leaves its own signature on the reaction behaviour. Seeing the curves side by side makes these differences easier to appreciate.

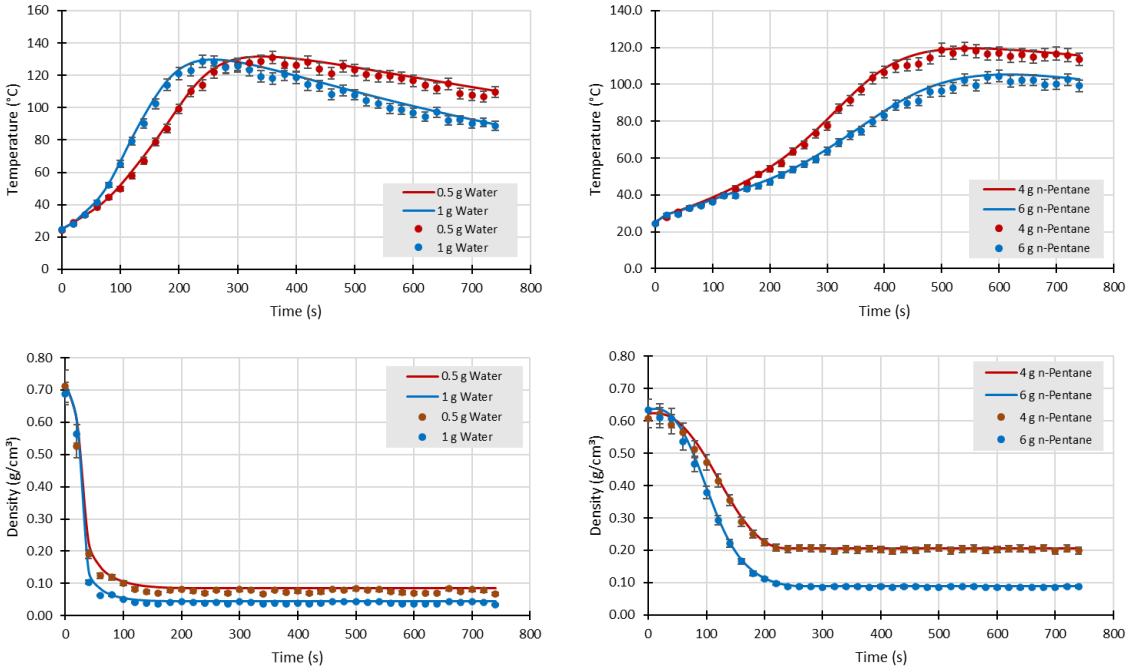
For the water-blown system, the temperature curves rise quickly after mixing, showing just how strongly exothermic the polyurethane reaction can be. The formulation with 1 g of water will have a faster rise and a slightly higher peak, which is consistent with the hypothesis that an increase in CO_2 formation in the process of water-isocyanate reaction will cause the process to quicken. Although the extra gas only enhances the expansion of the foam, it is also capable of modulating the reaction kinetics in a subtle way. The numerical model follows this temporal development very well. There is a slight deviation found to approach the terminal phase, which presumably can be explained by heat-loss processes in the actual foam that are difficult to describe analytically, but this doesn't weaken the overall concordance, which is strong and encouraging.

The density profiles support this account in the complementary view. Both formulations undergo a strong density decrease when the foam begins to rise, but the stabilization of the 1.2 g water sample is realized at a relatively low density. The high sensitivity of the system at the nucleation and coalescence stages of bubble formation is expected to be accompanied by the initial experimental scattering. However, the simulated density trajectories follow the empirical data well and essentially recapitulate the key transitions in both rate and morphology.

The behavior changes with the use of n-pentane. Since pentane is not reacted in the reaction, the temperature traces show a slower rise. The mixture with 6 g of pentane has a low peak, and it gets it a little later—a fact that indicates that part of the heat of the reaction is used in the vaporization of the extra pentane. This reduced profile with the minor plateau before the peak is recreated in the simulation.The shape of particles is revealed by density curves. With the volatilization of the pentane, the foam volume increases quickly, but the density decrease is slower than it is with the water-blown analog. The final density in the 6-pentane sample is

significantly less because the vapor volume available to push the expansion is large. The simulated curves have the same path that is concordant with the rapid decline, as well as the stabilized terminal region, thus achieving an acceptable level of accuracy.

The contrast between chemical and physical blowing is more distinctive when the two systems are taken together. Water pushes the reaction harder, leaving a strong imprint on the thermal behaviour, whereas n-pentane influences the foam structure more through its evaporation than through any change in reaction kinetics. Nonetheless, the model manages to reproduce the main characteristics of both routes. The agreement between the simulations and experimental data over temperature, density, and two very different blowing mechanisms indicates that the modelling approach has enough flexibility and physical grounding to serve as a reliable predictive tool for polyurethane foaming under varied formulations.



(a) (b)

Figure 2. Simulation and experimental data of reaction temperature and foam density of polyurethane foam blown with different loadings of (a) water and (b) n-Pentane. Straight lines represent simulation results and dots represent experimental data.

5.2 Cyclo-Hexane Simulation

The behaviour displayed by the cyclohexane-blown system turns out to be quite different from what the model predicts, and the gap between the simulation results and the experimental curves is noticeable in both the temperature and density plots (Figure 3). On one hand, the temperature profiles show the expected rise, but the measured points remain well below the corresponding simulated lines for most of the reaction. This mismatch appears already in the early stages, which suggests that something is cooling the mixture more than the model accounts for. Given the high boiling temperature of cyclohexane, this explanation fits reasonably well: at the beginning of the reaction, the cyclohexane absorbs a substantial amount of heat while it warms up, effectively delaying the temperature rise of both A and B components. The simulation, however, assumes a more idealized evaporation behaviour and does not fully capture this initial cooling effect.

There is a similar complication during the density evolution. The empirical density becomes less smooth, the values subside at a slower rate, and what they calculated is not the same as what the theoretical model shows. The excessively

strong cooling effect of cyclohexane during the first few seconds of the reaction probably slows down the rate of gas formation and delays the expansion initiation, thus extending the expansion curve relative to the simulation. Predicated on a lower liquid-vapor transition, simulations of profiles can overestimate the expansion velocity and reach the terminal density plateau too soon.

The thermal properties of cyclohexane seem to cause the difference between the experimental and simulation results. Due to its relatively high boiling point, cyclohexane takes up warmth at a relatively low temperature, and, as a result, it suppresses the initial rise in temperature that directly influences foam ascending and density change. This part of the mechanism is abstracted by the model and does not encompass the observed cooling and subsequent slowed expansion. However, the number is still informative enough in showing the strong effect of blowing-agent properties on the reaction temperature and the foam morphology.

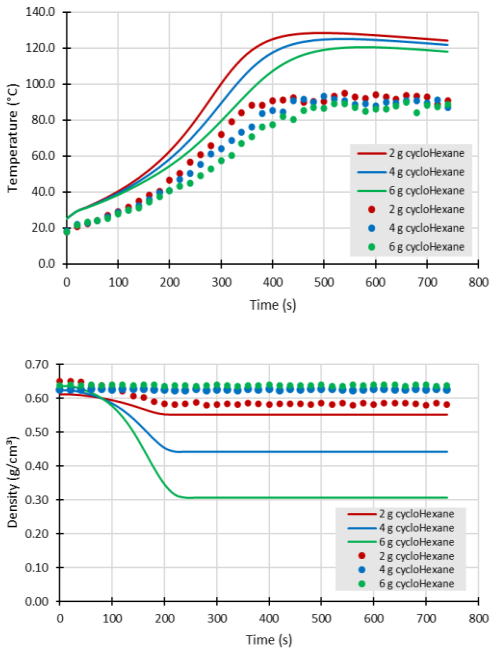


Figure 3. Simulation and experimental data of reaction temperature and foam density of polyurethane foam blown with different loadings of cyclohexane. Straight lines represent simulation results and dots represent experimental data.

5.3 Blowing Agent Mixture

As shown in Figure 4, there is a significant deviation in the system behavior when water is added with cyclohexane. The temperature traces become much more consistent than those of the case with cyclohexane alone; the thermal increase is less bumpy and begins to increase earlier and more converged with the results of the simulation. This enhanced correspondence is credited to the CO_2 emitted in the interaction of water with isocyanate that introduces the necessary thermal impetus in the system that is not present in the case of cyclohexane by itself. Water, therefore, helps the system to traverse through the first cooling dip due to the relatively high boiling point of cyclohexane.

The density curves that were achieved in the experiments have an outstanding resemblance. When water is introduced, a sharp decrease in foam density is exponential and becomes stabilized, after which it enters a plateau, which signifies the final structural regime. It is interesting to note that the model that has hitherto exhibited either an overshoot or undershoot effect along the density line shows significant improvement of conformability to the empirical data. The mixtures with 2 g, 4 g, and 6 g of cyclohexane become increasingly predictable, and the simulation no longer takes off as it did before. Apparently, the addition of water stabilizes the initial reaction stages, thus allowing the cyclohexane evolution to prevail without interfering with the equilibrium of the system.

Using the two blowing agents together suggests a more synergistic system numerically. Water is what starts the process by creating heat and CO_2, which is then followed by the action of cyclohexane that also further promotes the growth of foams. The concomitant action of these mechanisms is the effect of correcting the extreme cooling, which had slowed down the reaction before. The simulation with a more homogeneous thermal profile is closer to the experimental observations; although it cannot be called perfect, the overall enhancement is evident.

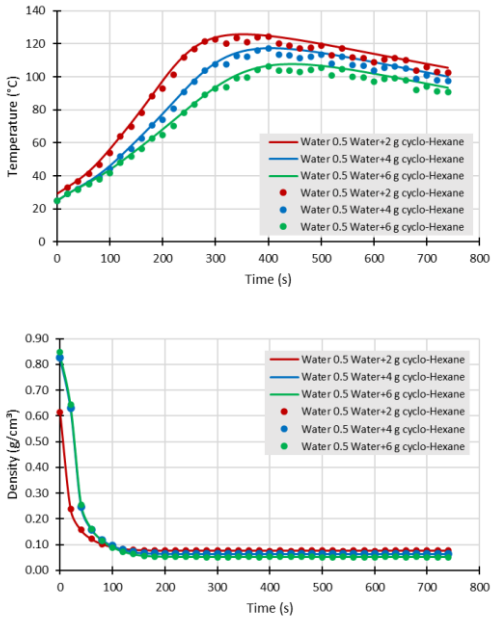


Figure 4. Simulation and experimental data of reaction temperature and foam density of polyurethane foam blown with different loadings of water and cyclohexane. Straight lines represent simulation results and dots represent experimental data.

5.4 Simulating Degree of Polymerization

Since the simulation code already showed that it can follow the reaction temperature and foam density with reasonable accuracy, it made sense to push it a bit further and see whether it could also track the degree of polymerization (DP). Once those larger physical behaviors—heat buildup and foam expansion—are modeled well, the polymer growth curve becomes the next logical thing to look at. Figure 5 is basically the first attempt at doing that for mixtures blown by both water and cyclohexane.

What the figure shows (Figure 5) is actually quite encouraging. All three curves rise in a steady, coherent way, and the differences between them look exactly like what you would expect when you vary the cyclohexane loading. The combination of 0.5 g water + 2 g cyclohexane reaches the highest DP and does so more quickly, which makes sense because the reaction gets a strong early push from the water–isocyanate step. When the cyclohexane increases to 4 g and then 6 g, the curves slow down noticeably. Higher amounts of cyclohexane tend to cool the mixture more at the start, and that cooling delay shows up very clearly in the DP curves.

Even though the model isn't necessarily aiming for a perfect numerical match, their relative behavior is exactly in line with the recipes. That in itself is a good sign. What this really means is that the simulation framework is not only capable of predicting temperature and density but can also follow the actual polymer network development in a physically meaningful way.

The results herein obtained show that this simulation framework still has much room to grow. Since it can already follow the main polyurethane reactions, foam temperature, density changes, and even the degree of polymerization, it should not be too much work to extend the code by adding other side reactions during foaming, introducing refined or newly measured kinetic parameters, and eventually predicting physical properties of the final foam structure. With each layer added, the model becomes a more complete tool for understanding and optimizing polyurethane foam behavior.

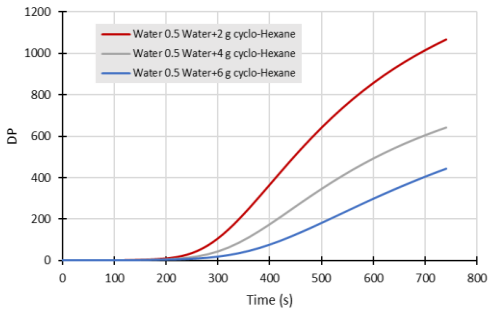


Figure 5. Simulation results of the degree of polymerization of polyurethane reaction using different loadings of blowing agents.

6. Conclusions

The present study demonstrated that the developed simulation framework can follow a polyurethane foaming process in a fairly detailed way. Starting from temperature and density—two of the clearer indicators of how a foam evolves—the model was able to reproduce the main behavior of the reaction for several blowing-agent systems. The foams produced by the blowing of water were found to have the highest concordance, which is compatible with the enhanced reaction kinetics of the water-isocyanate system. The difficulties that surrounded cyclohexane were more enlightening than discouraging since, with its high boiling point and the cooling effect that it had, it was very well

able to explain the initial deviation between simulation and experimentation. When the water was added to the cyclohexane medium, the foam behavior had significantly more stability, and the simulation was then able to predict experimental measurements in coherent ways. It was beneficial to extend the computational model to provide polymerization degree estimations. The framework addresses both bulk foam properties and the less pronounced, slower changes within the polymer network. These results underscore the extensiveness of the model. It seems possible to incorporate more side reactions, optimize kinetic parameters, and predict end foam physical properties. Overall, the simulation can be viewed as an expedient tool for explaining the mechanistic aspect of blowing agents and indicating improvements in performance. It also outlines a more distinct path for further experimental and modeling activities, which is the general goal.

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Conflict of interest

The authors declare no conflicts of interest concerning this research.

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AI Declaration Statement

The authors confirm that the manuscript has been written without the assistance of generative AI or AI-based writing tools.

Author Contribution

Ahmed K. Al-Kamal proposed the research problem, developed the theoretical framework, verified the analytical methods.

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