Emerging Trends in Engineering and Sustainability (ETES) Volume 02 (No. 01), 2026, pp. 51-64

Emerging Trends in Engineering and Sustainability (ETES)
https://etes.alnaji-uni.edu.iq

https://doi.org/10.65505/ETES-26-0004

ISSN 3105-1723 (Print)
ISSN 3105-1731 (Online)

Simulation Approaches for Polyurethane Materials: A Multiscale Review

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Article Info

Received: 14 March 2026
Revised: 28 March 2026
Accepted: 29 March 2026
Available online:
31 March 2026

Keywords:

Polyurethane;
Finite element;
Multiscale coupling;
Optimization;
Simulation.

ABSTRACT

Polyurethane (PU) products enjoy remarkable versatility due to their tunable chemistry, segmented structure, and a wide range of mechanical properties, making them useful in flexible foam products, structural systems, and biomedical applications. However, the complex multiphase morphology and the strong interaction between reaction and processing processes make experimental characterization incomprehensible on its own. In turn, computational studies have become essential to study and design PU systems at a range of spatial and temporal scales. The current review provides an overview of simulation methodologies that are relevant to polyurethane, including atomistic molecular dynamics (MD), coarse-grained (CG), and mesoscale simulations, including dissipative particle dynamics (DPD), finite element method (FEM) modeling, and computational fluid dynamics (CFD) simulations. Atomistic models provide data on molecular interactions, hydrogen bonding, and thermomechanical behavior, and CG and mesoscale methods on phase separation and morphological evolution. At the bigger length scale, nonlinear mechanical response can be predicted using FEM, whereas foaming and mold-filling processes can be predicted using CFD that is coupled with reaction kinetics and population balance equations. Its focus is on multiscale modeling strategies, which combine these apparently different approaches, hence allowing the explanation of structure-property-process links. New trends and modern issues, including the integration of machine learning and tool models of digital twins, are also mentioned, highlighting new opportunities in predictive design, based on simulations, of polyurethane materials.

1. Introduction

Polyurethane (PU) is one of the most universal families of polymer which is used in a wide range of applications, including automotive seating and insulation foams, biomedical devices and structural composites. Due to its multi-phase architecture, reaction chemistry and non-linear behavior of mechanical response, computational simulation has served to become an unavoidable supplement to experiment in elucidating, designing and optimization of PU systems. The review is a survey of the major simulation strategies used in polyurethane, based on length and time scale: molecular dynamics (MD), coarse-grained (CG) and mesoscale methods, finite element modelling (FEM), and process-level computational fluid dynamics (CFD) simulations, and more importantly the strategies of multiscale coupling methods that span between these scales. [1-5]

The connectivity of different modeling strategies at length and time scale is demonstrated by a hierarchical multiscale simulation framework of polyurethane materials. On a microscopic scale, quantum chemical computations and atomistic MD reaction captures the formation of bonds, hydrogen bonding and segmental dynamics. The results guide CG and dissipative particle dynamics (DPD) models, which are models of the separation of the microphase and the mesoscale morphology. Foaming, mold filling, and processing dynamics at the macroscopic scale is modelled with CFD with phase-field or population balance equation (PBE), whereas the dynamics of global mechanical behaviour of the system is predicted by FEM simulations. The information enters the system and spreads upwards by transfer of the parameters by-parameter fields, constitutive laws and downwards in terms of boundary conditions and validation and allows an integrated design of materials and processes. Table 1 provides a comparative overview of the main simulation techniques applied to the modeling of polyurethane material, their descriptive length and time scales, strengths and weaknesses. This review is to guide selection of methodology and also to contextualise the multiscale framework addressed in this review.

Table 1. Comparison of simulation approaches for polyurethane materials across length and time scales

Method	Time Scale	Key Strengths	Key Limitations	Typical PU Applications
Atomistic Molecular Dynamics (MD)	ns–µs	High chemical fidelity; captures hydrogen bonding, chain dynamics, diffusion	High computational cost; limited time/length scales	Tg prediction, HB analysis, diffusion, nanocomposites
Coarse-Grained MD (CG)	µs–ms	Larger systems; captures phase separation and morphology	Reduced chemical detail; parameterization complexity	Microphase separation, hysteresis, network formation
Dissipative Particle Dynamics (DPD)	µs–ms	Efficient mesoscale morphology prediction; good for soft matter	Limited molecular specificity; coarse interactions	Domain morphology, shape-memory behavior
Monte Carlo (MC)	Not time-resolved	Efficient equilibrium structure prediction	No real-time dynamics	Phase diagrams, thermodynamic studies
Finite Element Method (FEM)	ms–s	Accurate macroscopic mechanical response; engineering relevance	Requires constitutive models and experimental calibration	Foam mechanics, elastomers, structural behavior
Computational Fluid Dynamics (CFD)	ms–min	Captures flow, heat transfer, and reaction coupling	Highly sensitive to input parameters; complex coupling	Foaming, mold filling, RIM processes
Population Balance Equation (PBE)	ms–min	Predicts bubble size distribution and evolution	Requires coupling with CFD; kernel assumptions	Foam structure prediction
Multiscale Approaches	ns–min	Bridges chemistry to processing; predictive design	Complex implementation; data transfer challenges	Integrated PU design and process optimization

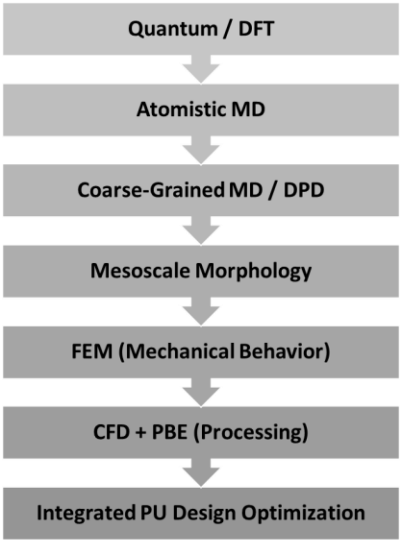

Figure 1. Multiscale simulation framework for polyurethane materials.

2. Atomistic Molecular Dynamics Simulations

Atomistic molecular dynamics (MD) simulation forms the major computational technique that has been used to study the underlying structure-property relationship of polyurethane at the molecular level. In such simulations, explicit models are used to represent individual atoms and their time evolution is modeled by solving Newton equations of movement in the presence of empirical force field terms such as COMPASS, DREIDING or OPLS [6, 7]. One of the main uses of atomistic MD is prediction of thermomechanical properties. E.g. Yeh and Hsieh (2023) used atomistic MD to study HDI-PTMO and MDI-PTMO polyurethane systems and again showed higher glass transition temperatures (T g) in MDI-PTMO, qualitatively in agreement with experimental results. They explained this trend by the fact that more rigid chain structures are available, and differences in hydrogen-bonding interactions occur. In the MDI-PTMO systems, more hydrogen bonds were identified between the amide-hydrogen atom and ether-oxygen atom of PTMO, in contrast to the HDI-PTMO in which more hydrogen bonds were found to be persistent between the carbamate groups. [6, 8, 9]

Talapatra and Datta studied graphene-reinforced thermoplastic polyurethane (Gr/TPU) nanocomposites using the COMPASS force field in Materials Studio, finding that MD simulations could predict glass transition temperature, coefficient of thermal expansion, heat capacity, and thermal conductivity with results in reasonable agreement with experimental values [7]. Their work showed that the incorporation of graphene into the TPU matrix increases the Tg due to stronger interlocking between graphene and TPU molecules, and volumetric coefficient of thermal expansion ranged between 2.6×10-5 and 2.4×10-4 K-1[7]. MD simulations are also used to study stress-strain behavior: Zhang et al. (2012) simulated a shape memory polyurethane (SMPU60) with 60 wt% hard segments, finding the computed Tg of 328 K in good agreement with the DMA-measured value of 316 K, and revealed that hydrogen bond dissociation with increasing temperature leads to decreased moduli [10]. Wang et al. (2022) further showed through MD simulation that the content and strength of hard segments directly govern the viscoelasticity of the PU elastomer, with phase separation between hard and soft segments being the mechanistic origin of these effects. [11-13]

Molecular dynamics has also been applied to study diffusion phenomena within PU matrices. Wang (2013) investigated the diffusion of nitroglycerin (NG) in elastomeric polyurethane via MD with the COMPASS force field, finding that diffusion coefficients are on the order of 10-8 cm2/s in agreement with experiment, and increase with chain flexibility and temperature above 308 K [14]. Pebdani and Miller (2021) used MD to study pull-out of halloysite nanotubes (HNTs) from a PU matrix, employing machine learning particle swarm optimization to parameterize the force field from DFT data and demonstrating that interfacial energy variation can serve as a cohesion strength metric between matrix and nanoparticle [15]. More recently, Pebdani (2022) applied MD to study the Mullins effect in HNT-reinforced PU, showing that residual strain increases with cyclic stretch loading and that increasing hard segment content or HNT volume fraction reduces permanent set. [16-19]

3. Coarse-Grained and Mesoscale Simulations

While atomistic MD captures molecular-level detail, its computational cost limits accessible length and time scales. Coarse-grained (CG) models address this by replacing groups of atoms with single interaction beads, enabling simulation of larger systems and longer timescales[20]. Uddin and Ju (2017) proposed an enhanced coarse-graining method for thermoplastic polyurethane (TPU) using three beads, incorporating pressure-correction to the force field and demonstrating that the resulting CG model captures bulk properties such as density variation with temperature, phase separation, and mechanical moduli, with bulk modulus substantially exceeding shear modulus as expected for elastomers[20]. In related work, Uddin and Ju (2016) used coarse-grained MD to predict the hysteresis of TPU by varying hard segment weight % from 34.90% to 62.30%, correlating hysteresis losses with bulk moduli and Poisson's ratios across different strain amplitudes and loading frequencies. [21]

The MARTINI force field has been applied to polyurethane step-growth polymerization. Ghermezcheshme et al. (2019) developed a fully automated MARTINI-based CG simulation method for cross-linked PU networks, capable of simulating the cross-linking reactions up to very high conversions and under complex conditions such as non-stoichiometric reactant ratios, solvent evaporation, and multi-step reactant addition [22]. They presented a new network-analysis paradigm akin to size exclusion chromatography carried out via graph theory, which observed that a two step addition strategy gives the greatest integrated network structure and that the dangling chains repress the glass-transition temperature in comparison with networks that exclude such chains. Similarly, Wu et al. (2024) performed a study to describe the three-dimensional cross-linked network of foamed polyurethane by using classical molecular dynamics and coarse-grained modeling and graph-theoretical methods. Their results point to the fact that the improved network connectivity leads to the high rate of shorter simple cycles that restrict the deformation and thus, gives a more homogeneous strain field and higher tensile strength of polyurethane closed cells. [23-26]

Mesoscale simulation methods such as dissipative particle dynamics (DPD) have become a formidable method of explaining phaseseparated morphologies in segmented polyurethane (PU). Hu et al. (2016) used DPD simulations in a recent study to define the nanoscale unit-cell morphological architecture of shape-memory polyurethane in which 30 wt% content of hard segment was used (HSC). Their analysis showed that there was a linked-spherical netpoint structure that consisted of diphenylmethane diisocyanate (MDI) hard segments, a matrix-switch phase that was dominated by polycaprolactone (PCL), and an interphase that was connected and spider-like in nature and composed of 1,4-butanediol (BDO). [27]. Park et al. (2024) applied DPD to understand the shape-memory mechanism of TPU, finding that as hard segment content increases, the hard-segment domain transitions from isolated to lamellar to interconnected to continuous, providing critical insights into how microstructure governs macroscopic shape-memory behavior [28]. Vakili et al. (2020) used CG-MD to demonstrate microphase separation between polycarbonate and polyethylene glycol soft segments in segmented PUs, showing a core-shell structure where hard segments are squeezed between two incompatible soft segments. [29-32]

Shape-memory PU nanocomposites have also been investigated by CG-MD. Park et al. (2024) studied the thermo-mechanical behavior of semicrystalline SMPU-silica nanocomposites, revealing that elevated silica content triggers nanoparticle clustering that degrades shape recovery, and that HSC determines matrix-nanoparticle compatibility and nanoparticle agglomeration . [33-36]

4. Reaction Kinetics and Polymerization Simulations

Computational simulation of polyurethane reaction kinetics addresses the complex thermoset polymerization that involves dozens of degrees of freedom. Al-Moameri et al. (2015) developed a computer-based simulation framework for rigid PU foam-forming reactions, comparing predictions against experimental data for six blowing agents including methyl formate and C5-C6 hydrocarbons [37]. The evaporation of blowing agents was modeled as an overall mass transfer coefficient time the activity difference between gas foam cells and resin walls, and successful simulation required this coefficient to decrease to near zero as foam approached its gel point. In subsequent work, Al-Moameri et al. (2017) [38] introduced a viscosity-dependent frequency factor in the Arrhenius equation to account for the increase in viscosity during thermoset polymerization, which can span several orders of magnitude, reducing the number of fitted parameters required and improving the transferability of kinetic models across different polyol systems[38]. The simulation was based on simultaneous solution of over two dozen ordinary differential equations for the many reaction and physical processes occurring during foaming. [39-41]

Al-Moameri et al. [37] explored the effect of maximum foam reaction temperature on decreasing the percentage of shrinkage in rigid polyurethane foams made out of soy based polyols and, as such, demonstrated that simulation is an enabling technology in green chemistry in the polyurethane industry, as it enables the rapid mapping of optimal formulations [42]. A new approach to the simulation of polyurethane foam in the form of a baseline model based on the population balance equation (PBE) was proposed by Karimi and Marchisio (2015), who follows the distribution of bubble sizes (BSD) changes over time as a fundamental determinant of the final thermal and mechanical characteristics. The model predictive results were compared to experimental results based on twelve different chemical formulations, with tolerable concordance found; the next step is to make the PBE a part of a computational fluid dynamics (CFD) program to run the simulations of the mold-filling.[43-45]

5. Finite Element Method (FEM) Simulations

The single most important numerical system used to forecast the macroscopic mechanical behavior of polyurethane (PU) materials is the finite element method (FEM), especially foams and elastomers that possess nonlinear viscoelastic behavior. Petru and Novak (2017) provide a detailed description of FEM-based models of PU foams, but include constitutive relations; rheological models, such as the modified Kelvin model and the Ogden-rubber model; and their implementation into commercial modeling platforms, such as PAM-CRASH, LS-Dyna, Abaqus, and ANSYS. Their model of dynamically compressed PU foam specimens illustrates the high level of correlation with the experimental data, which has a correlation coefficient of 0.961 up to 37.5% deformation, and the FEM method allows visualizing the contact-pressure distributions and internal stresses that cannot be measured directly. [46-48]

Widdle (2017) combined microstructural and continuum approaches for modeling flexible PU seating foam, representing microscopic structural irregularity with Voronoi tessellations and capturing the nonlinear elastic and linear viscoelastic response through a hereditary-type stress decomposition [46]. Mashhadi (2018) developed a multiscale modeling strategy for rigid PU foams using Laguerre tessellation of representative volume elements (RVEs) to capture cell size distributions, anisotropy, cell wall thickness, and strut shape as determined by SEM and X-ray microtomography, finding that elastic modulus and critical stress at the onset of plastic instability are predominantly controlled by relative density, mass fraction in struts and walls, and cell aspect ratio. [49]

For shape memory PU, Liang et al. (2019) used ABAQUS to simulate the thermo-mechanically coupled deformation of SMPU, finding that the forming of localized plastic flow and temperature rise originate from initial defects and propagate outward, with simulated average temperature rise curves in good agreement with infrared thermometer measurements across different loading rates[50]. Sheikhi et al. (2021) evaluated four hyperelastic material models (Mooney-Rivlin, Ogden, neo-Hookean, and Gent) for FEM analysis of PU elastomers, using the Valanis-Landel method to estimate biaxial and shear data from uniaxial tests, and concluded that the Gent model best described uniaxial stress behavior while neo-Hookean performed optimally for pure shear. [14, 51-53]

6. CFD and Process Simulation of Polyurethane Foaming

Computational fluid dynamics (CFD) simulation of the PU foaming and mold-filling process is critical for reducing manufacturing defects and cutting prototyping costs [54]. Geier and Piesche (2014) developed a macro-scale mold-filling simulation tool for PU foams in complex geometries, coupling it with a micro-scale bubble-growth model through tracer particles that record local density, temperature, and flow history along particle trajectories, providing a foundation for predicting the evolution of local foam microstructure [55]. Samkhaniani et al. (2013) implemented a numerical model for PU foam reaction injection molding (RIM) in OpenFOAM, treating the foam as a compressible fluid with a volume-of-fluid (VOF) free-surface tracker and incorporating chemical reaction, heat generation, and blowing agent evaporation, establishing a tool for reducing experimental runs with expensive prototypes. [56]

Seo et al. (2003) developed a finite volume method (FVM) for RIM of polymeric foam, predicting mold filling with variable-density fluid, and found that the expanding foam produces a flatter flow front and more complex particle trajectories compared to constant-density fluids [57]. Karimi et al. (2016) further extended the baseline PBE model into a full 3D CFD framework using OpenFOAM, coupling PBE solved by the quadrature method of moments (QMOM) with a VOF solver, and applied the model to predict apparent density and viscosity, bubble size distributions, and polymerization kinetics during mold filling[43]. Abdessalam et al. (2016) employed the Finite Pointset Method (FPM) for 3D mold-filling simulation of PU foam, using an inverse analysis to identify model parameters from FOAMAT system measurements and validating against short-shot foams from both a panel mold and an automotive underlay carpet cavity.

Population balance modeling was advanced by Ortiz et al. (2021), who coupled a pressure-dependent growth kernel with a 3D CFD arbitrary Lagrangian-Eulerian model to track bubble size distributions during foaming, comparing favorably with experimental data including diffusion wave spectroscopy measurements and post-test SEM analysis [58]. Hershey and Jayaraman (2020) demonstrated through simulation that the lag time introduced during batch mold coating is significant: in molds with complex geometries that force flow bifurcation, different filling lag times predict significantly different weld line locations that cannot be captured by instantaneous-filling assumptions in standard CFD codes. [59-62]

7. Reaction Injection Molding (RIM) Simulation

Simulation of the RIM process for PU requires coupling of reaction kinetics, heat transfer, and rheology. Domine and Gogos (1980) provided one of the earliest comprehensive simulations of non-isothermal, transient reactive flow in RIM molds, investigating the effects of operating, chemical, and rheological variables on process stability and product quality for linear PU systems [63]. Kim and Kim (1987) developed a computer simulation model for RIM of PU-unsaturated polyester blends using reaction kinetics and viscosity models in cylindrical coordinates, demonstrating that feed temperature, wall temperature, and catalyst level significantly affect the maximum exothermic temperature and demolding time [64]. Lee (1980) provided an early and influential review of PU RIM processing, emphasizing that mold filling is governed by the coupled polymerization reactor analysis and melt injection molding dynamics, and that impingement mixing quality is critical to product quality. [63, 65-67]

More recent CFD-based approaches use finite volume methods with more sophisticated constitutive descriptions. Wittemann et al. (2018) proposed a finite volume method for reinforced reactive thermoset injection molding using OpenFOAM, modeling multiphase flow with phase-dependent boundary conditions and incorporating fiber orientation, curing, and viscosity models; the method showed high potential compared to Finite-Element-based approaches and agreed well with experimental pressure data during mold filling [67]. Lee et al. (2002) used a 2D control volume FEM analysis for PU hybrid foam mold-filling, assuming creeping flow and constant viscosity, with theoretical predictions showing good agreement with digital camcorder observations of flow front advancement. [68]

8. Phase Separation and Morphology Studies by Simulation

The unique properties of segmented PU originate from microphase separation between hard segments (HS) and soft segments (SS), forming discrete hard domains dispersed in a soft matrix. Molecular simulation has been used extensively to quantify and understand this phenomenon. Tao et al. (1994) applied a modified Flory-Huggins Monte Carlo method incorporating the orientational contribution of hard segment rigidity to predict phase diagrams of model MDI-PPG polyurethanes, showing that both chain rigidity and thermodynamic incompatibility determine the degree of phase separation [69]. Sahebi Jouibari and Haddadi-Asl (2019) combined MD simulation with spectroscopic, rheological, thermal, and microscopic experiments to study how soft segment molecular weight and molecular architecture influence microphase separation in TPUs, finding that high molecular weight polyether-based TPUs exhibit the highest degree of phase separation and that competition between enthalpic and entropic factors produces different results depending on the analytical method used. [70]

Grujicic et al. (2013) used coarse-grained MD to study shock-wave mitigation in polyurea (PU), attributing its superior ability to attenuate shock waves to shock-induced ordering and crystallization of hard domains and coordinated shuffle-like lateral motion of soft-matrix segments. Zhou et al. (2018) investigated damping property enhancement in TPU/phenolic resin blends through MD simulation, quantifying hydrogen bonds, binding energy, and fractional free volume, finding that at 40% phenolic resin content the system exhibits the largest H-bond number and highest binding energy, which explains the experimentally observed improvement in loss factor and broadening of the effective damping temperature range. [71-74]

9. Nanocomposite Polyurethane Simulations

Simulation of PU-based nanocomposites has become a growing research area as nanofiller reinforcement offers a path to enhanced properties. Pebdani et al. (2023) used MD with DREIDING and Tersoff force fields to study PU-graphene nanocomposites with defective graphene nanosheets, finding that the introduction of defective nanosheets increases Young's modulus to 22.00 MPa and ultimate tensile strength to 71.39 MPa[16]. Talapatra and Datta (2024) performed a comprehensive MD study of Gr/TPU nanocomposites, showing that enhanced mechanical properties depend on graphene concentration, aspect ratio, orientation, and clustering effects, and that interfacial mechanical properties improve with higher aspect ratio due to enlarged surface area[7]. Park et al. (2024) provided a multiscale CG-MD study of semicrystalline SMPU-silica nanocomposites, demonstrating how nanoparticle clustering at elevated silica content degrades shape recovery, and how HSC governs nanoparticle agglomeration and, consequently, the shape-memory performance. [28, 33]

Drug delivery matrices based on PU have also been explored computationally. Campiñez et al. (2017) used a 3D cellular automaton model to simulate drug release from novel PU sustained-release matrices, revealing that even at only 10% w/w excipient concentration, the polymer creates an almost continuous geometric barrier around the drug particles comparable in efficacy to lipid or waxy excipients, a mechanism undetectable without in silico modeling. [66]

10. Multiscale Modeling Approaches

Single-scale simulations are inherently limited—atomistic models cannot reach the length scales of foam cells or the time scales of processing, while continuum models lack molecular detail. Multiscale methods that bridge these scales are therefore highly valued. Mashhadi (2018) developed a multiscale strategy for rigid PU foams that starts from nanoindentation-measured solid PU properties, passes through Laguerre-tessellated RVEs, and delivers macroscopic elastic moduli and critical stresses in compression, capturing the large influence of cell anisotropy on mechanical behavior [49]. Uddin and Ju (2017) proposed a coarse-grained to continuum bridge: by equating potential energy densities of the CG model to strain energy functions at volumetric and isochoric deformation modes, bulk and shear moduli of TPU were directly extracted and used to estimate macroscopic Young's modulus and Poisson's ratio [20]. The coupled macro/micro approach of Geier and Piesche (2014) links CFD mold-filling simulation at the part level with bubble-scale microstructure simulation in representative volumes, providing a path to predict local foam microstructure (and hence local thermal conductivity and impact strength) throughout complex mold geometries. [54, 55]

11. Challenges, Limitations, and Future Directions

Irrespective of the significant progress, there are still enduring issues that are prevalent at all the levels of simulation. At the atomistic level, the mechanism of the dynamic formation of hard domains during reactive polymerization remains a difficult challenge to solve, since molecular dynamics time scales (nanoseconds to microseconds) are orders of magnitude lower than phase separation kinetics [75]. The question of transferability of force fields remains an issue: force fields calculated with one polyurethane chemistry will not necessarily be a good model of other chemistries, and force fields calculated with very polar urethane bonds will have to compromise between electrostatic interactions and chain flexibility [6, 22]. The coarse-grained models are bounded by the cost of chemical specificity, and the process of inverting the model to atomistic resolution is not yet a simple one when trying to predict fine-sensitive properties [20, 21].At the macro scale, polyurethane foam constitutive models would have to support the large strains, viscoelastic model, rate dependence, and densification, which would require a large scale of experimental characterization in order to parameterize it correctly [46]. Mould-filling process-level computational fluid dynamics models are highly sensitive to rheological and kinetic model parameters, the computation of which is an expensive undertaking. [29, 54, 55]

Looking forward, several directions appear most promising. Machine learning interatomic potentials parameterized on quantum chemical data offer a path to more transferable and accurate force fields for PU systems[15]. The combination of DPD morphology predictions with atomistic MD for property extraction provides a practical route to structure-property design of segmented PU at the mesoscale[28, 33]. The continued development of PBE-CFD coupling for foam process simulation, together with more refined bubble nucleation and coalescence kernels, will improve the predictive power for cell size distributions that determine final foam performance [58]. Finally, the integration of digital twin frameworks—in which simulation models are continuously updated by experimental sensor data—represents an emerging opportunity to bring polyurethane simulation from the research environment into industrial process control.

12. Conclusions

Polyurethane simulation spans an exceptionally wide range of length and time scales, from quantum chemical force field parameterization through atomistic MD, coarse-grained and mesoscale modeling, finite element mechanical analysis, to CFD process simulation. Atomistic MD has established quantitative links between PU chemistry (isocyanate type, soft segment molecular weight, hard segment content) and thermomechanical properties, hydrogen bonding, and diffusion. Coarse-grained methods, particularly DPD and MARTINI-based approaches, have illuminated the nanoscale morphology of phase-separated PU and enabled simulation of polymerization up to high conversions. FEM has provided the engineering community with tools to predict nonlinear viscoelastic foam behavior, hyperelastic elastomer response, and shape memory effects under complex loading. CFD-based process simulation, incorporating reaction kinetics, heat transfer, and population balance equations, is increasingly capable of predicting foam expansion, mold filling, bubble size distribution, and density in industrially realistic geometries. Multiscale methods that bridge these domains remain an active frontier, with the ultimate goal of enabling the computational design of PU formulations and processes with predictive confidence across all relevant scales.

Acknowledgements

Authors appreciate the library team of the Materials Engineering Department of University of Duisburg Essen.

Conflict of interest

The authors declare no conflicts of interest concerning this research.

Funding

The authors did not receive support from any organization for the submitted work.

Author Contribution

A.K. Al-Kamal proposed the review, developed the framework, verified the analytical methods.

AI Declaration Statement

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

Abbreviations

Abbreviation	Definition
PU	Polyurethane
TPU	Thermoplastic Polyurethane
SMPU	Shape Memory Polyurethane
MD	Molecular Dynamics
CG	Coarse-Grained
DPD	Dissipative Particle Dynamics
MC	Monte Carlo
FEM	Finite Element Method
CFD	Computational Fluid Dynamics
RIM	Reaction Injection Molding
PBE	Population Balance Equation
QMOM	Quadrature Method of Moments
VOF	Volume of Fluid
FVM	Finite Volume Method
FPM	Finite Pointset Method
RVE	Representative Volume Element
HB	Hydrogen Bonding
Tg	Glass Transition Temperature
HSC	Hard Segment Content
HS	Hard Segment
SS	Soft Segment
DFT	Density Functional Theory

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