

Modelling, Parameterization, and Validation of Simulation Approaches for Deformable Packages in Conveyor-Based Bulk Scenarios

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Deformable packages such as polybags pose significant challenges for sorting and conveyor systems because their motion and contact behaviour are more complex than those of rigid cardboard parcels. This study validates two simulation approaches for such packages in a controlled conveyor-based 2D-bulk obstacle scenario. A detailed shell-based and a simplified volume-based Multi-Flexible Body Dynamics (MFBD) model are compared against 100 repeated experiments involving four representative package types. Validation considers transition time, lateral end position, experimental variability, and spatial occupancy, while a rigid-body multibody simulation (MBS) model and Demo3D are included as contextual references. Across the eight scalar evaluations, both MFBD approaches yielded five good, two acceptable, and one not acceptable median classification. The volume-based model more frequently remained within the experimental interquartile-range envelope and achieved a pooled Earth Mover's Distance of 45 mm, compared with 47 mm for the shell-based model and 46 mm for the rigid-body MBS; Demo3D showed a larger deviation of 85 mm. Computational effort differed substantially, with the shell model requiring approximately one order of magnitude more computation time than the volume model, while the rigid-body MBS was more than two orders of magnitude faster. The results demonstrate that increasing physical model detail does not necessarily improve global logistics-level predictions. For the investigated bulk-level quantities, volume-based MFBD therefore provides a favourable compromise between deformability, validation performance, and computational effort, while shell-based MFBD remains relevant for deformation-specific analyses.

[Keywords: Multi-Flexible Body Dynamics; deformable packages; Polybag; parcel bulk simulation; Demo3D; deformable bodies; conveyor systems]

1 INTRODUCTION

Flexible and non-rigid packages, such as polybags, kraft paper and bubble-wrap bags, are increasingly relevant in

courier, express and parcel (CEP) logistics. In contrast to quasi-rigid cardboard parcels, their geometry and contact conditions vary more during transport than those of quasi-rigid cardboard parcels. Deformation, local folding (non-linear deformation), variable friction and package-package interactions lead to motion behaviour that is difficult to predict and challenging for conveyor and sorting systems designed for geometrically stable parcels.

Physics-based simulation is an established tool for the design and evaluation of material handling systems, because it enables systematic investigations of geometries, operating points and initial conditions without extensive physical prototyping [1]–[5]. However, most established parcel-bulk simulation approaches rely on rigid-body, Discrete Element Method (DEM)-based or macroscopic flow representations and therefore simplify or neglect package deformation [6]–[9].

Multi-Flexible Body Dynamics (MFBD), which combines multibody dynamics (MBD) with finite element method (FEM) formulations, provides a physically richer modelling approach for deformable packages [10], [11]. Previous studies have shown that MFBD models can reproduce relevant deformation and motion effects of individual deformable packages and can be parameterized using targeted real-world tests [12]–[14]. However, validation has so far mainly focused on individual packages.

Deformation makes package motion highly path-dependent: small differences in initial shape or local contact conditions can alter the contact topology and lead to qualitatively different passage outcomes, rather than merely causing small quantitative changes in an otherwise unchanged trajectory. Following an inductive model-building strategy, the present four-package obstacle scenario is therefore treated as a controlled minimal model rather than as a direct representation of an industrial 3D parcel bulk [2]. Following Fritz [6], a 2D-bulk state is reached when all packages lie on the conveyor plane and their projections onto this plane no longer overlap. The present scenario is initialized according to this condition. However, temporary overlap, lifting, or local stacking may occur during obstacle

passage. This setup preserves package-level observability while introducing controlled package–package and package–obstacle interactions relevant to bulk handling and singulation. It therefore provides an intermediate validation step between isolated-package experiments and future denser 2D- and 3D-bulk scenarios. On this basis, the present paper addresses this requirement by validating two MFBD modelling approaches in a controlled conveyor-based 2D-bulk scenario. A detailed shell-element model is compared with a simplified volume-element model. Both models are initialized using the same trial-specific measured initial conditions and evaluated against repeated obstacle-passage experiments with four deformable package types. The comparison uses transition time, lateral end position and occupancy heatmaps, complemented by numerical stability and computation time.

The contribution of this paper is threefold. First, it transfers MFBD validation from isolated packages to a repeated, contact-rich 2D-bulk scenario. Second, it compares shell- and volume-based MFBD models under identical experimental boundary conditions. Third, it applies a variance-aware validation perspective in which simulation quality is assessed not only through agreement in the central tendencies of scalar key performance indicators (KPIs), but also through experimental spread and spatial occupancy patterns.

The study addresses the following research questions:

- RQ1: How accurately do shell- and volume-based MFBD models reproduce experimentally observed transition times and lateral end positions?
- RQ2: To what extent do the models reproduce spatial occupancy patterns observed in repeated real-world tests?
- RQ3: What trade-off between physical model detail, validation performance, and computational scalability results from simplifying the shell-based MFBD representation to a volume-based model?

2 RELATED WORK AND RESEARCH GAP

2.1 SIMULATION OF PARCEL BULK BEHAVIOUR

Previous work on parcel bulk simulation has investigated the motion of piece goods in bulk, singulation and transfer processes using rigid-body, DEM-based or macroscopic flow approaches. Fritz [6] analysed the movement behaviour of piece goods in bulk in the context of singulation using multibody simulation. Prims and Katterfeld [9] and Kaefer [7] applied DEM to parcel-bulk handling, representing parcels as rigid bodies through sphere conglomerates or superquadric shapes. These representations approximate parcel geometry and bulk-contact behaviour but do

not resolve packaging deformation or relative motion between packaging and content. Prims et al. [8] investigated macroscopic flow models as an efficient simulation approach for parcel handling in bulk mode. Active conveying concepts, such as peristaltic parcel transport, have also been investigated using DEM and multibody simulation [15].

For deformable packages, these assumptions are often insufficient. The package may fold, compress, bend or locally stick to surrounding objects. Therefore, the relevant validation target is not only a single object trajectory, but the resulting distribution of transport outcomes under repeated nominally identical conditions.

2.2 DEFORMABLE-PACKAGE SIMULATION APPROACHES

Leitner et al. [13] introduced MFBD models for form-unstable small packages and demonstrated the feasibility of shell-based package representations. MFBD couples flexible finite-element bodies with multibody dynamics and therefore provides a physics-rich modelling framework for representing deformation and contact-driven motion [10], [11]. For contact-rich conveyor scenarios, robust contact modelling is essential, especially when deformable packages interact with obstacles, conveyor surfaces or other packages [16]. The approach was later extended to representative real packages using bottom-up modelling of packaging and content and parameterization based on targeted real-world tests [12]. Stadlthanner et al. [14] further validated MFBD models against independent single-package experiments.

In parallel, faster deformable-body simulation approaches are gaining relevance. Position-Based Dynamics, GPU-accelerated FEM and real-time physics engines such as Isaac Sim / PhysX are attractive for bulk-scale studies, design-of-experiments and digital-twin-oriented applications [17]–[20]. Related work in robotics also uses physics-based and real-to-sim modelling for deformable packages in manipulation tasks [21].

Further approaches to modelling deformable bodies include bonded-particle DEM and lumped-mass models. While these approaches are capable of representing deformable bodies in principle, limitations remain in terms of exterior contact geometry, which is still based on discrete particle proxies. The resulting surface discretisation can introduce artificial roughness and mechanical interlocking during contact. MFBD also employs a discretised contact surface, but its faceted finite-element mesh provides a more continuous representation of the package boundary, although this representation remains dependent on mesh resolution [22].

Building on these developments, Leitner et al. [22] proposed a KPI-oriented multi-fidelity framework in which

MFBD serves as the high-fidelity reference and faster deformable-body models, such as PBD cloth or GPU-FEM, serve as low-fidelity candidates. High fidelity denotes a comparatively detailed representation of package deformation, packaging-content interaction, and frictional contact relative to the investigated simplified alternatives. It does not imply the exact reproduction of every physical quantity.

2.3 RESEARCH GAP

The reviewed literature reveals three limitations. First, established parcel-bulk simulation approaches mainly rely on rigid-body, rigid-particle DEM, or macroscopic flow representations and therefore do not resolve deformation effects of flexible packages. Second, existing MFBD models for deformable packages have mainly been validated in individual-package or otherwise simplified scenarios. Third, the benefit of increasing the physical modelling detail of deformable-package simulations has not yet been established for repeated bulk scenarios. In particular, it remains unclear whether representing additional deformation, packaging-content interaction, and contact effects leads to measurably better agreement with experiments, or primarily increases numerical complexity and computational cost.

What remains insufficiently addressed is therefore the validation of deformable-package models with different levels of physical detail in repeated, contact-rich bulk-conveyor scenarios. The present study addresses this gap by comparing two deformable modelling approaches implemented in RecurDyn: a detailed shell-based MFBD model

and a simplified volume-based MFBD model. Both are evaluated against repeated obstacle-passage experiments in a controlled 2D-bulk scenario using transition time, lateral end position, occupancy heatmaps, numerical stability, and computation time.

For context, two rigid-body reference implementations are additionally included: a multibody dynamics model implemented in RecurDyn, representing established scientific parcel-bulk modelling practice, and a material-flow model implemented in Demo3D, representing common industrial simulation practice.

3 MATERIALS AND METHODS

The study follows a comparative validation design comprising two primary deformable models and two contextual rigid-body references. The primary comparison concerns a shell-based and a volume-based MFBD implementation, both developed in RecurDyn and evaluated against the repeated experimental reference dataset. The contextual references comprise a rigid-body multibody dynamics implementation in RecurDyn and a rigid-body material-flow implementation in Demo3D.

The two MFBD models were parameterized using the targeted deformation and contact experiments described below. The rigid-body reference implementations were not subjected to the deformation- and material-specific parameterization applied to the MFBD models; experimentally determined contact and friction inputs were transferred

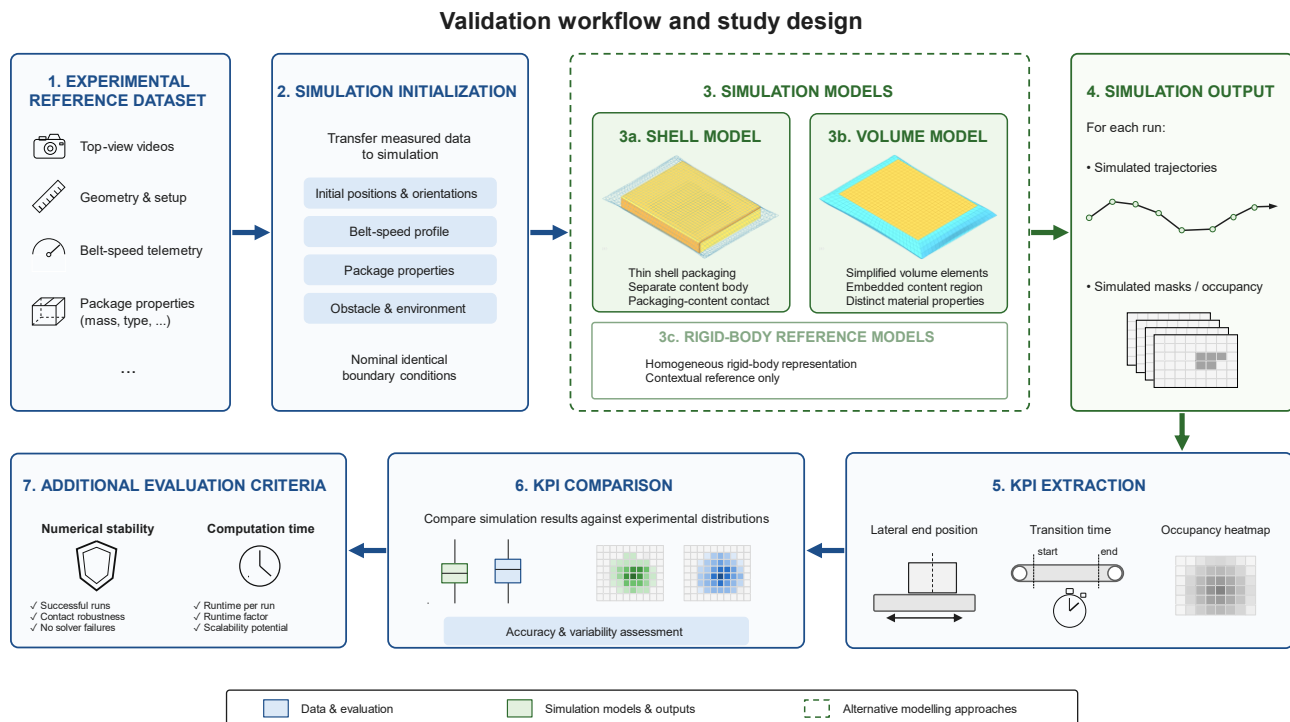


Figure 1. Validation workflow and study design.

where applicable. They are therefore interpreted as contextual baselines rather than as equivalently parameterized competitors and are not used for an absolute ranking of the modelling approaches.

3.1 VALIDATION WORKFLOW AND STUDY DESIGN

The validation workflow is shown in Figure 1. The experimental reference dataset provides measured initial conditions, belt-speed data and validation KPIs. These data are transferred into the simulation environment and used to initialize corresponding shell- and volume-based MFB simulations. The resulting simulated package motion is then evaluated against the experimental distributions of transition time, lateral end position and occupancy. Numerical stability and computation time are assessed as additional model-selection criteria.

3.2 EXPERIMENTAL REFERENCE DATASET

The experimental reference dataset was obtained from a controlled 2D-bulk obstacle-passage experiment. The test rig consisted of a 3.0 m long and 1.5 m wide belt conveyor with a cylindrical obstacle mounted centrally above the belt surface. A gap of 2 mm was maintained between the obstacle and the belt. During each trial, the belt was accelerated from rest to approximately 1.3 m/s before the packages reached the obstacle. The trial-specific belt-speed profile was recorded through the motor-controller telemetry. The scenario was selected to isolate deformation- and contact-driven interaction mechanisms under controlled and observable conditions.

Four representative deformable package types were investigated: kraft paper with bubble wrap (KP/BW), polybag (PB), kraft paper (KP) and bubble wrap (BW), as shown in Figure 2. The package types were derived from representative mixed-mail consignment classes [12], [23].



Figure 2. Deformable packages used in the study [12]

Figure 3 illustrates a representative passage of the four packages at three time points. The scenario induces package-package and package-obstacle contacts, deformation, lateral diversion, and temporary stagnation while retaining top-view observability of the individual packages.

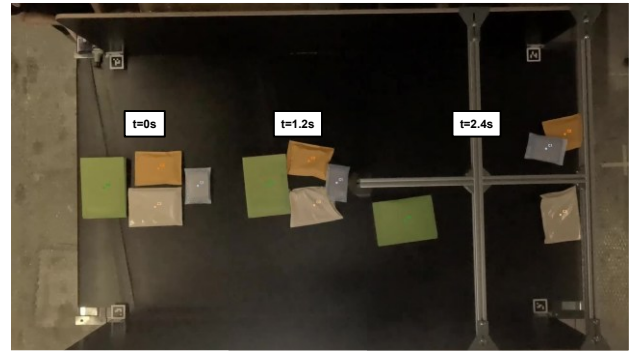


Figure 3. Representative obstacle-passage trial at $t=0$, 1.2, and 2.4 s. The four deformable packages are transported from left to right and interact with each other and with the centrally mounted cylindrical obstacle [22].

In total, 100 trials were conducted using ten independently prepared specimen sets. Each set contained one specimen of each of the four package types and was subjected to ten consecutive repetitions under nominally identical conditions. After the tenth repetition, the packaging of all four packages was fully replaced with previously unused packaging material, and a new specimen set was prepared using the same prescribed package contents.

This repeated design provides distributions of passage outcomes rather than a single deterministic reference trajectory. The present study uses the complete set of repeated trials as the experimental reference for simulation validation. A detailed statistical attribution of the observed variability to initial placement, belt operation, trial order, and specimen-set differences is outside the scope of the present paper.

The experiments were recorded using a downward-facing top-view camera at 60 frames per second. The moving packages were segmented and tracked using the SAM 2 video-segmentation model [24]. The resulting image-space masks were transformed into conveyor-fixed metric coordinates using a planar homography defined by stationary reference AprilTags, following the image-to-world mapping principle applied by Stadlthanner et al. [14]. Unlike the earlier marker-based application, no tags were attached to the moving packages. For each world-aligned package mask, the package centre was approximated by the centre of its minimum-area rotated bounding box.

Figure 4 summarizes the derivation of the three experimental validation quantities used in this study. The centre trajectories in Figure 4(a) are expressed in conveyor-fixed coordinates. Transition time is defined as the elapsed time between $x = -640$ mm and $x = 460$ mm. These limits capture the principal obstacle-interaction region while excluding most of the upstream initialization and downstream transport. The lateral end position is defined as the lateral coordinate of the package centre at the downstream evaluation line.

In addition to these scalar trajectory quantities, package-specific occupancy heatmaps were generated by accumulating the world-aligned binary package masks from all frames in which the corresponding package centre was located between the two evaluation limits. The occupancy value at each spatial location represents the proportion of included frames in which that location was occupied by the respective package mask.

Figure 4(b) illustrates this representation for BW in one representative experimental trial. For the subsequent validation analysis, aggregate experimental heatmaps were generated separately for BW, KP/BW, PB, and KP using the corresponding package masks from all 100 trials. Thus, each package-specific experimental heatmap represents 100 package passages, corresponding to 400 individual package passages across all four package types.

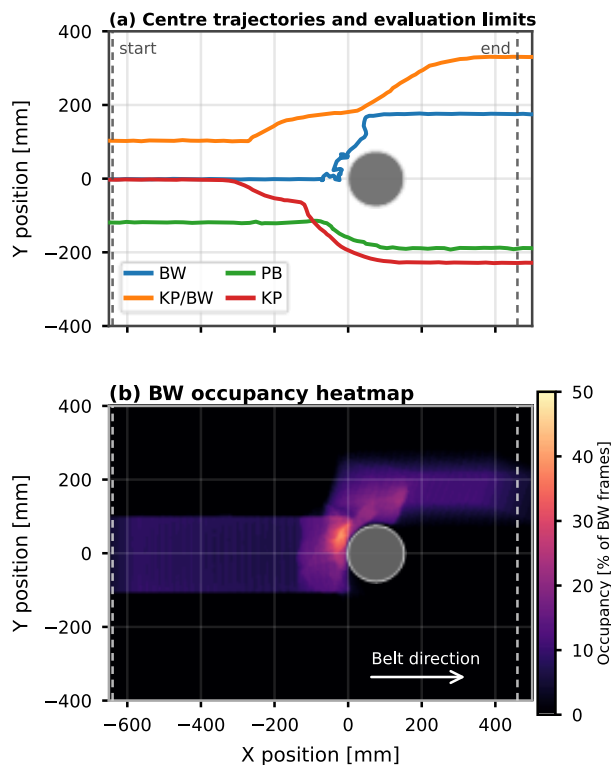


Figure 4. Extraction of the experimental validation quantities for one representative obstacle-passage trial. (a) Centre trajectories of the four deformable packages and the upstream and downstream evaluation limits at $x = -640$ mm and $x = 460$ mm. Transition time is determined between these limits, while lateral end position is evaluated when the package centre crosses the downstream limit. (b) Corresponding occupancy heatmap for BW, expressed as the percentage of included BW frames in which each spatial location was occupied by the world-aligned package mask. The grey circle represents the cylindrical obstacle, and the belt moves from left to right.

In contrast to the centre trajectories, the occupancy heatmaps retain the projected package extent and temporal

residence distribution. They therefore represent occupied transport corridors, lateral spread, and regions of prolonged obstacle interaction that are not captured by the centre trajectories alone.

The experimental transition times, lateral end positions, and occupancy heatmaps are used as the reference quantities for the subsequent simulation comparison.

3.3 SIMULATION-EXPERIMENT ALIGNMENT

Each simulation run is aligned with a corresponding real-world trial. The simulation uses the measured initial position of the respective package configuration, the recorded belt-speed profile, and the same obstacle geometry as the experiment. The recorded belt-speed profile is represented by spline interpolation and implemented as a time-dependent conveyor-motion input. In the simulation, this input drives a translational joint that moves a cuboid representing the conveyor-belt surface. Package masses are assigned according to the measured properties.

3.4 SIMULATION MODELS

Both deformable simulation approaches are implemented as MFBF models. MFBF couples flexible finite-element bodies with multibody dynamics and is therefore suitable for representing deformation and contact-rich motion of flexible packages [10], [11]. The contact formulation follows the compliant contact approach for bodies with complex geometry described by Choi et al. [16].

All RecurDyn-based implementations were developed in RecurDyn 2025. The MFBF formulation combines multibody dynamics with an incremental finite-element formulation based on a corotational procedure, allowing the gross translation and rotation of the finite elements to be separated from their deformation [10]. The deformable regions were assigned linear-elastic material behaviour.

Contact between packages, packaging and content, the conveyor belt, and the obstacle was represented using a compliant contact-force formulation acting on faceted contact surfaces. All RecurDyn implementations used the same velocity-dependent Coulomb-friction formulation, including static and dynamic coefficients and a smoothed transition with relative sliding velocity. The underlying MFBF, normal-contact, and friction formulations have been described previously and are therefore not repeated here [14], [16]. All RecurDyn simulations were performed using the same solver configuration, with an error tolerance of $8 \cdot 10^{-5}$ and four CPU cores.

3.4.1 SHELL-ELEMENT MODEL

The shell-based model represents the packaging as a thin flexible structure and the content as a separate rigid or flexible body, depending on the package type (Figure 5).

The packaging was discretized using four-node quadrilateral shell elements with bilinear shape functions and connected along their boundary nodes. Explicit packaging-content contact allows relative motion and local changes in the package shape. The rigid contents of KP/BW, KP, and BW are represented by rounded cuboids with package-specific geometry and mass, whereas the flexible content of PB is represented using volume elements [12], [14].

The shell models were developed using the bottom-up modelling workflow described in previous work, in which packaging and content are first modelled separately and subsequently assembled through contact [12]. The previously parameterized package models were retained for the present study; only the package-package contacts and the alignment with the bulk-conveyor scenario were added.

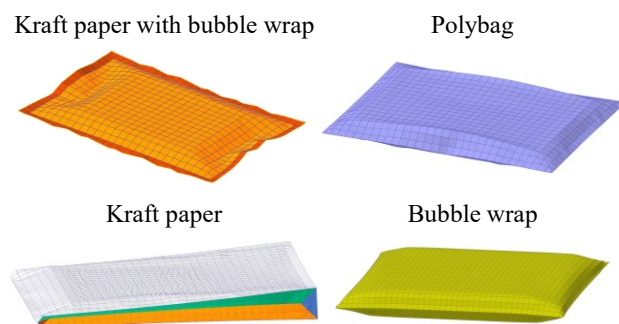


Figure 5. Shell-based MFBD models of the four deformable package types [12].

3.4.2 VOLUME-ELEMENT MODEL

The volume-element model is introduced as a simplified MFBD alternative. Its purpose is to reduce modelling complexity and computation time while preserving the main transport-relevant deformation characteristics. In contrast to the shell model, the package is represented by a simplified volumetric body with assigned material properties for packaging and content regions.

The FEM volume models were generated using a workflow based on the external geometry of the real-world packages, with the surface of the shell model serving as a reference. The general modelling workflow is illustrated in Figure 6 using the bubble-wrap package as a representative example. In the CAD modelling stage, only a one-eighth section of the geometrically non-trivial outer structure was created. This section was then imported and discretized, while the complete outer geometry was reconstructed by mirroring it across the symmetry planes. To represent the enclosed content, an additional cuboid volume was introduced. Finally, all parts were merged to obtain the final FEM volume model. Different material properties were assigned to the outer part (light blue) representing the packaging and to the inner volume (purple) representing the content. The same procedure was applied to all investigated packages with individual geometry-specific adaptations.

The resulting FEM volume models for all four real-world packages are shown in Figure 7.

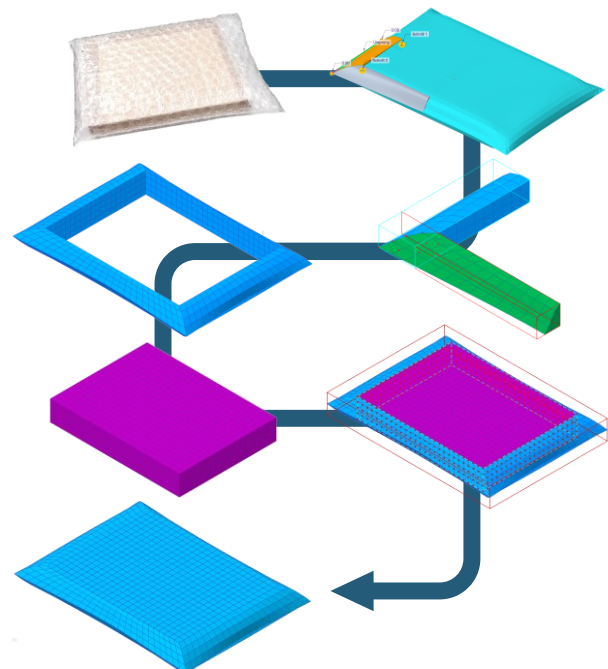


Figure 6. Modelling workflow for the volume-based MFBD representation, illustrated for the bubble-wrap package.

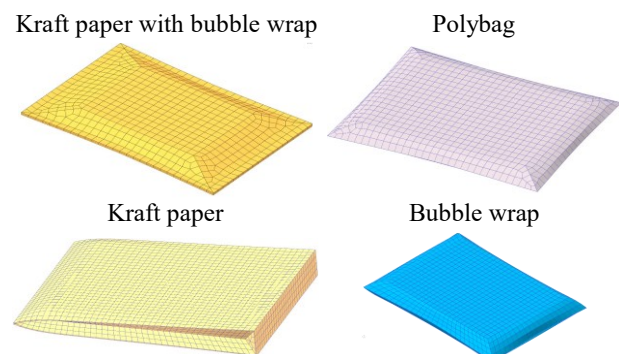


Figure 7. Volume-based MFBD models of the four deformable package types.

The volume-element model is expected to reduce computational effort and improve scalability. However, local folding and detailed interaction between packaging and content are represented less explicitly than in the shell-element model.

3.4.3 RIGID-BODY REFERENCE MODELS

Two homogeneous rigid-body implementations were included as contextual reference models. Both used the same CAD geometries as the corresponding volume-based MFBD models. However, the contact surfaces were faceted independently in the respective simulation environments, resulting in different triangular surface discretizations.

The rigid-body model in RecurDyn was implemented as a representation of the scientific lineage of earlier parcel-bulk simulations based on multibody dynamics. Fritz et al. [25], for example, simulated parcel bulks using homogeneous rigid package representations in MSC ADAMS. The present model transfers this general modelling principle, but does not reproduce the original implementation. It uses the same package geometries, masses, initial conditions, conveyor input, contact parameters, and friction formulation as the corresponding volume-based MFBFD model. The main difference is the omission of package deformation and a separate representation of packaging and content.

The second reference model was implemented in Demo3D, which is commonly applied to the modelling, simulation, and emulation of material-handling systems [26], [27]. The simulation used the PhysX physics engine with a fixed physics time step of 0.01 s. The implemented friction model assigns a single Coulomb friction coefficient to each material pairing. Because separate static and dynamic coefficients, as used in the RecurDyn models, were not available, the experimentally determined static coefficient was assigned to each material pair.

3.5 PARAMETERIZATION STRATEGY

The parameterization follows the methodology developed in previous work on modelling flexible packages [12], [19]. Simple real-world tests are used to determine material and contact parameters. The parameterization is not

repeated at the level of the full obstacle scenario. Instead, simplified tests are used to obtain physically interpretable parameter values that can be transferred to the validation scenario.

3.5.1 MATERIAL AND CONTACT PARAMETERS

The material and contact parameterization was based on compression under self-weight, vertical-orientation drop tests, horizontal-orientation drop tests, and overhang tests. The terms vertical and horizontal refer to the initial package orientation—the drop direction is vertical in both configurations. The tests isolate characteristic compression, rebound, bending, and relaxation responses while remaining more reproducible than the complete conveyor scenario. Not every test was required for every package type; the selected tests depended on the dominant deformation and contact behaviour of the respective package.

Figure 8 summarizes the four parameterization tests. Panel (a) characterizes quasi-static compression and relaxation under self-weight. In panel (b), the package is dropped in a vertical orientation onto a narrow side. The packaging between the content and the impact surface can therefore fold and compress before the content approaches the surface. Maximum compression and, where present, rebound consequently provide target values primarily associated with packaging stiffness and damping. In panel (c), the package is dropped in a horizontal orientation onto its

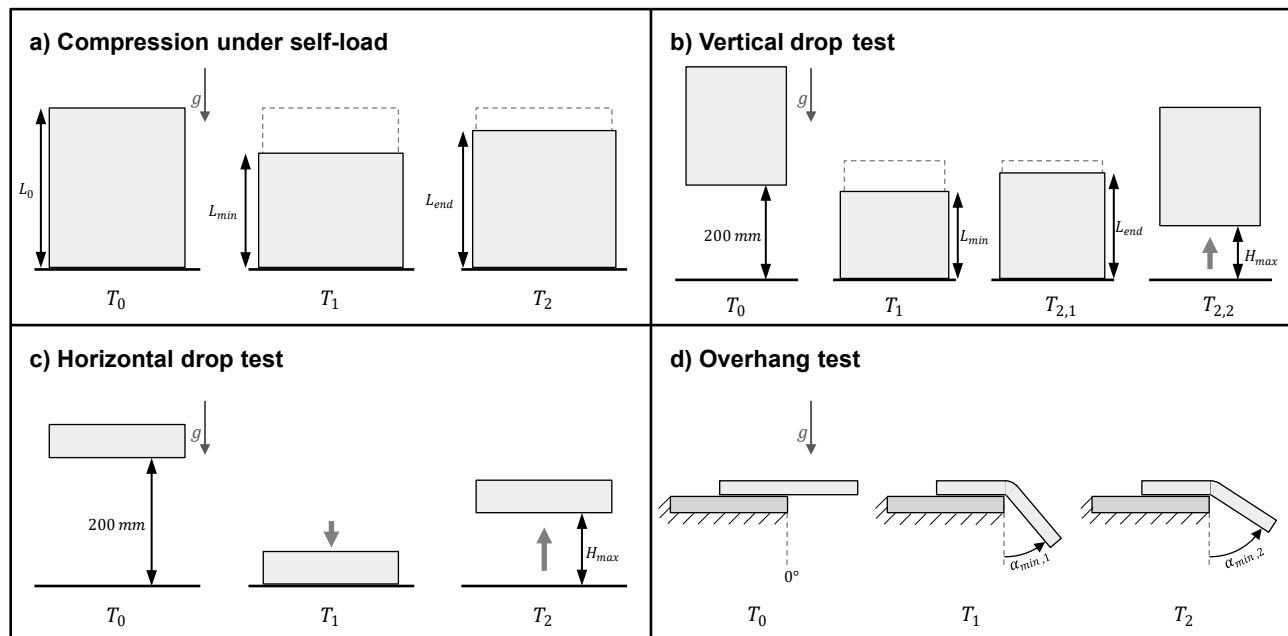


Figure 8. Schematic definition of the parameterization tests and extracted target values. (a) Compression under self-load: T_0 denotes the initial state with length L_0 , T_1 the state of maximum compression with length L_{min} , and T_2 the relaxed state with length L_{end} . (b) Vertical drop test from 200 mm: T_0 denotes the initial drop position, T_1 the state of maximum compression at impact with length L_{min} , $T_{2,1}$ the relaxed post-impact state with length L_{end} , and $T_{2,2}$ the alternative rebound state with rebound height H_{max} . (c) Horizontal drop test from 200 mm: T_0 denotes the initial state before impact, T_1 the impact state, and T_2 the rebound state with rebound height H_{max} . (d) Overhang test: T_0 denotes the initial undeformed state, T_1 the first maximum deflection characterized by $\alpha_{min,1}$, and T_2 the second maximum deflection characterized by $\alpha_{min,2}$.

broad side. Because the content is located close to the impacted packaging surface, only limited global deformation of the packaging occurs. Maximum compression is therefore not used as a target; instead, the rebound response primarily informs the stiffness and damping of the external contact formulation. Panel (d) shows the overhang test used to characterize bending stiffness and relaxation behaviour.

Figure 9 illustrates the parameterization procedure for the kraft-paper package KP. The real-world specimen, shell-element model and volume-element model are compared at the characteristic states T_0 , T_1 and T_2 . This example shows how the target values are extracted consistently from experiment and simulation. The same principle was applied to the other tests and package types, while the full optimization workflow is described in the referenced previous studies.

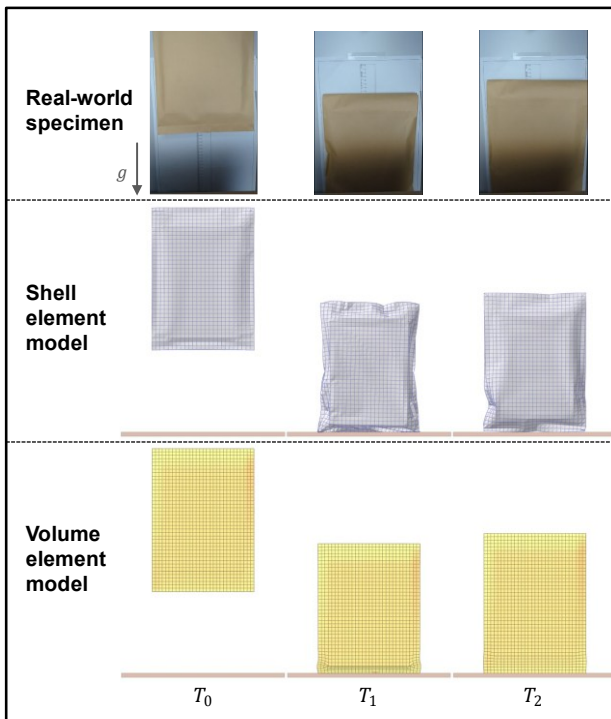


Figure 9. Exemplary parameterization test for the kraft-paper package KP. The vertical-orientation drop test is shown for the real-world specimen, the shell-element model and the volume-element model at the characteristic states T_0 , T_1 and T_2 .

3.5.2 FRICTION COEFFICIENTS

In addition to the material and contact parameters obtained from the compression, drop, and overhang tests, material-pair-specific static and dynamic friction coefficients were determined. In the RecurDyn models, friction was represented using a velocity-dependent Coulomb formulation in which the transition between static and dynamic friction was smoothed as a function of relative slip velocity to improve numerical robustness [2], [28], [29].

Figure 10 summarizes the two friction-test methods. Static coefficients μ_0 for package-package and package-obstacle contacts were determined using inclined-plane tests. The lower contact partner was fixed to the platform, which was tilted quasi-statically until sliding began. The coefficient was derived from the critical angle φ_0 . Because the result depends on both tilt velocity and detection of the onset of sliding, the inclination was increased smoothly and slowly [30]. This method was preferred for μ_0 because it avoided extracting a short breakaway-force maximum from a pulling-force signal.

Dynamic coefficients μ_d were determined using load-cell pulling tests. The package was pulled at approximately constant velocity, and the mean force F_d during steady sliding was evaluated, following the horizontal-plane friction-measurement principle described in TAPPI/ANSI T 549 om-20 [31]. Since complete packages and package-specific contact partners were tested, the procedure was based on the standard's measurement principle rather than performed in full accordance with it.

For package-belt contacts, both coefficients were measured directly on the installed belt. The force maximum F_{peak} was used for the static belt coefficient, while the mean steady-sliding force F_d was used for the dynamic coefficient. Each material pairing was tested five times, and the mean value was assigned as the simulation input.

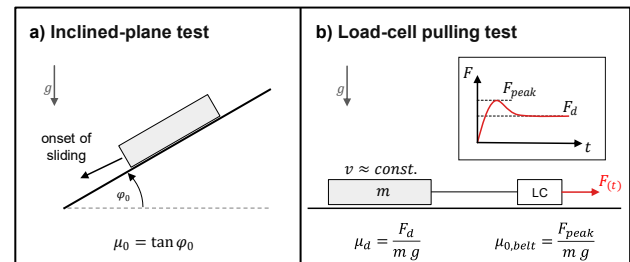


Figure 10. Experimental methods for determining friction coefficients. (a) Inclined-plane test for determining the static friction coefficient μ_0 from the critical inclination angle φ_0 at the onset of sliding. (b) Load-cell pulling test for determining the dynamic friction coefficient μ_d from the mean force F_d during approximately steady sliding. For package-belt contacts, the maximum force F_{peak} was used to determine the static coefficient $\mu_{0,belt}$ directly on the installed belt.

3.6 VALIDATION METRICS AND COMPARISON PROCEDURE

The validation uses three primary KPI groups and two additional simulation criteria. The primary KPIs are transition time, lateral end position and occupancy heatmaps. The additional criteria are numerical stability and computation time.

Transition time and lateral end position are compared based on their median and interquartile range (IQR). For

the lateral KPI, quantitative agreement is assessed based on the absolute distance from the belt centreline $|y_{\text{end}}|$. Median deviations within $\pm 10\%$ of the experimental value are classified as good, deviations between $\pm 10\%$ and $\pm 25\%$ as acceptable, and deviations above $\pm 25\%$ as not acceptable. Variability is assessed using the simulation-to-experiment IQR ratio. Ratios below 25% are interpreted as a low-IQR limitation, indicating limited model sensitivity to the experimentally observed variability. Ratios between 25% and 100% indicate variability within the experimental envelope, whereas ratios above 100% indicate variability above the experimental envelope.

For occupancy heatmaps, experimental and simulated mask overlays are normalized and compared spatially. The comparison assesses whether the simulations reproduce the relevant transport corridors, stagnation zones, and lateral spread observed in the experiments. Spatial agreement is quantified using the two-dimensional Earth Mover's Distance (EMD), equivalent to the first Wasserstein distance for the normalized discrete distributions used here. EMD is well suited for comparing image-like distributions because it measures the minimum transport effort required to transform one spatial distribution into another [32]. The interpretation follows the optimal-transport formulation described by Peyré and Cuturi [33].

For the EMD calculation, heatmaps are cropped to the common transition domain. The cropped heatmaps are normalized to unit mass so that the comparison reflects spatial distribution rather than the number of frames. Native 5 mm pixels are pooled into 25 mm bins, and the transport cost is defined as the Euclidean distance between bin centres. Consequently, EMD has units of length and is reported in millimetres, with lower values indicating closer spatial agreement. The discrete two-dimensional transport calculation was performed using OpenCV's *cv2.EMD* implementation [34], while directional marginal distances were calculated using SciPy's weighted one-dimensional Wasserstein distance implementation [35].

Numerical stability is evaluated separately from physical agreement. A simulation run is classified as numerically stable if the solver completes without divergence, crash, or abnormal termination. Contact-detection artefacts are classified as model-robustness issues rather than solver failures if the solver remains stable but the resulting contact state is physically implausible. All completed simulation runs are retained in the KPI evaluation, including runs with such contact artefacts, to avoid post-hoc exclusion and preserve an objective comparison between the modelling approaches.

Computation time is analysed as an indicative operational cost measure rather than as a controlled hardware benchmark. The simulations were not executed under standardized benchmarking conditions, because different workstations were used, several simulations were executed

in parallel, and additional background simulations may have influenced the elapsed times. Therefore, the reported runtimes indicate only the order of magnitude and relative practical feasibility of the model classes, not exact speed-up factors. Computational scalability with increasing package number is additionally assessed for the RecurDyn-based modelling approaches using 1, 4, 10, and 25 identical PB packages over 3 s of simulated physical time.

4 RESULTS

This section compares the experimental reference data with the investigated simulation models. Figure 11 provides a qualitative illustration of the deformability observed in the experiment and reproduced by the two MFBD formulations. A representative obstacle-passage run is shown at selected time instances for the experiment, shell-based MFBD model, and volume-based MFBD model. The figure is intended to illustrate package deformation and interaction with the obstacle rather than to compare all investigated simulation approaches.



Figure 11. Representative obstacle-passage sequence comparing the experiment with the shell- and volume-based MFBD models at selected time instances.

The quantitative comparison is then structured according to the validation criteria defined in Section 3.6. Section 4.1 reports transition time and lateral end position using distribution plots and aggregated classification counts. Section 4.2 evaluates spatial agreement using occupancy heatmaps, two-dimensional Earth Mover's Distance values and directional Wasserstein diagnostics. Section 4.3 reports numerical stability and indicative computation time.

4.1 TRANSITION TIME AND LATERAL END POSITION

Figure 12 shows distinct model- and package-specific differences. For transition time, the shell-based MFBD model remains within $\pm 18\%$ of the experimental median for all four package types, with deviations below 8% for KP/BW, PB, and KP. The volume-based MFBD model similarly agrees within $\pm 10\%$ for these three package types, but overpredicts the BW median by approximately 50%. The rigid-body MBS reproduces BW and PB closely but deviates by -12% for KP/BW and $+40\%$ for KP. Demo3D shows the largest transition-time deviations for KP/BW ($+56\%$) and PB ($+36\%$), while agreement is closer for BW ($+23\%$) and KP (-5%).

For lateral position, the volume-based MFBD model reproduces the experimental distance from the belt centre-line $|y_{\text{end}}|$, within 22% for all four package types. The shell-based MFBD model agrees closely for KP/BW and KP, but underpredicts the BW centrality by approximately 50%. The rigid-body MBS shows its largest deviation for PB ($+46\%$), whereas Demo3D deviates strongly for KP/BW ($+72\%$) and PB ($+75\%$). The signed distributions in Figure 12 additionally show that several models reproduce the lateral distance while selecting the opposite side of the obstacle.

The variability comparison further separates the two MFBD approaches. The shell-based MFBD model exceeds the experimental IQR envelope in four of eight evaluations, particularly for the lateral distributions of BW and PB. In contrast, the volume-based MFBD model remains within the experimental envelope in five evaluations, with two low-IQR cases and only one above-envelope case. The rigid-body MBS shows both low and strongly increased variability (2 / 3 / 3), while Demo3D exceeds the experimental envelope in four evaluations. Table 1 summarizes these median and IQR classifications across all eight package-specific KPI evaluations.

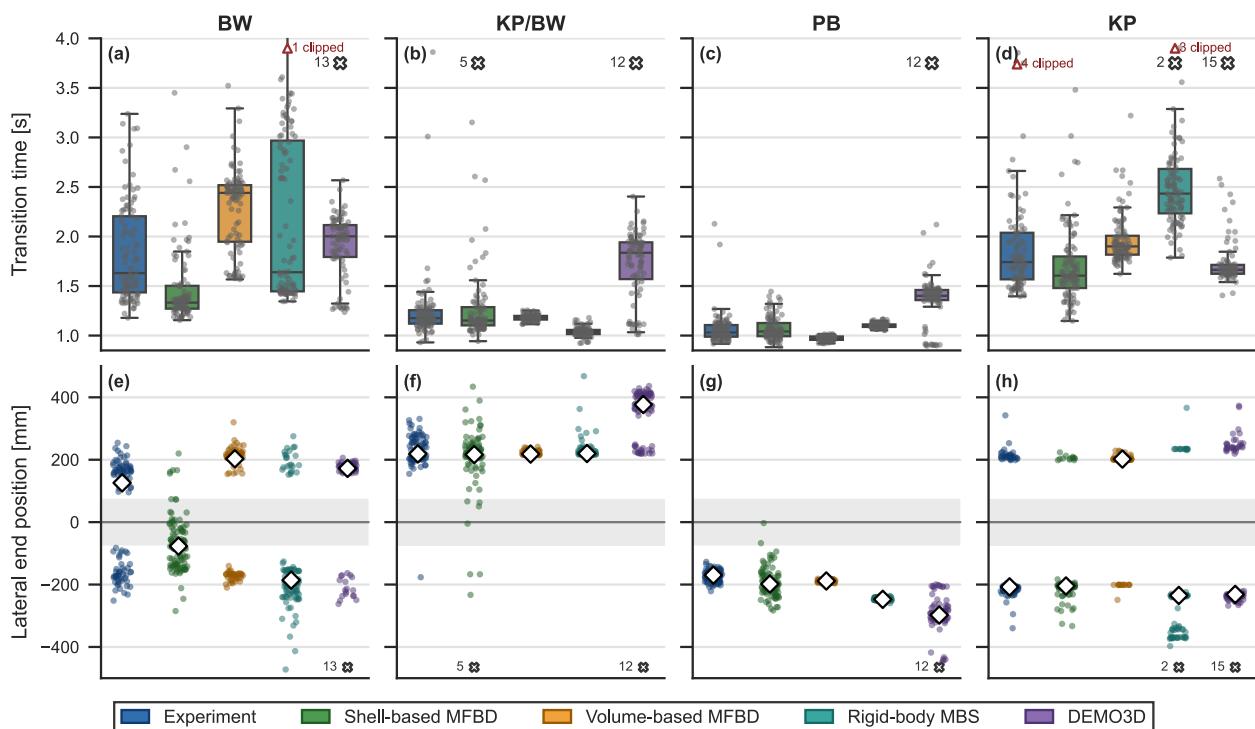


Figure 12. Experimental and simulated distributions of transition time and lateral end position for BW, KP/BW, PB, and KP. Upper panels show transition time and lower panels the signed lateral end position. Individual points represent single runs and boxplots summarize the corresponding distributions. Positive and negative lateral positions indicate passage on opposite sides of the obstacle. Counts at the panel boundaries indicate observations that could not be represented as regular data points because the transition-time plotting limit was exceeded or the respective KPI was unavailable.

Table 1. Summary of scalar KPI validation classifications across eight package-specific evaluations per model. *G* = good, *A* = acceptable, *NA* = not acceptable; *IQR* categories are within experimental envelope / low-IQR limitation / above experimental envelope.

Model	Median: G / A / NA	IQR: within / low / above
Shell-based MFB	5 / 2 / 1	4 / 0 / 4
Volume-based MFB	5 / 2 / 1	5 / 2 / 1
Rigid-body MBS	3 / 3 / 2	2 / 3 / 3
Demo3D	2 / 2 / 4	3 / 1 / 4

4.2 OCCUPANCY HEATMAPS

Figure 13 compares the normalized experimental and simulated occupancy heatmaps for the four package types. The heatmaps provide a qualitative overview of the reproduced transport corridors, stagnation regions, and lateral spreading. The RecurDyn-based models generally reproduce the experimental occupancy patterns more closely than Demo3D, although the agreement varies between package types.

Spatial agreement was quantified using the two-dimensional EMD defined in Section 3.6. For the pooled bulk, the volume-based MFB model showed the lowest EMD (45 mm), followed closely by the rigid-body MBS (46 mm) and shell-based MFB model (47 mm), whereas Demo3D showed a substantially larger deviation (85 mm). Thus, the three RecurDyn-based approaches provide similar overall spatial agreement, while Demo3D shows clearly larger deviations.

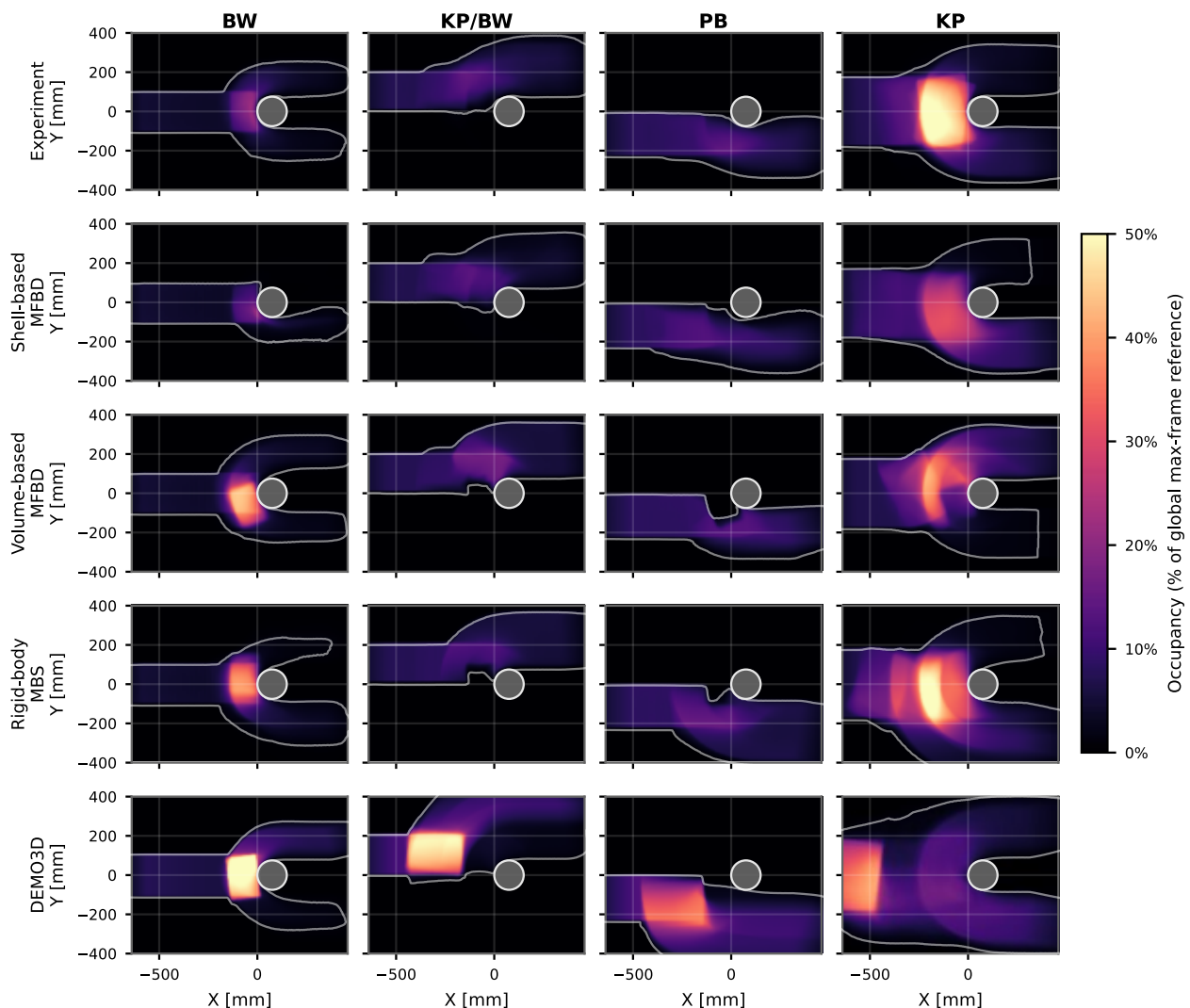


Figure 13. Experimental and simulated occupancy heatmaps for the four package types. Occupancy is normalized by the largest number of included frames contributed by any single package within the corresponding experiment or simulation.

To further resolve the spatial differences, Figure 14 shows the longitudinal and lateral Wasserstein distances defined in Section 3.6. Lateral deviations can largely result from differences in the side selected when passing the obstacle, whereas longitudinal deviations more directly indicate differences in transport progression and stagnation along the belt. Demo3D exhibits predominantly longitudinal deviations for KP/BW, PB, and KP, with longitudinal distances of 122, 84, and 135 mm, respectively, compared with lateral distances of 17, 52, and 32 mm. This pattern is also visible in the heatmaps, where temporary stagnation before the obstacle is visible for all four package types in Demo3D. In the experiment and the RecurDyn-based models, comparable stagnation occurs only occasionally and predominantly for KP. The RecurDyn-based models consequently show smaller longitudinal deviations overall.

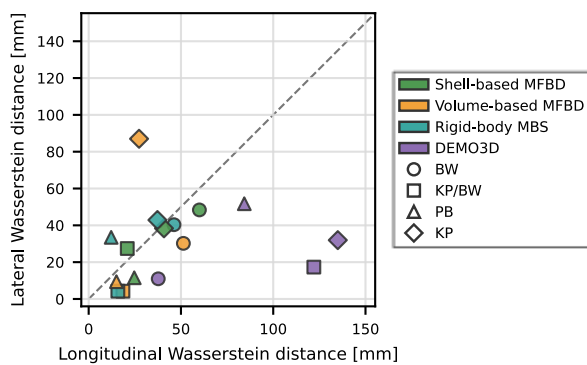


Figure 14. Directional Wasserstein distances between simulated and experimental occupancy heatmaps. Longitudinal and lateral distances are shown on the horizontal and vertical axes, respectively. Lower values indicate closer spatial agreement, and the dashed diagonal indicates equal longitudinal and lateral deviation.

4.3 NUMERICAL STABILITY AND COMPUTATION TIME

Numerical stability was not a differentiating limitation, as all models completed without solver divergence or abnormal numerical termination. Computational effort, however, differed substantially. For the four-package validation scenario, median runtimes were 0.011 h for the rigid-body MBS, 8.20 h for the volume-based MFBD model, and 79.4 h for the shell-based MFBD model. Demo3D was not quantitatively benchmarked but operated faster than real time.

To assess computational scalability, the same obstacle-passage scenario was additionally simulated with 1, 4, 10, and 25 identical PB packages, with each run covering 3 s of physical time. Figure 15 shows a strong increase in real-time factor with package number for all three RecurDyn approaches. At 25 packages, the shell-based MFBD model required approximately 360 h of computation, compared with 105 h for the volume-based MFBD model and 0.40 h for the rigid-body MBS.

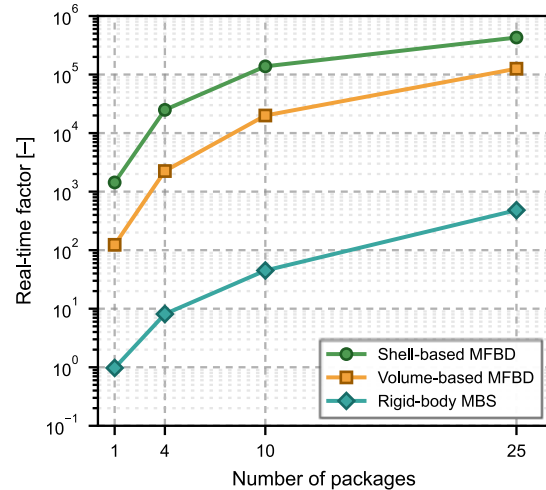


Figure 15. Real-time factor as a function of package number for the investigated RecurDyn models. Each run represents 3 s of simulation time using identical PB packages.

5 DISCUSSION

5.1 VALIDATION PERFORMANCE AND FIDELITY

The results do not show a monotonic relationship between physical model detail and agreement with the investigated bulk-level KPIs. The shell- and volume-based MFBD models achieve the same overall median classification of 5 good, 2 acceptable, and 1 not acceptable evaluation, while the volume model more frequently remains within the experimental IQR envelope (Table 1). Thus, the additional physical detail of the shell formulation does not provide a systematic advantage for transition time or lateral end position. Although the representative sequence in Figure 11 qualitatively suggests a more realistic local deformation of the shell model, this advantage cannot be confirmed with the global quantities investigated here.

This result can be interpreted in the context of pseudo-accuracy: additional numerical and representational detail only increases predictive value if the corresponding physical effects and parameters are sufficiently well characterized and relevant to the target quantity [36], [37]. This is particularly relevant here because the experiments exhibit substantial run-to-run variability, while increasing model detail introduces additional uncertain parameters and contact states. Part of the observed variation may be aleatory, whereas uncertainties in friction, stiffness, damping, and surface properties are epistemic and potentially reducible [36], [37]. In addition, large deformation and folding make robust self- and inter-package contact of the shell surfaces challenging, particularly for evolving triangulated geometries [16], [38]. Physically implausible contact states could therefore not be eliminated completely in the present implementation. Consequently, higher shell-model fidelity also introduces additional robustness requirements that must be justified by the intended validation quantity.

The two rigid-body references reveal that the lower accuracy of Demo3D cannot be attributed to the absence of deformation alone. While the RecurDyn rigid-body MBS performs worse than the MFBD models for several scalar KPIs, its pooled spatial agreement remains close to the deformable models, whereas Demo3D shows approximately twice the pooled spatial deviation (85 mm compared with 45–47 mm). Differences in contact and friction formulation, contact-surface discretization, numerical implementation, and parameter transfer are therefore likely additional contributors, although the comparison remains contextual because the rigid references were not parameterized equivalently and may behave differently in other scenarios. The directional Wasserstein analysis further shows that the larger Demo3D deviations for KP/BW, PB, and KP are predominantly longitudinal and correspond to increased upstream occupancy and different stagnation behaviour at the obstacle, whereas lateral deviations may partly result from stochastic variation in passage-side selection despite otherwise comparable transport progression.

5.2 COMPUTATIONAL SCALABILITY AND APPLICATION-ORIENTED MODEL SELECTION

Computational effort substantially changes the practical interpretation of the validation results. In the four-package scenario, the shell-based MFBD model required approximately one order of magnitude more computation time than the volume-based model, while the rigid-body MBS was more than two orders of magnitude faster than the volume model. These differences remain substantial as package number increases (Figure 15), confirming the limited scalability of the MFBD formulations for larger bulk studies. A comparable limitation was reported by Fritz et al. [25], who observed a strongly nonlinear increase in computation time for rigid-body parcel simulation in MSC

ADAMS, compared with an approximately linear development for LIGGGHTS. Absolute runtimes are not directly comparable because solver settings, implementation, and hardware differ.

The rigid references illustrate the resulting accuracy–scalability trade-off particularly clearly. The RecurDyn rigid-body MBS retains comparatively good agreement for several global quantities at substantially lower computational cost, but cannot reproduce deformation. Demo3D shows the weakest agreement in the present validation, especially for spatial occupancy and stagnation behaviour, but operated faster than real time in the investigated scenario. Its role is therefore fundamentally different: it is suited to rapid material-flow studies, control development, commissioning, and emulation rather than detailed prediction of deformable-package mechanics [26], [27].

Taken together, the results support purpose-dependent model selection rather than a universal fidelity ranking [2]. The investigated approaches differ in physical representation, validation performance, pre-processing and solving effort, and required expertise. Shell-based MFBD provides the highest physical detail, including explicit packaging–content interaction, but also requires the greatest modelling effort, computational cost, and combined MBD/FEM expertise. Volume-based MFBD reduces these demands while retaining deformability and therefore provides the most favourable compromise for the investigated bulk-level KPIs. Rigid-body MBS offers substantially lower computational effort, whereas Demo3D provides the simplest and most accessible implementation for rapid material-flow studies but with a simplified physical representation and lower agreement in the present validation. Table 2 summarizes the resulting roles, recommended use, and main limitations of each approach.

Table 2. Application-oriented comparison of the investigated modelling approaches. Effort and expertise ratings are qualitative and relative to the implementations evaluated in this study.

Comparison criterion	Shell-based MFBD	Volume-based MFBD	Rigid-body MBS	Demo3D
Role in study	Detailed deformable model	Simplified deformable model	Scientific rigid-body reference	Industrial rigid-body reference
Physical representation	Flexible packaging and separate content	Deformable packaging and content regions	Homogeneous rigid body	Homogeneous rigid body
Pre-processing effort	Very high	High	Moderate	Low
Solving effort	Very high	High	Moderate	Low; real-time capable
Required expertise	Very high	Very high	High	Low–moderate
Recommended use	Detailed single-package analyses	Deformable bulk simulations	Bulk systems with secondary deformation	Rapid bulk studies, controls, emulation
Main limitations	High effort and runtime; limited scalability	Substantial effort and runtime; simplified local deformation	No deformation	No deformation; simplified physical representation

The conclusions are specific to the controlled 2D-bulk obstacle scenario, and their transferability to other scenarios, particularly dense industrial 3D bulks, should therefore be assessed with caution. The top-view validation does not assess full three-dimensional deformation, local stresses, contact forces, or packaging-content motion, while the rigid-body references were not subjected to the same deformation- and material-specific parameterization as the MFBD models. Computation times indicate practical orders of magnitude rather than standardized benchmark performance. Future validation should therefore address denser bulk states and deformation-specific quantities.

6 CONCLUSION AND OUTLOOK

This study validated shell- and volume-based MFBD models against repeated obstacle-passage experiments in a controlled 2D-bulk conveyor scenario. Regarding RQ1, both MFBD approaches showed comparable agreement in scalar KPI central tendencies, each achieving five good, two acceptable, and one not acceptable median evaluation. The volume-based model showed closer agreement with the experimental variability, remaining within the experimental IQR envelope in five of eight evaluations compared with four for the shell-based model. Regarding RQ2, both MFBD models reproduced the main experimental occupancy patterns with similar pooled spatial agreement, with EMD values of 45 mm for the volume-based and 47 mm for the shell-based model. The directional Wasserstein analysis additionally distinguished deviations caused by lateral side choice from those associated with longitudinal progression and stagnation. Regarding RQ3, simplifying the shell representation to a volume-based MFBD model substantially reduced computational effort without a systematic loss of agreement for the investigated global KPIs.

Overall, the results do not support a general assumption that increasing physical model detail necessarily improves logistics-level predictions. For repeated deformable-package bulk simulations based on global motion and occupancy quantities, the volume-based MFBD model provides the most favourable compromise in the investigated scenario. The shell-based formulation remains relevant when local deformation or packaging-content interaction is itself the analysis target, while rigid-body approaches remain efficient alternatives where deformation is secondary.

Future work should extend the validation to denser 2D and 3D bulk states and include deformation-specific measurements that can directly assess local folding, package-shape evolution, and relative packaging-content motion. Improved robustness of contact handling and dedicated investigation of rare stagnation events are additional priorities. For larger design spaces and statistical studies, combining validated detailed models with computationally efficient reduced approaches within a multi-fidelity framework represents a promising next step.

AUTHOR CONTRIBUTIONS

For brevity, the authors' initials are used. Conceptualization, G.L. and C.L.; methodology, G.L.; software, G.L.; validation, G.L.; formal analysis, G.L.; investigation, G.L.; data curation, G.L.; writing – original draft, G.L.; writing review and editing, G.L. and C.L.; visualization, G.L.; supervision, C.L.; project administration, G.L. and C.L.; funding acquisition, G.L. and C.L. All authors have read and agreed to the published version of the manuscript.

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DECLARATION OF GENERATIVE AI AND AI-ASSISTED TECHNOLOGIES IN THE MANUSCRIPT PREPARATION PROCESS

During the preparation of this work, the authors used ChatGPT by OpenAI to support language and manuscript-structure refinement, as well as the development and revision of code used for data processing, statistical analysis, and visualisation. All AI-assisted outputs, analyses, and code were reviewed and verified by the authors, who take full responsibility for the content of the manuscript.

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