

A novel simulation-based framework for predicting the basic performance data of structured packing

Halina Murasiewicz¹ , Jerzy K. Maćkowiak^{*2,3} , Jan F. Maćkowiak^{2,3} 

¹ West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering, Department of Chemical and Process Engineering, Piastów 42, 71-065 Szczecin, Poland

² ENVIMAC Engineering GmbH, Im Erlengrund 27, 46149 Oberhausen, Germany

³ ENVIMAC Polska Sp. z o.o., Niska 1A, 63-400 Ostrów Wlkp., Poland

* Corresponding author, e-mail:
j.mackowiak@envimac.de

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Abstract

Generally, establishing design guidelines for structured packings has required prolonged empirical testing inside pilot-scale columns. While vital for mapping multi-phase fluid dynamics and mass transfer, these physical trials drain financial resources, take excessive time, and create major bottlenecks. Specifically, determining foundational Basic Performance Data (BPD) – such as pressure drop in packed bed and capacity range of the packing – remains shackled to physical experiments. Crucially, the flooding line, which defines the ultimate hydrodynamic operating limit and maximum gas throughput capacity of the column before operational failure, is traditionally not estimated by standard Computational Fluid Dynamics (CFD) simulations. Without the ability to predict this vital parameter, utilizing predictive mathematical tools for column design and scale-up remains deeply restricted.

This paper presents a virtual engineering strategy to leapfrog traditional trial-and-error workflows. By embedding a mechanistic “Suspended Bed of Droplets” (SBD) model directly within a high-resolution CFD domain, this cohesive tool permits the standalone determination of the complete BPD profile, including direct flooding line prediction. Consequently, counter-current pressure gradients and hydrodynamic capacity boundaries are computed directly from first principles, stripping away the need for preliminary laboratory measurements. To verify accuracy, these digital predictions are rigorously cross-examined with archival field data from commercial-grade structured packing installations. This methodology represents a profound shift toward a nimble, software-centric discovery model in thermal separation engineering, radically shortening performance profiling timelines, mitigating infrastructure expenses, and providing a powerful digital platform to optimize future packing geometries.

Keywords

structured packing; CFD modelling; basic performance data; distillation; flooding line prediction

1. INTRODUCTION

For over forty years, packed columns containing random and structured internals have been extensively utilized in thermal separation operations. These internals revolutionized mass transfer technology by offering outstanding performance characteristics, such as minimal gas-phase resistance and remarkably high separation efficiencies per unit height when contrasted with conventional tray columns. Despite this technical superiority, the engineering development and geometric optimization of these internals have historically been hindered by the intricate, non-linear coupling that exists between complex surface architectures and multi-phase fluid hydrodynamics.

To safely scale up and engineer industrial-scale installations, acquiring precise Basic Performance Data (BPD) is an absolute necessity. Historically, mapping these parameters required exhaustive, labor – intensive experimental campaigns. Researchers relied on established multi-component distillation test systems – such as those detailed by Zuideweg (1969) – alongside atmospheric air-water simulators to generate empirical design equations (Maćkowiak, 2010; 2022a). While these

classic empirical correlations provided foundational blueprints, this purely experimental approach is increasingly viewed by modern industry as cost-prohibitive, rigid, and time-intensive.

To complement or entirely bypass traditional laboratory testing, Computational Fluid Dynamics (CFD) has emerged as a transformative engineering methodology. Over the past two decades, CFD has advanced from a simple optimization tool used for non-active tower internals (such as gas distributors) (Chen et al., 2009; Ngo and Lim, 2020; Spiegel and Meier, 2003) into a high – fidelity predictive framework capable of evaluating active random and structured packing performance.

The Mellapak family of structured packings has established itself as the definitive industry benchmark for counter-current column internals, driving continuous advancements in materials science and geometric configuration. This structural framework has expanded from standard commercial configurations – such as the widely utilized Mellapak 250Y and 500Y series – to high-capacity variations like Mellapak Plus, which are optimized to reduce gas-phase resistance while maximizing liquid distribution. Consequently, due to its status as an industry



standard, a vast body of literature features combined experimental and CFD studies specifically dedicated to validating, testing, and performance-mapping various Mellapak configurations (Basden et al., 2013; Haroun and Raynal, 2016; Isoz and Haidl, 2018; Salten et al., 2021; Szulczewska et al., 2003).

A primary focus of structure-resolved CFD is capturing the exact physical mechanisms governing film stability, liquid spreading, and localized gas-liquid interactions within structured packing channels. Understanding these phenomena at a fundamental level allows for the precise optimization of column internals where conventional macroscopic models rely heavily on empirical estimation. Modern research focuses on resolving the complex, micro-scale interfacial mechanics occurring on the surface of structured packings, while simultaneously seeking macro-scale workflows that can predict overall column performance without excessive computational overhead.

A foundational breakthrough in combining these spatial scales was achieved by Li and Zeng (2025), who developed a multi-scale hydrodynamic framework that bridges small-scale 3D representative elementary units with a macroscopic node network model. By training a Back Propagation Neural Network (BPNN) directly on datasets generated from two-phase CFD simulations, they successfully mapped localized wall-boundary and interlayer conversion effects that traditional models often neglect. This dual-neural network approach achieved high predictive reliability for macroscopic parameters, yielding an average relative deviation of 8.63% for dry pressure drop and 9.63% for liquid holdup when compared to experimental benchmarks.

Evaluating these boundary layer mechanisms, Dechert and Kenig (2025) isolated the geometric influence of surface microstructures on liquid film behaviour using single inclined plates. Their numerical simulations demonstrated that the spatial orientation of microstructures relative to the primary flow vector exerts the most dominant effect on localized liquid flow patterns and the resulting wetted area size. This structural sensitivity was further contextualized by Dechert et al. (2024), who expanded the microscopic modelling framework to incorporate physical fluid property variations alongside complex surface texturing. Their findings revealed that under specific operational conditions, standard smooth packing surfaces can outperform microstructure surfaces due to complex variations in surface tension and viscous forces. They demonstrated that the local liquid flow angle is not dictated solely by the packing's macroscopic corrugations, emphasizing that microstructure reorientation serves as a highly sensitive mechanism for local fluid diversion and film stability.

This complex geometric relationship is further modified by the presence of macroscopic sheet perforations. Wang et al. (2026) focused specifically on mechanical perforation parameters within Mellapak 250.Y corrugated sheets for post-combustion CO₂ capture. Their microscale simulations indicated that reducing perforation spacing significantly enhances the effective gas-liquid mass transfer area under lower hydraulic

loads, as the liquid-perforation edge interaction creates localized droplets and film disruption. However, this advantage diminishes at higher liquid loads because the increased liquid volume completely submerges the perforations, bridging the gaps to form continuous liquid curtains rather than discrete films. To account for this shifting hydraulic mechanism, they established modified empirical correlations that incorporate corrugated sheet porosity as a critical variable, successfully restricting prediction deviations for both liquid holdup and effective interfacial area to within $\pm 10\%$ of their structure-resolved simulation data.

To contextualize the extensive body of CFD and numerical research compiled across both microscale surface investigations and macroscale column scaling frameworks, it is necessary to evaluate these models against classical chemical engineering definitions of column capacity. A complete and functionally useful hydrodynamic profile of any packed column configuration must explicitly define its operational envelope. According to established chemical engineering benchmarks (Maćkowiak, 2010), this entire operating range is plotted as a function of the gas load factor (F_V) versus the specific irrigated pressure drop ($\Delta p/H$), bounded strictly between the lower dry pressure drop line and the upper hydraulic flooding line.

Table 1 provides a structured, chronological audit of the foundational papers to assess if current literature successfully bridges the gap between local geometric optimization and full-scale capacity mapping. This matrix isolates the specific hydrodynamic parameters investigated by each research group, identifying whether authors explicitly determined or omitted the baseline dry resistance and high-load phase inversion thresholds necessary to establish a true operating range.

Despite these computational advancements, a major bottleneck persists in all existing literature, as seen in Table 1: predicting the maximum operating capacity (the ultimate hydraulic flooding line) using purely numerical CFD simulations remains impossible without pre-existing empirical validation data.

Because the absolute flooding boundary cannot be simulated autonomously, current CFD models are equally incapable of predicting the sub-critical operating thresholds of the packing (Figure 1). This includes the vital "loading line", which typically occurs at approximately 65% of the total flooding gas velocity as described by Maćkowiak (2010). Resolving this predictive limitation remains a major requirement for achieving autonomous, simulation-driven column design.

The fundamental dependency of the pressure drops per unit of packing height ($\Delta p/H$) as a function of the gas load factor (F_V) is systematically illustrated in Figure 1a. In this comprehensive hydraulic profile, the specific liquid load (u_L) serves as the primary operational parameter. The active hydrodynamic operating regime of any packing geometry is strictly bounded between the flooding line and the baseline for dry pressure drop curve characteristic of single-phase gas flow.

Table 1. Comprehensive operating range evaluation matrix.

Author & Year	Scope of Hydrodynamic Data Defined	Addressed Dry Pressure Drop?	Addressed Flooding Limit?	Formally Defined Full Range?
Szulczewska et al. (2003)	Local film wave formations and phase velocity profiles.	No (Focused on isolated irrigated film growth).	No (Omitted counter-current phase inversion).	No (Operational boundaries undefined).
Basden et al. (2013)	Neutron-scan mapping of localized interlayer liquid holdup.	No (Purely experimental irrigated holdup tracking).	No (Flooding velocity thresholds not recorded).	No (Limited to local spatial distributions).
Lassauce et al. (2014)	Interfacial area evaluation criteria for carbon capture.	No (Addressed generic design guidelines).	No (Omitted maximum capacity tracking).	No (No quantitative hydraulic limits).
Lautenschleger et al. (2015)	Gas-phase flow vectors and optimization of PD 10 packing.	Partial (Modelled dry pressure loss trends).	No (Two-phase flooding limits omitted).	No (Upper boundary capacity undefined).
Amini et al. (2016)	Film uniformity tracking on PACε2100 geometry.	Partial (Modelled wet pressure drops at stable loads).	No (Did not identify hydraulic runaway limits).	No (Upper operational threshold missing).
Haroun and Raynal (2016)	Large-scale distributor flow patterns and geometry maps.	No (Focused on distributor boundary conditions).	No (Omitted column-wide flooding points).	No (Restricted to inlet distribution zones).
Isoz and Haidl (2018)	Single-phase gas flow profiles across corrugated channels.	Yes (Validated dry pressure loss equations).	No (Liquid phase entirely absent from models).	No (Lower baseline defined; upper boundary missing).
Lavalle et al. (2018)	Cross-flow packing layout via a single REU domain.	Partial (Calculated baseline pressure drop shifts).	Partial (Identified delayed flooding trends).	No (Identified a delayed trend but did not chart the full envelope).
Basha et al. (2020)	Full-scale Eulerian absorber grid tracking for CO ₂ capture.	No (Simulated stable, steady-state absorption points).	No (Solver kept well below flooding velocities).	No (Operational extremes completely omitted).
Macfarlan et al. (2021)	Specific area, inclination, and opening angle trade-offs.	Partial (Tracked stable pressure drop slopes).	No (Phase inversion boundaries not simulated).	No (Envelope limits left unquantified).
Salten et al. (2021)	Multi-regime analogy modelling (film, jet, drop flow).	No (Addressed stable irrigated holdup parameters).	No (Analogy correlations omit loading limits).	No (Operating range boundary left unmapped).
Zeng et al. (2022)	Dynamic vs. static interfacial area distributions (VoF).	No (Isolated local surface tension boundaries).	No (Counter-current loading limits omitted).	No (Focused on wet area physics).
Bertling et al. (2023)	Tomography-validated VoF simulation of RTD and holdup.	No (Captured stable irrigated parameters).	No (Flooding instability point not modelled).	No (Operational limits omitted).
Dechert et al. (2024)	Micro-scale film trajectories and fluid properties.	No (Focused on single-phase local film paths).	No (Omitted counter-current gas drag).	No (Restricted to fundamental surface layers).
Dechert and Kenig (2025)	Micro-scale film spreading on solitary inclined plates.	No (Isolated single-phase liquid wetting tracks).	No (Counter-current gas interaction omitted).	No (Limited to pre-column isolated film mechanics).
Li and Zeng (2025)	Gas-liquid node flows; holdup macro-distribution.	Yes (BPNN validated with an 8.63% deviation).	No (Upper hydraulic flooding limits not simulated).	No (Missing the upper boundary threshold).
Wang et al. (2026)	Perforation interactions, liquid holdup, and effective a_e .	Partial (Evaluated lower liquid load baseline boundaries).	No (Observed liquid curtains but omitted flooding velocity).	No (Focused on parametric trends over boundary limits).

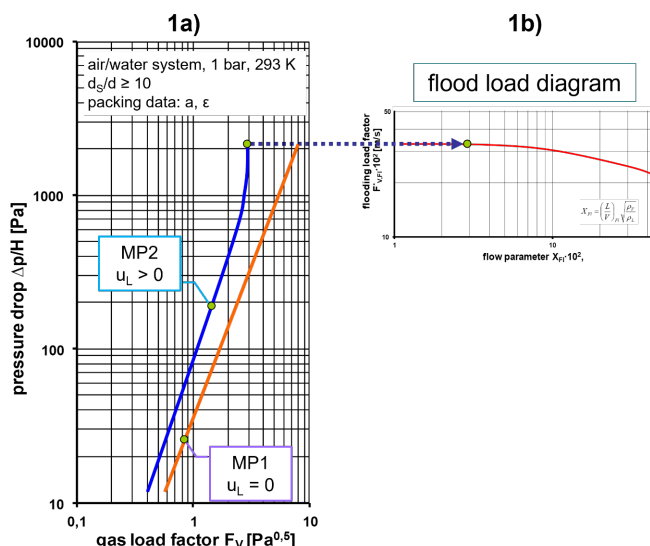


Figure 1. A comprehensive methodology for characterizing the hydraulic performance and operating range of all types of packing geometries, as established in the foundational work of Maćkowiak (2010).

Utilizing the experimental hydrodynamic data compiled in Figure 1a, a generalized flooding diagram can be generated, as presented schematically in Figure 1b. This diagram maps the flood load factor ($F_{V,fl}^*$) directly against the dimensionless Sherwood-type flow parameter (X_{fl}), related to the flooding condition (Eq. 1).

$$F_{V,fl}^* = \frac{F_{V,fl}}{\sqrt{\rho_L - \rho_V}} = f(X_{fl}) = f\left(\frac{L}{V} \sqrt{\frac{\rho_V}{\rho_L}}\right) \quad (1)$$

Developing and mastering this flooding load diagram is an absolute prerequisite for the safe design, structural scaling, and column sizing of industrial-scale chemical separation plant.

Consequently, establishing these operational boundaries provides the baseline validation necessary to model multi-phase hydraulics and localized mass transfer rates within advanced numerical solvers. However, a critical evaluation of the current state of the art reveals a major limitation: the vast majority of CFD investigations presented in the literature fail to predict these macroscopic boundaries autonomously. Because traditional CFD models cannot reliably determine the absolute flooding capacity range without pre-existing empirical data, their ability to model mass transfer across the full operating range is severely compromised.

As a result, current numerical simulations do not yet offer a sufficiently secure, standalone foundation for deriving generalized mass transfer correlations suitable for industrial equipment design. This significant gap in predictive separation technology heavily restricts the utility of high-fidelity simulations, forcing engineers to remain reliant on expensive pilot plant trials.

This work directly addresses and resolves this persistent computational bottleneck. We introduce a novel transition away

from computationally prohibitive, micro-scale high-fidelity multiphase models, moving instead toward the rapid, standalone prediction of Basic Performance Data (BPD) for industrial-scale structured packings, as presented in Figure 2.

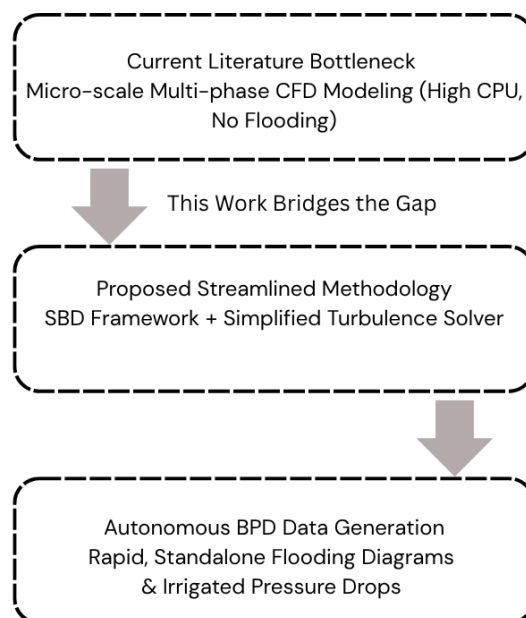


Figure 2. Methodological transition framework demonstrating the shift from computationally restrictive, micro-scale CFD models to an autonomous BPD generation workflow utilizing an integrated SBD model and RANS turbulence closures.

This study achieves this acceleration by proposing a streamlined, macroscopic CFD methodology coupled with simplified Reynolds–Averaged Navier–Stokes (RANS) turbulence closures, specifically the standard two-equation k – ϵ model. By strategically prioritizing computational throughput and algorithmic efficiency without sacrificing core physical relevance, this synergetic approach provides an autonomous mathematical pathway to predict foundational performance parameters. Ultimately, this framework drastically reduces the traditional reliance on long-term, capital-intensive experimental campaigns, paving the way for agile digital twin optimization of next generation packing architectures.

2. EXPERIMENTAL SETUP

Quantifying the dry pressure drop is a critical prerequisite for characterizing packed column hydraulics and establishing a baseline for rigorous CFD model verification and validation. To anchor these numerical simulations in physical data, baseline pressure drop measurements were systematically gathered from vacuum distillation plants utilizing diverse distillation and absorption test systems.

The operation conditions, physical properties of the used systems, and technical data of the investigated R500Y (RVT) structured packing – including its specific surface area (a) and void fraction (ϵ) are detailed in Table 2. Furthermore, the systematic layout of the laboratory distillation plant and the physical structure of the packing elements are illustrated in Figure 3.

The comprehensive experimental methodology and validation protocols applied in this study align with the recent collaborative academic-industrial framework established by Neumann et al. (2025), alongside the classic foundational guidelines outlined by Billet et al. (1978) and Maćkowiak (2022b). Prior to this investigation, no published experimental data was available concerning the hydraulic behaviour of the R500Y packing. To address this gap in literature, rigorous hydraulic

measurements were executed using a laboratory distillation column with an inner diameter of 0.05 m.

The total packing height was systematically varied between 0.5 m and 1.50 m. The investigations were carried out under atmospheric and low pressure ranging from 300 mbar to 1 bar (as catalogued in Table 2). To ensure high data fidelity during counter-current operation, the vapour flow rate and corresponding vapour load factor were calculated continuously via heat balance across the condenser loop. These heat balance calculations were verified in real-time using an Endress+Hauser (E+H) inductive flow meter (IDM). Simultaneously, the specific irrigated differential pressure drop across the structured bed was captured using a high-precision E+H pressure transmitter, ensuring reproducible hydraulic capacity limits.

Table 2. Physical properties of the used test systems and technical data of the structured packing.

Packing data	d_s	H	p_T	T	ρ_v
Packing R 500Y (RVT), $a = 500 \text{ m}^2/\text{m}^3$, $\epsilon = 0.970 \text{ m}^3/\text{m}^3$	[m]	[m]	[mbar]	[K]	[kg/m ³]
air	0.05	1 / 1.5	1013	293	1.2
cyclohexane / <i>n</i> -heptane	0.05	1 / 1.5	950 / 300	360 / 327	2.9 / 1.0
ethanol / <i>n</i> -butanol	0.05	0.5	950 / 300	364 / 345	1.62 / 0.6
ethanol / water	0.05	0.5	950 / 300	363 / 345	0.85 / 0.45

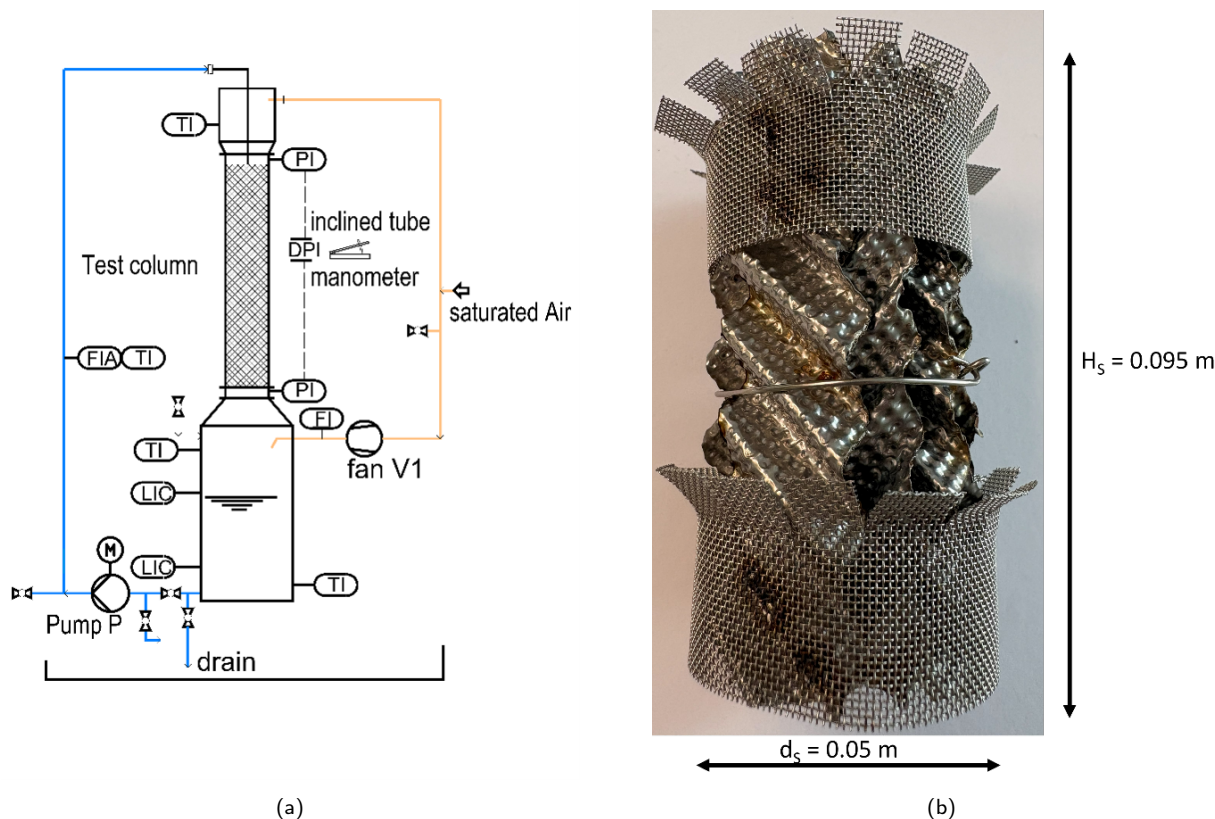


Figure 3. a) Laboratory test plant for air – water test, $d_s = 0.05 \text{ m}$, $H = 1.5 \text{ m}$; b) a photo of one element of packing R500Y.

3. THEORETICAL

Predicting the resistance of structured packings under non-irrigated conditions is a fundamental prerequisite for comprehensive column optimization. Prior to resolving complex multi-phase interfaces, characterizing the single-phase gas dynamics allows researchers to isolate the raw geometric impact of the corrugated matrix.

The dry pressure drop serves as the hydraulic baseline of the column, directly influencing the operating cost, vapour capacity, and overall separation efficiency. By utilizing structure resolved CFD, the highly complex, anisotropic resistance generated by intersecting corrugated sheets can be evaluated from a fundamental fluid mechanics perspective. To evaluate this dry pressure drop and map localized velocity profiles, the transport behaviour of the gas phase is resolved by enforcing the conservation of mass and momentum over discrete spatial volumes.

The mathematical description of single-phase gas transport through structured packings rests on the fundamental conservation laws of fluid mechanics (Bird et al., 2006). Assuming an incompressible gas phase under typical low-vacuum or atmospheric distillation regimes, the flow field is governed by the continuous Navier–Stokes equations and the continuity equation:

$$\nabla \mathbf{u} = 0 \quad (2)$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (3)$$

where $\mathbf{u}$ represents the velocity vector, p is the static pressure, ρ is the gas density, and μ is the dynamic viscosity of the working fluid. This differential framework balances local momentum flux against pressure gradients and viscous shear stresses, providing the strict mathematical foundation required to map localized skin friction and form drag before introducing counter-current liquid films.

To simulate turbulent, high-velocity gas fields through the corrugated matrix without incurring prohibitive computational penalties, the standard Reynolds–Averaged Navier–Stokes (RANS) equations are employed. The closing of the turbulent transport equations is achieved using the standard two-equation k - ϵ turbulence model (Launder and Spalding, 1974), a widely used model for turbulent flow in Ansys Fluent. This framework tracks the transport of turbulent kinetic energy (k) and its corresponding isotropic dissipation rate (ϵ) via the following coupled partial differential equations:

$$\frac{\partial}{\partial t}(\rho k) + \nabla(\rho \bar{\mathbf{u}} k) = \nabla \left(\frac{\mu_{\text{eff}}}{\sigma_k} \nabla k \right) + P_k - \rho \epsilon \quad (4)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \nabla(\rho \bar{\mathbf{u}} \epsilon) = \nabla \left(\frac{\mu_{\text{eff}}}{\sigma_\epsilon} \nabla \epsilon \right) + \frac{\epsilon}{k} (C_1 P_k - C_2 \rho \epsilon) \quad (5)$$

Within this formulation, P_k denotes the volumetric production rate of turbulent kinetic energy arising from velocity gradients,

while μ_{eff} represents the effective viscosity, combining the molecular dynamic viscosity (μ_m) with the turbulent eddy viscosity (μ_t). The turbulent viscosity is derived algebraically as follows:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (6)$$

The closure coefficients for these transport formulations are set to their standard established empirical values (Launder and Spalding, 1974): $C_\mu = 0.09$; $C_1 = 1.44$; $C_2 = 1.92$; $\sigma_k = 1$; $\sigma_\epsilon = 1.314$.

To resolve boundary layer separation and skin friction along the complex corrugated metallic sheets without over-refining the computational mesh within the viscous sublayer, scalable wall functions are integrated (Farmer et al., 2005; Launder and Spalding, 1974). These functions mathematically extend the applicability of standard boundary definitions to low mesh-density regions by limiting the dimensionless wall distance parameter ($y_{\text{limit}}^* = 11.225$). This configuration prevents numerical instability and avoids the excessive computational overhead of full boundary layer mesh resolution. Compared to higher-order Reynolds stress models, the k - ϵ framework provides a highly stable, computationally efficient approach for sweeping broad gas load factor operational envelopes. Detailed information, mathematical derivations, and boundary layer formulations for this specific turbulence model are extensively documented in the foundational literature. For a comprehensive review of the transport equations and closure coefficients, readers are referred to the pioneering work of Launder and Spalding (1974), the advanced fluid dynamics framework by Pope (2001), and the classic boundary layer treatment by Wilcox (2006).

The governing conservation equations describing the single-phase gas dynamics within the structured packing matrix were discretized and numerically solved utilizing the commercial CFD software ANSYS Fluent 2023 R2.

4. SETUP OF CFD MODELLING

This section is dedicated to detailing the precise geometric configuration and the specific mesh topology utilized throughout the current numerical study. Furthermore, the foundational boundary conditions, physical constraints, and the iterative numerical procedures deployed within the solver environment are systematically presented to ensure full reproducibility of the hydrodynamic simulations.

4.1. Geometry and mesh

The high-fidelity three-dimensional CAD geometries representing the R500Y structured packing matrix were constructed within a standardized pilot column domain featuring an inner diameter (d_s) of 0.05 m and a total axial length of 0.30 m. To investigate the localized boundary layer bypass effects and

disruptions caused by peripheral internals, the computational domain was established in two distinct configurations: a standard core packing block and a specialized assembly integrated with wall wipers.

The detailed spatial configurations, boundary interfaces, and assembly domains are visualized in Figure 4. The initial 3D geometric modelling of the intricate corrugated packing sheets and their corresponding boundary-layer wiper attachments was executed using AutoCAD.

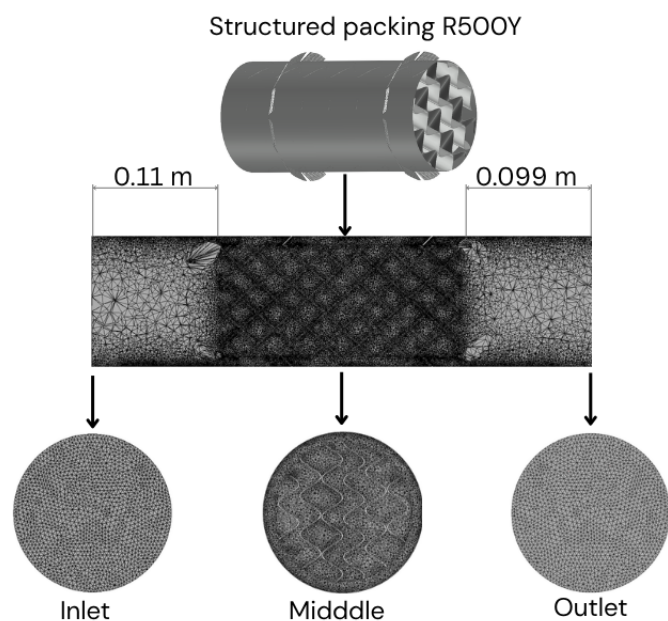


Figure 4. Structural representation of the computational domains utilized for the R500Y structured packing with wipers within a 0.05 m diameter column.

Following geometric compilation, the fluid domain was exported into ANSYS Meshing, the high-performance pre-processing suite within the ANSYS 2023 R2 software environment, to undergo spatial discretization. An unstructured tetrahedral mesh topology was selected to accommodate the sharp angle transitions, complex channel intersections, and narrow crimp apexes characteristic of structured packing R500Y corrugation profiles.

To resolve localized high-gradient fluid phenomena without incurring excessive computational overhead throughout the entire column volume, strategic mesh refinement zones were implemented. High-density cell distributions were embedded in critical transport regions, including the solid-fluid boundary layers along the metallic packing elements, the narrow gaps surrounding the wall wipers, and the flow development zones near the main inlet section.

This localized clustering allows the numerical solver to accurately capture boundary layer separation, secondary vortex generation, and localized skin friction profiles while keeping global element counts mathematically manageable.

To isolate the numerical solutions from spatial discretization artifacts and guarantee that the resulting flow fields are not functions of mesh density, a systematic grid independence study was performed in accordance with established numerical verification protocols (Picardi et al., 2016). This iterative optimization framework involved systematically inflating the total cell count across three independent mesh densities for each physical geometry while monitoring the convergence trajectories of primary hydrodynamic variables, specifically the specific dry pressure drop and the cross-sectional average velocity profiles.

The exact element counts evaluated during this grid sensitivity audit for the modified column geometry were distributed as follows: 4.51 million, 6.66 million, and 7.92 million elements, capturing the added geometric complexity of the peripheral wall attachments. Definitive grid independence was verified when further mesh refinement yielded negligible changes in the simulated static pressure drop and localized velocity vector distributions.

Quantitative cross-examination revealed that the relative error deviations between the coarse (4.51 M) and intermediate (6.66 M) mesh levels were strictly restricted to below 6%. While a 6% deviation may be considered significant in some idealized flow scenarios, it is important to contextualize this value within the complexities of structured packing modelling. Modelling R500Y packing is computationally demanding, requiring the resolution of thin boundary layers and intricate interactions within narrow, corrugated channels. The 4.51 M grid was selected as a pragmatic balance between computational resource availability and numerical accuracy; it provides sufficient resolution to capture primary flow characteristics, turbulence transition behaviour, and stable convergence for pressure drop and velocity profiles. Given that this 6% deviation signifies that results lie within the asymptotic range of the grid convergence study, the 4.51 million element configuration was utilized for all subsequent ANSYS Fluent simulations to establish an optimal baseline between spatial accuracy and CPU wall-clock efficiency. The quality of the generated mesh was verified using standard metrics (Wilcox, 2006). For the selected 4.51 M element mesh, the average orthogonal quality is 0.7518, with a minimum value of 0.18. Regarding skewness, the average value is 0.2467, with a maximum value of 0.82. These metrics indicate that the mesh quality is sufficient for accurate flow resolution within the corrugated channels of the R500Y packing, as all cells fall within the recommended limits for stability in ANSYS Fluent.

4.2. Boundary conditions

To establish a physically realistic numerical framework representing the single-phase gas dynamics through the R500Y structured packing, appropriate boundary conditions were prescribed at all peripheral interfaces. The computational domains are bounded by a fluid inlet zone, a fluid outlet zone,

and solid boundaries representing the column shell and internal packing surfaces. All boundary conditions were configured within the ANSYS Fluent 2023 R2 software environment to ensure strict continuity with the physical laboratory conditions.

The explicit mathematical and physical constraints applied to the boundaries of the computational domain are defined as follows:

1. Inlet boundary condition (velocity inlet): The gas phase inlet was designated as a Velocity Inlet profile. The operational parameters were directly informed by the experimental velocity ranges to ensure data alignment. Air was utilized as the working fluid, with uniform inlet velocities systematically varied from 0.5 m/s to 4.0 m/s in discrete increments of 0.5 m/s. This incremental sweep matches the experimental gas load factor distribution. The Reynolds number, Re_V , calculated using the formula provided by Maćkowiak, 2010, spans a range from 200 to 4000 for the R500Y packing.
2. Outlet boundary condition (pressure outlet): A Pressure Outlet boundary condition was specified at the column exit plane. The gauge pressure at this boundary was fixed at a constant 0 Pa, allowing the fluid to exhaust freely into a standard reference pressure environment and preventing artificial backpressure waves from disrupting the upstream flow field.
3. Wall boundary condition (no-slip constraint): The outer column shell, internal corrugated sheet faces, and wall wiper surfaces were modelled as stationary solid boundaries. A strict no-slip condition was enforced, setting the fluid velocity vector at the solid-fluid interface to zero. To account for micro-structural friction along the metallic sheets, a uniform wall roughness factor of 0.5 was applied across the surfaces.

4.3. Numerical model

To optimize computational efficiency and minimize CPU overhead while maintaining a high degree of simulation fidelity, the numerical framework incorporates several core engineering hypotheses:

1. The gas phase transport through the corrugated structured packing matrix is modelled as a steady-state flow regime, wherein the working fluid (air) is treated as a viscous, incompressible Newtonian fluid.
2. The velocity profile at the inlet boundary is assumed to be entirely uniform, treating the incoming gas as a fully developed turbulent flow immediately upon entering the domain.
3. The structured column is assumed to operate under strictly isothermal conditions at an ambient temperature, thereby neglecting thermal energy variations across the entire column domain.

These simplifying assumptions provide a vital computational baseline that significantly improves numerical efficiency and ensures solver stability without compromising the underlying fluid mechanics of the system.

The governing conservation equations, subject to these defined boundary conditions, were numerically solved within the segregated solver framework of the commercial CFD package ANSYS 2023 R2. To resolve the pressure-velocity coupling, the classic iterative Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm, originally developed by Patankar and Spalding (1972), was deployed to sequentially compute each dependent variable. To suppress numerical diffusion and enhance spatial stability across the complex, intersecting flow channels, a second-order upwind differencing scheme was strictly enforced for the continuity, momentum, and turbulence transport equations. This numerical configuration was further modulated using standard RANS under-relaxation factors to guarantee smooth matrix convergence throughout the iterative loop.

Strict convergence criteria were enforced to ensure data fidelity, requiring the normalized sum of residuals for all variables to drop below a tolerance threshold of 10^{-5} alongside completely stabilized column pressure profiles. Under these rigorous convergence constraints, each individual production run required approximately 3000 iterations to achieve steady-state conditions.

Ultimately, a total matrix of 8 independent simulations was performed. This systematic sweep generated a comprehensive dataset of dry pressure drops, allowed for the comprehensive analysis of localized gas-phase flow vectors, and quantified the specific impact of the integrated wall wipers within the packing structure. The predictive accuracy of the numerical model was fully validated by cross-examining the simulated dry pressure drop values against physical pilot-plant measurements collected under identical operating conditions, where the strong alignment between the datasets confirmed the reliability of the established CFD framework.

5. RESULTS

The simulated CFD hydrodynamics are evaluated using mainly primary indicators: total pressure drop, localized static pressure contours, and additionally velocity vector fields. In separation processes like distillation, absorption, and stripping, the dry pressure drop establishes the baseline operating cost and vapour capacity. While a lower single-phase pressure drop generally implies a higher ultimate two-phase capacity, specific geometric drag components can increase resistance without improving separation efficiency.

To systematically deconstruct the internal dynamic of the R500Y packing matrix, the hydrodynamic analysis is partitioned into a multi-stage spatial and kinematic investigation. This structured diagnostic approach isolates specific

energy losses and flow distribution behaviours across the column domain through the following sequential evaluations: longitudinal static pressure profiles and multi-dimensional velocity distributions.

This numerical investigation focuses exclusively on the validation of dry pressure drop for air. By isolating the influence of the packing geometry and fluid velocity, we establish a fundamental hydrodynamic baseline independent of the complex mass and heat transfer phenomena present in the multi-component distillation systems detailed in Table 2.

This approach provides a reliable foundation for industrial applications; the results obtained for dry air pressure drop are sufficient for characterizing packing performance and can be adapted to other systems as described by Maćkowiak (2010). This methodology is particularly valuable for reducing experimental effort, as it allows for a precise validation of the turbulence modelling against clean, single-phase air flow, providing a necessary prerequisite for understanding the more complex behaviour observed in industrial distillation.

5.1. CFD dry static pressure and pressure drop

To evaluate the mechanical energy losses and localized transport phenomena within the R500Y structured packing matrix ($d_S = 0.05$ m), the longitudinal static pressure contours were extracted from the validated RANS k - ε turbulence simulations. Figure 5 illustrates the spatial distribution and development of the pressure fields across the structural elements from the pipeline inlet plane (left) to the discharge zone – pipeline outlet (right) under two contrasting gas kinetic energy regimes: low vapour $u_V = 1.5$ m/s load (Case a) and high vapour load $u_V = 3.5$ m/s (Case b).

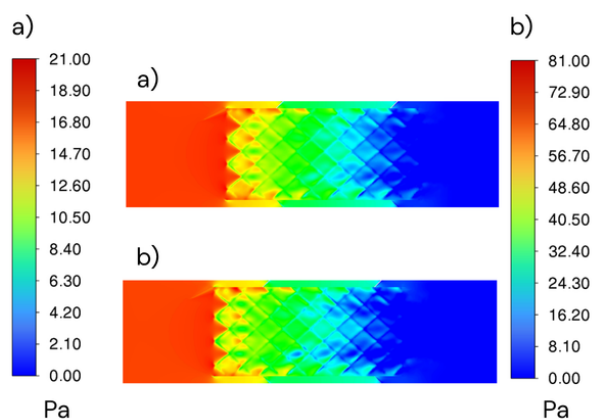


Figure 5. Static pressure profile in column equipped with standard metallic structured packing R500Y for inlet linear velocity of air: a) $u_V = 1.5$ m/s, b) $u_V = 3.5$ m/s. Column diameter: $d_S = 0.05$ m.

As anticipated, all evaluated cases demonstrate a distinct and continuous decrease in static pressure along the longitudinal axis of the packed column from the pipeline inlet plane to the

exhaust. This monotonic pressure drop reflects the cumulative resistance, skin friction, and form drag imposed on the gas phase as it is forced through the tortuous channels generated by the corrugated sheets of the R500Y matrix. The rate of this axial pressure declines scales directly with the incoming gas load, showing significantly steeper gradients as the inlet velocity steps up from 1.5 m/s to 3.5 m/s.

A macroscopic comparison of the two evaluated operational states reveals a highly non-linear evolution of the total dry pressure drop across the R500Y structured packing matrix. The discrete quantitative values derived directly from the structure-resolved computational grid are compiled. To systematically assess the impact of gas-phase kinetic energy on column mechanics, the primary hydrodynamic parameters were evaluated and compared across both simulated operating regimes. The primary independent operational variable, the superficial gas velocity, is increased from 1.5 m/s in Case a, representing the low vapour load condition, to 3.5 m/s in Case b, representing the high vapour load condition. This change establishes a dimensionless shift ratio of 2.33 for the incoming fluid velocity.

Due to the downstream atmospheric boundary constraint, both the peak static resistance at the column entrance and the total dry pressure drops across the packing matrix increase identically from 21.0 Pa under low vapour conditions (Case a) to 81.0 Pa under high vapour loads (Case b), representing a dimensionless shift ratio of 3.86. This proportional alignment between the maximum inlet pressure and the net domain pressure differential indicates that the overall system resistance is dominated by the structural characteristics of the packing matrix rather than localized exit effects.

In conventional, fully rough macroscopic turbulent systems, the pressure drop across a fixed packed bed scales strictly according to the quadratic velocity square-law ($\Delta p \propto u_V^2$), which would theoretically yield a pressure shift ratio of approximately 5.44 for the velocity increase investigated herein. However, a rigorous processing of the numerical datasets reveals a real-system scaling exponent, n , of approximately 1.59.

This specific exponent value provides critical scientific evidence that within the designated operational envelope, the internal micro-channels of the R500Y matrix experience a highly transitional flow regime. In this state, linear viscous dissipation layers along the metallic sheet boundaries still exert a significant dampening effect, actively competing with the quadratic inertial form drag induced by the macro-scale geometric corrugations and channel intersections. Consequently, the global resistance exhibits characteristics that lie between purely laminar friction and fully developed isotropic turbulence, emphasizing the necessity of structure-resolved numerical modelling to accurately capture these localized transport mechanisms.

Deconstructing the structure-resolved contours of static pressure presented in Figure 5 reveals several distinct localized fluid mechanic phenomena that directly influence macroscopic

column efficiency. Periodic stagnation and impact zones are discernible where the ascending gas phase encounters the leading edges of the corrugated packing elements. Upon impact, the initially uniform velocity field is forcibly split. As shown in Figure 5b, which displays the static pressure profile across the packing structure (ranging from 0.00 to 81.00 Pa), localized high-pressure zones pinpoint the coordinates where fluid flow impinges directly upon the inclined packing surfaces. This collision triggers a rapid deceleration of the gas stream, resulting in a partial conversion of dynamic pressure into static head.

Further inward, the interior core of both computational domains exhibits a highly symmetrical, periodic criss-cross channel tessellation. This geometric arrangement forms a repeatable "mosaic" pattern that accurately reflects the physical intersections of the cross-corrugated metallic sheets. Within this core matrix, the alternating high- and low-pressure cells map the microscopic pressure fluctuations that occur as the gas streams are continuously forced to bifurcate, twist, and recombine at the internal channel junctions. This continuous redirection prevents the formation of stable, unmixed core streams, promoting local gas-phase radial dispersion across the packing channels.

However, when evaluating the high vapour load condition, $u_V = 3.5$ m/s, phenomena related to boundary layer detachment and core channeling become highly pronounced. At this elevated velocity, the spatial pressure gradients intensify significantly across short physical distances, establishing sharp boundaries between the low-velocity wake regions and the high-velocity core flow vectors. The $k-\epsilon$ turbulence closure scheme effectively captures significant shear-stress accumulation at these critical geometric boundaries. These zones highlight the exact physical locations where macro-vortices are shed from the corrugated crests, converting primary mechanical energy into parasitic turbulent dissipation and driving up the overall dry pressure drop.

From an engineering and column design perspective, these micro-scale topological insights yield critical insights into the underlying transport trade-offs. The localized, high-gradient pressure fields along the geometric boundaries shown in Figure 5b represent areas of intense local shear, which are highly favourable for minimizing gas-side mass transfer resistance. Simultaneously, however, these exact zones serve as the primary source of dry pressure drop. This indicates that optimizing the corrugation base angle or smoothing the sharp transitions at the plate crests could significantly reduce overall energy consumption and form drag without sacrificing the effective gas-liquid contact area required for mass transfer.

5.2. Velocity fields

Additionally, CFD simulations provide an advanced, high-resolution framework to non-invasively investigate these intricate velocity patterns within the complex internal channels of structured packings, capturing micro-scale fluid behaviours

that are typically inaccessible via conventional experimental diagnostic techniques. To investigate the localized kinematic transitions and flow uniformity within the R500Y structured packing matrix, cross-sectional velocity profiles were evaluated at three distinct axial planes for the R500Y packing: inlet, the middle core matrix, and outlet. Consequently, Figure 6 demonstrates the structure-resolved velocity magnitude distributions extracted from these simulations for the same velocity range as presented for static pressure profile. The local velocity scales are adjusted independently to capture the precise hydrodynamic features unique to each operational regime.

A primary phenomenon observed across all evaluated cross-sections is the severe localization of gas velocity within the open channels of the corrugated sheets, which culminates in intense, localized interstitial jetting. To quantify this behaviour, a detailed analysis of the peak local velocities ($u_{loc,max}$) relative to the nominal superficial inlet velocities (u_V) was conducted. The resulting data reveals a highly consistent geometric acceleration ratio across disparate flow regimes, demonstrating an underlying kinematic scaling invariance within the R500Y packing matrix.

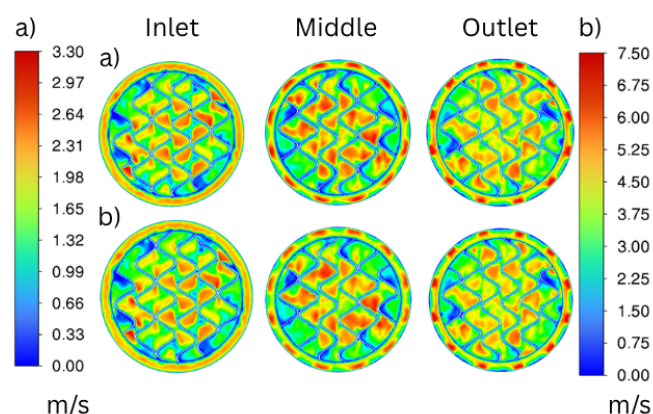


Figure 6. The velocity profile of cross-sectional area in standard metallic structured packing R500Y: a) $u_V = 1.5$ m/s, b) $u_V = 3.5$ m/s. Column diameter: $d_s = 0.05$ m.

When evaluating the primary independent operational variable, the u_V scales from 1.50 m/s in Case a under low vapour load conditions to 3.50 m/s in Case b under high vapour load conditions. This operational adjustment establishes a distinct baseline velocity scale factor of 2.33. Looking at the corresponding internal flow response, the $u_{loc,max}$ tracks this upward trend closely, rising from approximately 3.30 m/s under the low vapour load regime to approximately 7.50 m/s during the high vapour load execution. This yields a peak local scale factor of 2.27, which aligns closely with the baseline input scaling.

To establish a dimensionless framework for this localized phenomenon, the dimensionless acceleration ratio (R_{acc}) is utilized, defined by the hydrodynamic relationship:

$$R_{acc} = \frac{u_{loc,max}}{u_V} \quad (7)$$

Evaluating this parameter yields an R_{acc} value of 2.20 for Case a and 2.14 for Case b. The marginal variance between these two values represents a calculated deviation of less than 3%. This remarkably low deviation provides robust evidence of kinematic scaling invariance within the column. It confirms that the physical acceleration of the gas phase is fundamentally governed by the structural constraints and local void fraction variations of the cross-corrugated channels rather than macro-scale Reynolds number variations or turbulent velocity fluctuations. The narrow passages within the R500Y packing elements consistently force the localized gas streams to more than double their velocity to satisfy mass continuity, ensuring that high-shear micro-environments remain active across the entire stable operating envelope of the column.

Deconstructing the structure-resolved velocity fields sequentially from the packing inlet plane to the discharge zone reveals the highly complex spatial flow dynamics operating within the column. This axial evolution highlights how the gas phase transitions from an unconstrained stream into a highly ordered, geometrically restricted flow matrix before discharging into the column headspace.

Regarding the packing inlet plane, a high-velocity ring forms next to the column wall due to the wall-bypass effect. Because the corrugated sheets terminate against the smooth column shell, the local void fraction is highest here, creating a path of least resistance that causes gas to channel along the perimeter.

Deeper within the middle plane inside the core matrix, the flow adapts directly to the criss-cross geometry. High-velocity jets travel through the corrugation valleys are visible in Figure 6. The k - ϵ model effectively captures sharp velocity gradients between these core jets, which scale from 3.0 to 7.0 m/s in Case b, and the slow wake regions under 1.5 m/s, shown behind the corrugated peaks.

At the final packing outlet plane near the exit, the gas discharges as localized jet fingers rather than a uniform plug flow. The inclined packing plates act as internal guide vanes, forcing the gas along parallel planes up to the discharge point and leaving a clear pattern of macroscopic maldistribution.

These spatial variations create a direct trade-off between micro-scale efficiency and macro-scale maldistribution. On the micro-scale, the sharp velocity gradients generated in the packing core increase local shear stress and micro-mixing at the gas-liquid boundary. This behaviour thins the resistance layers and significantly increases the local gas-phase mass transfer coefficient (k_G).

On the macro-scale, however, the persistent wall-bypass streams and outlet jetting cause severe flow maldistribution. If the liquid feed is not tailored to match these local gas velocity variations, the high-velocity zones risk causing liquid entrainment or localized packing dry-out, while the low-velocity wakes suffer from poor mass transfer due to an insufficient driving force.

In conclusion, while the internal geometry of the R500Y packing successfully generates the turbulent shear needed for high local efficiency, its macro-scale channeling tendencies create a critical design constraint that requires high-performance peripheral liquid distributors to prevent overall performance loss.

5.3. Evaluation of dry pressure drop via experimental methods and CFD simulation

To validate this new method for predicting the flooding gas velocity using CFD, modelling of dry pressure drop and combination with SBD model experimental hydraulic investigations were conducted. These were performed using a laboratory distillation plant, which is shown in Table 3. Experiments were carried out under low and atmospheric pressures ranging from 0.3 bar to 1 bar, as detailed in Table 3 and shown in Figure 7.

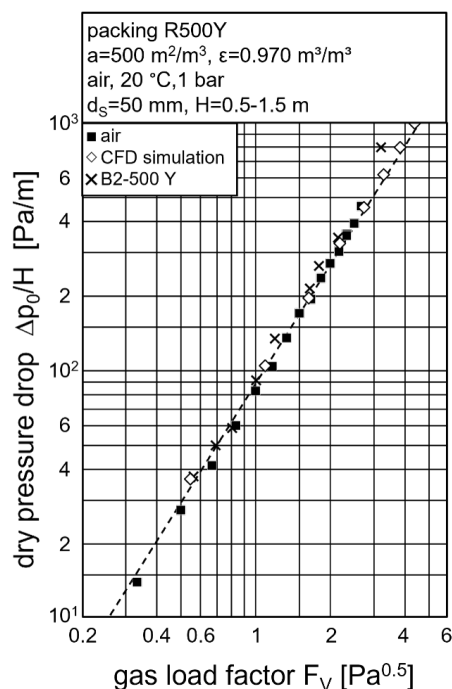


Figure 7. Comparison of experimental and CFD results for single-phase flow in a packed column filled with metallic structure packing R500Y and for comparison with structure packing of type B2-500Y (Montz) – data taken from literature (Maćkowiak, 2010).

A comprehensive description of the experimental procedure is provided in the collaborative study between academia and industry (Neumann et al., 2025).

In addition to the primary hydraulic parameters, this investigation elucidates the critical role of peripheral elements, specifically wipers, on the global hydrodynamic behaviour of the structured packing. The observed influence of these boundary features aligns with established literature, confirming their necessity in achieving uniform fluid distribution and minimizing wall effects (Figure 7 and Figure 8).

Table 3. Physical properties of the used test systems and technical data of the structured packing.

Packing data:	d_s	H	p_T	T	ρ_V	μ_V	$F_{V,fl,exp}$	$F_{V,fl,CFD}$	$\delta(F_{V,fl})$
Packing R500Y (RVT), $a = 500 \text{ m}^2/\text{m}^3$, $\varepsilon = 0.970 \text{ m}^3/\text{m}^3$, $\varphi_P = 0.795$	[m]	[m]	[mbar]	[K]	[kg/m ³]	[mPas]	[Pa ^{1/2}]	[Pa ^{1/2}]	[%]
air	0.05	1.0	1013	293	1.20	0.0181	—	—	—
	0.052	1.5	1013	293	1.20	0.0181	—	—	—
cyclohexane /		0.5	950	360	2.90	0.0079	2.20	2.23	−1.4
n -heptane	0.05	1.0	300	327	1.00	0.0069	2.33	2.43	−4.3
$\dot{L}/\dot{V} = 1$		1.5	300	327	1.00	0.0069	2.33	2.43	−4.3
ethanol / n -butanol			950	364	1.62	0.0098	2.40	2.54	−5.8
$\dot{L}/\dot{V} = 1$	0.05	0.5	300	345	0.60	0.0090	2.71	2.63	+3.0
ethanol / water			300	345	0.45	0.0140	2.60	2.80	−7.7
$\dot{L}/\dot{V} = 1$	0.05	0.5	300	345	0.45	0.0140	2.60	2.80	−7.7

The knowledge of the dependency of resistance factor $\psi = f(\text{Re}_V, \varphi_P)$, see Figure 8, is the most important factor for the prediction of the flooding condition of the packing and also BPD data for all types of random and structured packing (Maćkowiak, 2010; 2022a).

According to this model, the flooding gas load factor $F_{V,fl}$ was calculated from CFD data and compared with the experimental values (Table 2). Quantitative analysis reveals a superior level of agreement between the experimental observations and the simulated datasets, with a maximum relative error of $\pm < 8\%$, as detailed in Table 2.

On the base of the experimental and CFD simulated dry pressure drop data of Figure 7 the dependency of the resistance

of factor $\psi = f(\text{Re}_V, \varphi_P)$ as function of the gas Reynolds number (Eq. 8a–8c) was evaluated according to Maćkowiak (2022a) for both structure packing R500Y and B2-500Y and presented in Figure 8. According to experimental data of Figure 8, the packing form factor $\varphi_P = 0.795$ was estimated.

$$\frac{\Delta p_0}{H} = \psi(\text{Re}_V) \frac{1 - \varepsilon}{\varepsilon^3} \frac{F_V^2}{d_p} \quad (8a)$$

$$\psi(\text{Re}_V) = \psi_0(1 - \varphi_P) \quad (8b)$$

$$\psi_0 = \frac{725.6}{\text{Re}_V} + 3.203 \quad (8c)$$

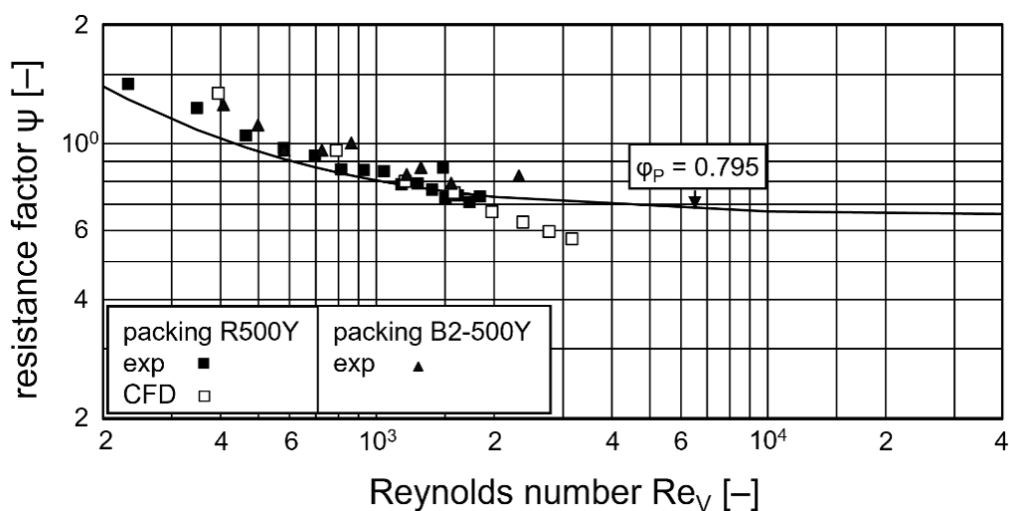


Figure 8. Resistance factor ψ as function of Reynolds number of gas $\psi = f(\text{Re}_V, \varphi_P)$ for investigated structured packing R500Y and for comparison the experimental data taken from literature (Maćkowiak, 2010).

5.4. Evaluation of flooding load diagram generated according to SBD model and CFD simulation

According to the SBD model (Maćkowiak, 2010) on the basis of the estimated form factor φ_P (Eq. 8b), the flooding gas load velocity $u_{V,fl}$ and often flooding gas load factor $F_{V,fl}$ can be predicted at different specific liquid loads u_L , Eq. (9).

$$u_{V,fl} = 0.566 \varepsilon^{\frac{6}{5}} \psi^{-\frac{1}{6}} \left(\frac{d_T \Delta \rho g}{\rho_V} \right)^{\frac{1}{2}} \left(\frac{d_h}{d_T} \right)^{\frac{1}{4}} K_{\rho_V} (1 - h_{L,fl}^0)^{3.5} \quad (9)$$

The dependency of the flood load factor $F_{V,fl}^*$ as function of the flow parameter X_{fl} (Eq. (1)) related to the operating condition on flooding point as maximum capacity range of the investigated packing R500Y is presented in Figure 9, and additionally for comparison for the structured packing B2-500Y. The experimental data was taken from the literature (Maćkowiak, 2010). The comparison shows that the basic performance data for both packings are very similar.

Ultimately, this research substantiates that the synergistic integration of CFD simulations and the SBD model provides a robust, rapid, and highly reliable methodology. By leveraging these high-accuracy CFD results as a primary predictive tool, the necessity for resource-intensive experimental campaigns is significantly mitigated, facilitating the streamlined modelling, optimisation, and scaling of structured packing performance data without the traditional reliance on extensive empirical testing.

5.5. Turbulence model selection and future directions

The selection of the $k-\varepsilon$ model for this investigation was driven by the necessity to balance physical accuracy with computational feasibility. While the Transition SST model is superior for resolving the precise physics of boundary layer detachment, the $k-\varepsilon$ model provides a robust framework for performing the extensive parametric studies required to establish macroscopic pressure drop baselines across varied vapour loads. The validation confirms that, when integrated with appropriate wall-treatment techniques, the $k-\varepsilon$ model effectively captures the dominant form drag effects induced by the R500Y packing geometry, the primary driver of resistance within our studied operational envelope. This approach ensures high-fidelity results for industrial-scale hydrodynamic modelling without the prohibitive computational costs associated with resolving the viscous sublayer in highly complex, multi-channel structures.

Building upon these findings, future work will focus on integrating mass transfer coefficients into the structure-resolved CFD framework. While this study characterizes the dry pressure drop and internal flow mechanics of the R500Y matrix, extending the model to include liquid-phase interactions, such as film thickness distribution and surface renewal rates, will provide a more holistic understanding of column efficiency. Additionally, we intend to perform a comparative study using the Transition SST model on a localized segment of the

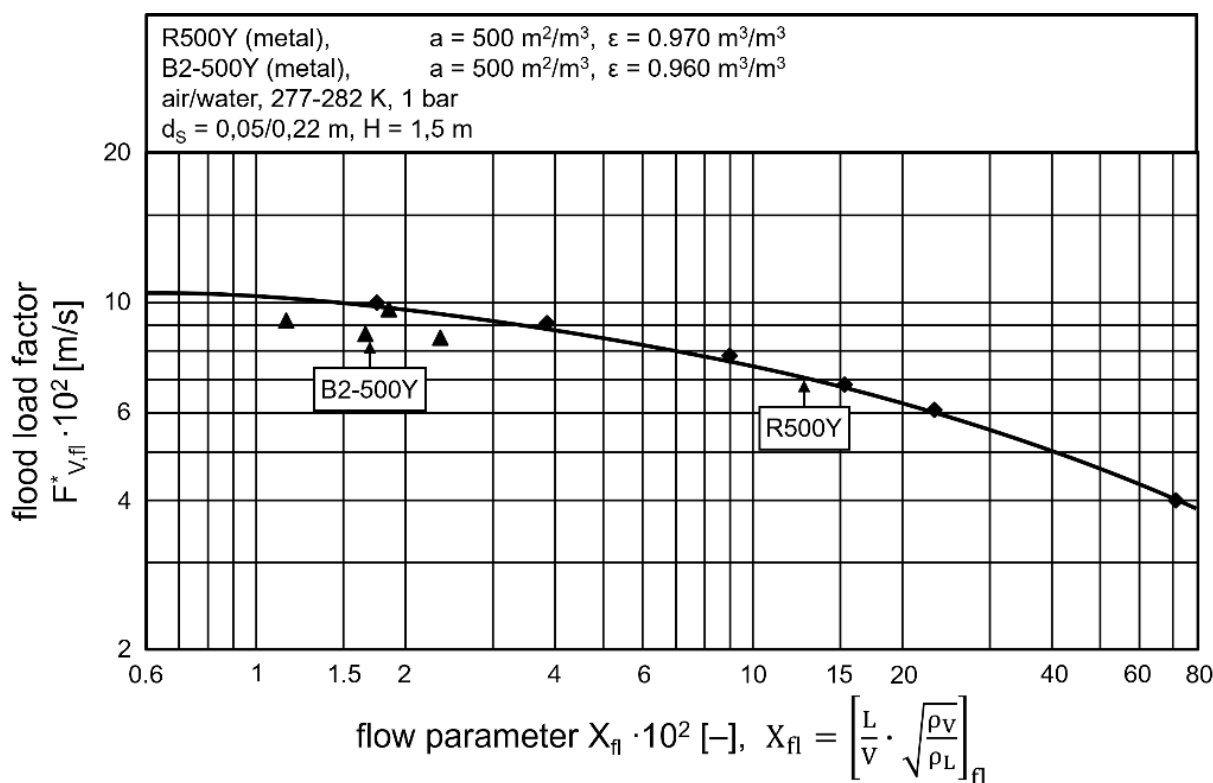


Figure 9. Capacity diagram for structured packing R 500Y and Montz B2-500 Y.

packing. This will validate the accuracy of the current k - ϵ model in capturing the nuances of boundary layer detachment at the corrugated crests and quantify the influence of transition-sensitive effects on the overall drag coefficient.

6. CONCLUSIONS

This study successfully introduces a novel predictive framework that couples high-resolution, structure resolved CFD simulations with the SBD model developed by Maćkowiak (2010) and 2022b. Operating in a systematic three-phase sequence, hydrodynamic baseline determination, resistance coefficient estimation, and flooding velocity prediction, this method achieves a mathematically rigorous transition from micro-scale local fluid dynamics to macro-scale column capacity forecasting.

The main findings and contributions of this work are summarized as follows:

1. By utilizing baseline dry pressure drop datasets from CFD to estimate the packing-resistance factor (ψ) and in the next form factor (φ_p), the framework analytically generates complete flooding gas load diagram for different operating conditions without relying on preliminary laboratory trials (Figure 9).
2. The main step is estimation of dry pressure drop of the investigated packing using CFD simulation as shown in Figure 1a and afterwards the resistance factor. At the end, the flooding load diagram as shown in Figure 9 can be generated.
3. The predictive workflow was rigorously validated against high-fidelity, independent CFD simulations configured for the commercial structured packing R500Y. The numerical grid successfully captured micro-scale gas-phase shear interactions and localized momentum transfer vectors, demonstrating excellent parity with physical pilot-plant measurements.
4. The described way for generation of the range of flooding gas velocity and flood load diagram under different operating condition as presented in Figure 9 and also the all BPD data using CFD simulation reduces extremely the time of the experimental investigations using different test system under distillation and absorption condition and as result also an experimental effort.
5. The determination of BPD – the basic performance data was executed via the SBD model, utilising the theoretical modelling established by Maćkowiak (2010) and 2022b.
6. The correlation between the CFD-derived values and the analytical model is very good; the simulation successfully captured the intricate gas-phase interactions and momentum transfer within the packing geometry with exceptional resolution.
7. The systematic nature of this method allows for the precise optimization of packed bed operations. A very good

agreement was observed between the experimental measurements and the numerical predictions. This successful validation demonstrates that the integrated simulation approach provides a simple, fast, and reliable alternative to traditional physical testing. By achieving high predictive accuracy, this method significantly reduces the experimental effort required for the modelling, optimization, and performance prediction of high-efficiency structured packings in industrial separation processes.

8. This is the first study to demonstrate that CFD and SBD can be used to determine both the flooding limits and the operating window of a column for any packing geometry, as illustrated in Fig. 9, thereby addressing a key gap in the published literature summarized in Table 1.

SYMBOLS

a	specific packing area, m^2/m^3
$C_{fi,0}$	universal flooding-point constant for packing, –
d_s	column diameter, m
d_h	hydraulic diameter of packing, m ($d_h = 4\epsilon/a$)
d_p	particle diameter, m
d_T	droplet diameter according to Sauter, m
f	external force exerted on the fluid, N
F_V	gas load factor in relation to full column cross section, $\text{Pa}^{0.5}$
$F_{V,fi}^*$	flood load factor, m/s
g	acceleration due to gravity, m/s^2
H	height of packed column, m
$h_{L,fi}^0$	liquid hold-up at flooding point, based on free column volume, m^3/m^3
K	wall factor (Maćkowiak, 2010), $K = 1$ for structured packing
k	turbulence kinetic energy, m^2/s^2
L, V	liquid and gas mass flow, kg/h
$\dot{L}, \dot{V}$	liquid and gas molar flow, kmol/h
p	pressure, Pa
P_k	rate of production of turbulent kinetic energy, $\text{kg}/(\text{ms}^3)$
p_T	top pressure, mbar
$\Delta p_0/H$	dry pressure drop per 1 m packing height, Pa/m
$\Delta p/H$	pressure drop per 1 m packing height for two phase flow and wetted packed bed, Pa/m
Re_V	gas-phase Reynolds number, –
t	time, s
$u, \mathbf{u}$	velocity / velocity vector, m/s
u_V	linear gas velocity in relation to full column cross section, m/s
$u_{V,fi}$	gas or vapour velocity at the flooding point, based on the cross-sectional area of an empty column, m/s
X_{fi}	flow parameter related to condition at flooding point, –
y^*	dimensionless distance from the wall, –

Greek symbols

α	flow channel angle, °
ε	energy dissipation rate, m^2/s^3
ε	void fraction of packing, m^3/m^3
$\mu, \mu_{\text{eff}}, \mu_t$	molecular, effective and turbulent dynamic viscosity, $\text{kg}/(\text{m} \cdot \text{s}^2)$
τ	deviatoric stress tensor, Pa
φ_P	packing form factor (Maćkowiak, 2010), –
ν_V	kinematic viscosity of gas or vapour, m^2/s
ρ	density, kg/m^3
ρ_L, ρ_V	densities of liquid and gas phase, kg/m^3
ψ	resistance coefficient for single gas flow, –

Dimensionless numbers

d_p	particle diameter, $d_p = \frac{6(1-\varepsilon)}{a}$
Re_V	Reynolds number for gas or vapour, $\text{Re}_V = \frac{u_V d_p}{(1-\varepsilon)\nu_V} K$
X_{fl}	flow parameter related to condition at flooding point, $X_{\text{fl}} = \left(\frac{L}{V}\right)_{\text{fl}} \sqrt{\frac{\rho_V}{\rho_L}}$
$F_{V,\text{fl}}^*$	flood load factor, $F_{V,\text{fl}}^* = \frac{F_{V,\text{fl}}}{\sqrt{\rho_L - \rho_V}}$

Abbreviations

BPD	basic performance data (Maćkowiak, 2022b)
CFD	computational fluid mechanics
SBD	suspended bed of droplets (Maćkowiak, 2010)

Subscripts

L, V	liquid and gas phase,
fl	at flooding point,

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