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## Pressure Vessel Optimization and Separator Internals Redesign Based on Fluid Dynamics and Structural Simulation

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### Abstract

This paper investigates the optimization of pressure vessels and separator internals through fluid dynamics and structural simulation techniques. In industries such as oil & gas, chemical processing, and petrochemicals, pressure vessels and separators are critical for ensuring safe, efficient, and cost-effective operations. As operational demands increase and regulations tighten, optimizing these systems for enhanced performance and reliability becomes imperative. Using advanced computational tools such as Computational Fluid Dynamics (CFD) and Finite Element Analysis (FEA), this paper explores methods for optimizing pressure vessel geometries and separator internals. The study highlights key optimization strategies, including the redesign of internal components to improve phase separation, reduce pressure drop, and minimize entrainment. Furthermore, structural simulations are used to analyze stress, fatigue, and buckling under dynamic loads, facilitating the reduction of material usage without compromising safety. Case studies demonstrate the practical application of these simulations in redesigning separator internals and optimizing pressure vessel wall and nozzle configurations. The integration of design tools into engineering workflows via CAD-CAE co-simulation and digital twin technologies offers significant advantages for real-time feedback and operational monitoring. The paper concludes with recommendations for best practices in incorporating simulations into the design and operational stages, emphasizing interdisciplinary collaboration and lifecycle analysis to ensure sustainable and efficient system designs.

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### 1. Introduction

#### 1.1 Overview of pressure vessels and separators in process industries

Pressure vessels and separators are fundamental components within a wide range of industrial systems, particularly in the oil and gas, chemical processing, and petrochemical sectors. These components are engineered to contain fluids under varying pressure and temperature conditions, making them essential for processes such as storage, phase separation, and chemical reactions <sup>[1]</sup>. Separators, often integrated within pressure vessels, are designed to facilitate the physical separation of mixed-phase fluids—typically gas-liquid or liquid-liquid—using internal devices like demisters, baffles, or cyclones <sup>[2]</sup>.

Given their critical function in process reliability, the design and operation of these systems must meet stringent codes and standards, such as those outlined in ASME Boiler and Pressure Vessel Code (BPVC) <sup>[3]</sup>. The structural integrity, pressure

containment capabilities, and separation efficiency directly influence plant safety, product quality, and operational continuity. Therefore, engineering efforts to improve these systems are central to maintaining high performance and minimizing the risk of catastrophic failures or process downtime <sup>[4]</sup>.

## 1.2 Need for optimization and redesign in modern engineering context

In recent years, the need to redesign and optimize pressure vessels and separators has become increasingly important due to evolving industry demands and external pressures. Environmental regulations are tightening across regions, requiring facilities to minimize emissions, reduce waste, and improve process efficiency—goals that can be achieved through better separation performance and lighter, more efficient pressure vessel construction <sup>[5]</sup>.

At the same time, process industries are shifting toward higher-pressure operations to maximize throughput and accommodate complex feedstocks, which requires more robust and precisely engineered vessels. Material cost and availability also drive the need for efficient use of structural materials without compromising safety <sup>[6]</sup>. Furthermore, the integration of digital design tools and sensor-based monitoring systems in modern engineering practices enables a data-driven approach to equipment optimization. In this context, conventional design methods are increasingly being replaced or supplemented by simulation-driven design, enabling faster iterations, better flow control, and more resilient structural performance under varied operational scenarios <sup>[7]</sup>.

## 1.3 Objectives and scope of the study

This paper aims to explore how advanced engineering simulations—specifically computational fluid dynamics (CFD) and structural simulations—can be systematically applied to optimize the geometry and internal design of pressure vessels and separators. The primary objective is to demonstrate how simulation models can lead to improved fluid flow management, reduced material stress concentrations, and increased separation efficiency within the constraints of real-world operational environments. Through a comprehensive analysis of internal flow behavior, pressure differentials, and stress distribution, the study seeks to inform engineering decisions related to vessel sizing, internal arrangement, and material specification.

Additionally, the paper investigates how simulation tools can be integrated into the design workflow to streamline engineering practices and ensure compliance with industry codes. By focusing on both fluid and structural performance, the scope encompasses the holistic redesign of vessel systems—improving reliability, safety, and cost-effectiveness in applications where performance and compliance are paramount.

## 2. Theoretical background and design principles

### 2.1 Fundamentals of pressure vessel design and failure mechanisms

Pressure vessel design is fundamentally governed by the principles of stress analysis and material mechanics, which ensure the vessel's ability to withstand internal pressure without yielding or failing. Key parameters influencing design include internal pressure, vessel diameter, wall thickness, material properties, and the nature of the contents

(e.g., corrosiveness, temperature) <sup>[8]</sup>. The vessel must be engineered to prevent catastrophic failures, adhering to design codes that define permissible stress limits and safety factors. These guidelines ensure that the structural capacity exceeds the maximum anticipated operational conditions <sup>[9]</sup>. Failure mechanisms in pressure vessels commonly include fatigue, which occurs due to cyclic loading; buckling, which results from compressive stresses in thin-walled sections; and brittle fracture, which is influenced by low-temperature operations and stress concentrations <sup>[10]</sup>. Corrosion and erosion also pose significant risks, especially when operating in chemically aggressive environments or with abrasive fluids. Accurate modeling of these failure risks is essential to determine inspection intervals, predict service life, and define appropriate maintenance strategies <sup>[11]</sup>.

Stress analysis, both analytical and simulation-based, plays a pivotal role in the design process. By assessing primary membrane stresses, bending stresses, and localized stresses around nozzles and supports, engineers can optimize wall thickness and reinforce vulnerable regions <sup>[12]</sup>. Modern structural simulations enable the evaluation of these stresses under complex loading conditions, including thermal expansion and seismic forces. This theoretical foundation ensures that pressure vessels are designed to operate safely over extended lifecycles while maintaining cost-efficiency and regulatory compliance <sup>[13]</sup>.

### 2.2 Separator internals: functions, flow regimes, and efficiency drivers

Separator internals are critical components that influence the phase separation process within multiphase flow systems. Their primary function is to promote the effective separation of gas, liquid, and sometimes solid phases by controlling fluid flow paths, reducing turbulence, and enhancing residence time <sup>[14]</sup>. Common internals include inlet diverters, demister pads, vane packs, cyclones, baffles, and weirs. Each internal component is tailored to a specific task—such as momentum reduction, droplet coalescence, or phase collection—ensuring a high-efficiency separation process <sup>[15]</sup>.

The effectiveness of these internals depends significantly on the prevailing flow regimes, which are determined by fluid properties, flow rates, and vessel orientation. For instance, stratified and annular flow patterns require different internal configurations than mist or slug flow. Understanding these regimes allows engineers to design internals that maximize droplet settling, minimize re-entrainment, and maintain stable liquid interfaces. Pressure drop and flow maldistribution must also be minimized to ensure consistent separator performance across operating conditions <sup>[16]</sup>.

Designing efficient separator internals requires a balance between hydraulic performance and mechanical robustness. Internals should not only improve separation but also withstand the dynamic loads and flow-induced vibrations inherent to high-capacity operations <sup>[17]</sup>. Innovations in internal geometry, such as 3D vane structures and high-surface-area mesh pads, have enhanced the efficiency of separation without significantly increasing pressure loss. These theoretical considerations guide the selection and placement of internals, ensuring optimal separator performance across a wide range of industrial applications <sup>[18]</sup>.

### 2.3 Application of fluid dynamics and structural mechanics in design

The application of fluid dynamics in vessel and separator design centers on solving the Navier–Stokes equations to predict flow behavior, pressure gradients, and turbulence characteristics. These equations govern the motion of fluids and are essential in modeling complex multiphase flow patterns encountered in separators. Computational simulations allow engineers to visualize flow fields, identify zones of stagnation or high turbulence, and optimize internal configurations to ensure even fluid distribution and efficient separation.

In parallel, structural mechanics provides the framework for analyzing stress and deformation under operational loads. Finite element analysis (FEA) is widely used to evaluate stress concentrations around nozzles, support brackets, and weld seams. This analysis is critical for preventing local failures due to fatigue, thermal gradients, or mechanical loads. Transient simulations further enhance the design process by accounting for pressure surges, start-up conditions, and operational transients that may not be captured in steady-state analysis<sup>[19, 20]</sup>.

Combining fluid dynamics with structural mechanics offers a powerful integrated approach to vessel and separator design. By coupling fluid simulations with structural response models, designers can assess the impact of dynamic flow forces on structural integrity in real time. This holistic methodology leads to more resilient and efficient designs, reducing the need for costly overengineering and minimizing operational risks. These principles form the theoretical backbone of simulation-driven design, enabling continuous improvement in industrial process equipment.

## 3. Simulation models and optimization techniques

### 3.1 CFD modeling of internal flow distribution and phase behavior

Computational fluid dynamics (CFD) modeling has become an indispensable tool in the analysis and design of pressure vessels and separators, particularly in the study of internal flow distribution and multiphase phase behavior. By numerically solving the Navier–Stokes equations and incorporating turbulence models such as  $k-\epsilon$ ,  $k-\omega$  SST, or Large Eddy Simulation (LES), CFD enables engineers to replicate the internal dynamics of fluids under a range of operating conditions. These simulations reveal how fluid streams interact with internals, where vortices form, and how momentum is transferred within the separator<sup>[21, 22]</sup>.

An essential aspect of CFD in this context is the modeling of multiphase flow regimes—typically gas-liquid or liquid-liquid—and their transition behaviors. Accurate phase tracking using Volume of Fluid (VOF), Eulerian-Eulerian, or Lagrangian multiphase models allows for detailed analysis of droplet separation, interface stability, and entrainment phenomena. Inlet momentum dampening structures such as perforated baffles or vane-type diffusers are tested virtually to optimize energy dissipation and flow homogenization before fluid reaches the separation zones<sup>[23, 24]</sup>.

The insights from CFD modeling not only improve the geometric placement and orientation of internal components but also reduce trial-and-error in physical prototyping. Design alternatives can be rapidly tested and compared based on performance metrics such as pressure drop, residence time, and separation efficiency. This simulation-led design approach allows for data-driven optimization of vessels,

reducing costly design errors and improving operational stability in demanding industrial environments<sup>[25, 26]</sup>.

### 3.2 Structural simulation for stress, fatigue, and buckling analysis

Structural simulation complements fluid dynamic analysis by validating the mechanical performance of the vessel under operational and accidental loads. Using finite element analysis (FEA), engineers can model the response of the vessel's shell, nozzles, and supports to static and dynamic stressors, such as internal pressure, thermal gradients, and seismic forces. These simulations verify that stresses remain within allowable limits as defined by regulatory codes, thereby ensuring the vessel's long-term integrity and safe operation.

Stress analysis includes evaluation of membrane stresses in cylindrical and spherical sections, as well as localized stress concentrations at discontinuities such as welds, manways, and flange connections. Fatigue analysis, especially critical in cyclic service conditions, predicts the number of operational cycles before crack initiation. This analysis helps define maintenance schedules and informs material selection to enhance fatigue resistance. Similarly, buckling simulations are crucial for thin-walled designs where external pressure or compressive forces can cause structural instability<sup>[27, 28]</sup>.

Thermal simulations further evaluate the effect of rapid temperature changes or prolonged thermal exposure, which can lead to expansion-induced stress, warping, or material degradation. Coupled fluid-structure interaction (FSI) models enable engineers to assess how internal flow turbulence can induce mechanical vibration or oscillation in internals and wall structures. Together, these simulations offer a comprehensive validation of vessel design, reducing the risk of failure under both normal and extreme conditions<sup>[29, 30]</sup>.

### 3.3 Design iteration and optimization algorithms

To achieve optimal design outcomes, simulation results are often integrated with computational optimization algorithms that automate and refine geometry and material usage. Topology optimization techniques, for example, iteratively remove unnecessary material from the vessel while preserving structural strength and functionality. This leads to weight reduction and cost savings without compromising safety. In the context of separator internals, topology optimization can produce novel baffle or vane configurations that maximize surface area while minimizing obstruction to flow.

Genetic algorithms—bio-inspired heuristic search methods—are used to explore large design spaces, particularly where multiple conflicting objectives exist, such as minimizing pressure drop while maximizing separation efficiency. These algorithms iteratively evolve design candidates by mimicking natural selection, allowing for convergence toward globally optimal solutions. Combined with CFD and FEA tools, they enable rapid prototyping of design concepts that would be time-consuming to evaluate manually<sup>[31, 32]</sup>.

Response Surface Methodology (RSM) provides a statistical approach to modeling relationships between design variables and performance outputs. Through design of experiments (DoE) and regression analysis, RSM identifies optimal parameter sets for vessel dimensions, inlet orientation, and internal placement. These optimization tools are applied in compliance with design codes such as ASME Section VIII,

ensuring regulatory adherence while innovating beyond traditional rule-based design. The integration of these computational techniques results in pressure vessels and separators that are not only code-compliant but also highly efficient, manufacturable, and durable [33-35].

#### 4. Case studies and engineering applications

##### 4.1 Redesign of vertical and horizontal separator internals

In industrial applications, separator internals play a pivotal role in optimizing phase separation efficiency, which directly impacts operational costs and system performance. In one case study, CFD-informed redesigns of both vertical and horizontal separators demonstrated significant improvements in separation efficiency and pressure loss reduction. Prior to the redesign, traditional internal layouts—comprising baffles, weirs, and cyclonic separators—had limitations in managing complex multiphase flow regimes, leading to issues like phase re-entrainment and uneven flow distribution. By applying CFD simulations, engineers tested a variety of new internal configurations that improved fluid mixing, momentum dissipation, and droplet coalescence.

The redesigned separator internals showed enhanced phase separation performance, achieving a reduction in entrained liquid and a decrease in overall pressure drop. Experimental validation through pilot-scale testing confirmed that the new configurations not only improved operational efficiency but also minimized energy consumption. These improvements were especially significant in separators operating under varying flow rates and temperatures, where the traditional designs often struggled to maintain stable performance. The case study demonstrated the potential of CFD to guide real-world redesigns, confirming that simulation-based optimization is crucial for improving separator functionality in complex industrial processes [36, 37].

##### 4.2 Pressure vessel wall and nozzle optimization under simulated loads

The optimization of pressure vessel walls and nozzle designs is essential to reducing material costs while maintaining safety margins. A case study focused on the redesign of pressure vessels subjected to internal pressure and dynamic thermal loads. Structural simulations, including finite element analysis (FEA), were employed to evaluate the vessel wall thickness, nozzle loading, and support design under various simulated conditions, such as fluctuating pressures and extreme temperature changes. Through this process, engineers identified areas where material could be reduced without compromising the structural integrity of the vessel [38].

By applying advanced optimization algorithms, such as topology optimization, the study successfully reduced the overall weight of the vessel by 10-15% while maintaining the required safety factors. In particular, the nozzle designs were optimized to minimize stress concentrations, a common weak point in pressure vessels. Material selection was also guided by simulation results, ensuring that the chosen materials offered the best performance under the expected operating conditions. This optimization led to a more cost-effective design, with reduced material waste and enhanced manufacturability, all while ensuring compliance with industry standards like ASME Section VIII [39, 40].

##### 4.3 Integration of design tools into engineering workflows

Incorporating simulation tools into early design stages is increasingly common in the engineering industry, enabling real-time analysis and optimization of pressure vessels and separator internals. In this case, a multidisciplinary engineering workflow integrated CAD (computer-aided design), CAE (computer-aided engineering), and digital twin environments for enhanced design feedback. By creating a digital twin of the separator or pressure vessel, engineers were able to simulate real-world operating conditions and make iterative design adjustments throughout the development process. This integration enabled continuous feedback loops, where design changes could be validated through simulation before physical manufacturing, significantly reducing the risk of errors and costly redesigns [41, 42].

The combination of CAD-CAE co-simulation allowed for seamless collaboration between design, structural analysis, and fluid dynamics teams. Engineers could explore multiple design alternatives in parallel, including modifications to vessel geometry, nozzle placement, and internal configurations, to identify the most efficient solutions. Furthermore, digital twins provided a dynamic platform for monitoring real-time operational performance, providing insights into long-term durability and efficiency under actual service conditions. This integrated approach to design enhances the decision-making process, ensuring that designs are not only optimized for performance but also aligned with practical manufacturing constraints and regulatory standards [43, 44].

#### 5. Conclusion

The application of simulation-driven optimization for pressure vessels and separator internals has demonstrated substantial improvements in both operational reliability and cost-efficiency. Through the use of computational fluid dynamics (CFD) and structural simulations, significant advancements have been made in the design of internal flow structures and vessel geometries, leading to better phase separation and reduced pressure losses. The optimization of nozzle designs, internal baffle configurations, and separator internals based on simulation results has not only increased separation efficiency but also minimized energy consumption, ensuring more sustainable operations.

Additionally, the ability to predict potential failure mechanisms such as fatigue, buckling, and material degradation using structural analysis has enhanced the safety and durability of pressure vessels. These simulations allow for material reduction without compromising strength, ultimately leading to cost savings in both material procurement and manufacturing. Moreover, the integration of digital twin technologies and real-time feedback mechanisms offers significant advantages in lifecycle management, improving asset monitoring, predictive maintenance, and operational performance. These engineering impacts highlight the growing importance of simulation in optimizing both design and operational performance within process industries.

To fully leverage the benefits of simulation-driven optimization, it is recommended that engineers adopt a holistic approach that integrates CFD, FEA, and optimization algorithms throughout the entire design cycle. Early-stage design should involve comprehensive simulation analysis to explore a range of possible configurations and identify the

most effective solutions for both performance and manufacturability. Additionally, multidisciplinary collaboration between fluid dynamics, structural, and materials engineers is critical to ensuring that each design component meets operational requirements while adhering to safety standards and regulatory guidelines.

The use of digital twin environments should also be encouraged to enable continuous monitoring and performance analysis during the operational phase. This allows for proactive identification of potential issues and facilitates predictive maintenance, reducing the risk of unplanned downtime. Furthermore, lifecycle analysis should be incorporated from the outset, ensuring that both short-term performance and long-term durability are considered in the design. By adopting these best practices, industry professionals can achieve more efficient, cost-effective, and safe pressure vessel and separator designs, while ensuring compliance with increasingly stringent environmental and safety regulations.

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