

# Chemical Reactor Design and Analysis: A Review

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## Abstract

*Chemical reactors play a critical role in industries such as oil and gas, chemical processing, and power generation, where they operate under extreme pressure and handle highly toxic, compressible fluids. The growing need for alternative energy sources has led to an increased demand for vessels capable of withstanding high pressure and temperature, especially in the chemical and petroleum industries. Recent innovations in chemical reactor technology have concentrated on creating new grades of materials, developing composites, and improving welding methods. Finite element analysis (FEA) has become an essential tool for examining fatigue and creep behavior, contributing to the enhancement of reactor designs. This review highlights recent advancements in the field of transient dynamic stress analysis, particularly focusing on the application of finite element analysis (FEA) as a tool for evaluating complex stress distributions in mixing chambers. FEA-based simulations have proven effective in predicting fatigue life and identifying critical failure zones, enabling engineers to redesign components for enhanced durability. Moreover, structural optimization techniques, such as topology optimization and design for fatigue resistance, are being increasingly integrated into reactor design workflows. Mixing chambers, a specific type of chemical reactor used in chemical industries, often experience deformation and distortion due to fluctuating pressure and temperature conditions, leading to high local stresses and reduced fatigue life. This review explores the latest advancements in transient dynamic stress analysis and the application of FEA for evaluating stress distribution, fatigue life prediction, and structural optimization of chemical reactors. By using computational fluid dynamics (CFD) and Multiphysics simulation tools such as ANSYS, engineers can analyze the impact of various nozzle configurations on both mechanical stress and fluid behavior. Additionally, the influence of nozzle design modifications on mixing efficiency is discussed, with a focus on computational validation using simulation tools such as ANSYS. By synthesizing recent developments in materials, design methodologies, and analytical techniques, this review provides insights into improving the resilience, efficiency, and operational safety of mixing chambers and high-performance chemical reactors across various industrial applications.*

**Keywords:** Reactors, finite element analysis (FEA), stress analysis, computational fluid dynamics (CFD), ANSYS

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## INTRODUCTION

Chemical reactors are vessels designed to handle highly toxic and compressible fluids at elevated pressures. These containers find applications across various sectors, including oil, gas, petroleum, beverage, chemical, power generation, food, and fertilizer industries [1]. The uses of chemical reactors extend to nuclear reactor vessels, pneumatic reservoirs, and storage units for liquefied gases. In recent decades, the growing demand for alternative fuels has necessitated the development of vessels capable of withstanding high pressures and temperatures in petroleum refineries and chemical plants. Significant advancements have

been made in the field of chemical reactors, particularly in areas such as new grade materials, composite materials, and welding techniques [2, 3]. Finite element analysis plays a crucial role in understanding fatigue and creep processes. In certain chemical industry applications, the mixing of liquid or gaseous chemicals occurs within enclosed chambers like chemical reactors.

A more comprehensive grasp of stress can be obtained through transient dynamic analysis [4–6]. This method is employed to assess structures under various time-dependent loads, enabling the determination of time-varying displacements, strains, and forces acting on components. In the context of mixing chambers, chemicals enter through nozzles at varying pressures and temperatures over time during operation [7].

These fluctuations in pressure and temperature lead to deformation and distortion, resulting in high localized stresses within the mixing chamber, which subsequently diminishes its fatigue life. Transient dynamic analysis is utilized to identify stress and deformation in chemical reactors. Consequently, the current research aims to conduct a transient dynamic stress analysis to evaluate stresses in structures subjected to general time-dependent loads. Additionally, fatigue life is predicted and improved through finite element analysis, which determines the time-varying displacements, strains, and forces acting on chemical reactors.

## LITERATURE REVIEW

A study employed a computational approach to model the initial transient flow in a vacuum ejector system. This system, which includes an ejector-diffuser, is commonly utilized in various applications, including refrigeration [8–10]. The researchers used numerical methods to simulate and examine the starting transient flows and performance characteristics of the supersonic vacuum ejector-diffuser system. Initial numerical findings indicate that chevrons have a beneficial impact on the vacuum ejector's performance, resulting in shorter starting times and lower secondary chamber equilibrium pressure compared to the convergent nozzle [11].

To simulate the equilibrium flows and flow dynamics behavior of the secondary chamber, researchers implemented a computational fluid dynamics (CFD) method utilizing a transient scheme. The design and development of tools for industry is a critical phase in the manufacturing process [12]. A study focuses on the design of filament-wound composite overwrapped chemical reactors, emphasizing their strength-to-weight advantages. Their tests show that these composite vessels withstand pressures up to 300 MPa with minimal deformation, offering a 25% weight reduction compared to traditional metal vessels [13]. The authors find that composite materials provide increased resilience under dynamic loading conditions, with failure strains reduced by 15–20% in optimized composite layers. These results support the use of composites in aerospace and marine applications where weight efficiency is paramount [14]. The study analyzes corroded pipelines with single defects under internal pressure, using finite element analysis (FEA) to quantify the impact of corrosion on structural integrity. They find that pipelines with defects of 5 mm depth experience a 30% reduction in burst pressure. For example, pipelines with this level of corrosion failed at around 150 MPa, whereas intact pipelines withstood pressures up to 220 MPa [15]. These results underscore the importance of regular inspections and timely repair in extending pipeline service life. An investigation examines the effects of varying winding angles on hoop stress in composite chemical reactors through FEA, aiming to enhance vessel design. They find that adjusting winding angles significantly reduces hoop stress, with optimal configurations decreasing stress by up to 20%. For instance, a winding angle of 55° showed the lowest stress concentrations, whereas non-optimal angles led to increases in stress by 10–15% [16]. The study highlights that adjusting winding angles not only enhances strength but also improves overall vessel stability under high-pressure conditions. These findings support the use of customized winding configurations to maximize performance in composite chemical reactors, particularly in aerospace and chemical applications where pressure tolerance is critical [17].

A study investigates crack-induced pressure intensity factors within cylindrical vessels using FEA, discovering that crack position plays a significant role. They find that cracks positioned closer to the vessel's midsection (within 10 cm) resulted in pressure reductions of 20–30%, compared to cracks located near the edges [18]. For example, a vessel with a midsection crack failed at 180 MPa, while one with an edge crack maintained structural integrity up to 250 MPa. This study provides valuable insights for optimizing vessel inspection and maintenance routines, with a focus on midsection crack management. A study investigates the influence of semi-elliptical cracks on chemical reactor failure, focusing on stress intensity and fracture patterns [19]. Using FEA, they find that crack depth and shape greatly impact failure risk, with vessels featuring deeper cracks (over 2 mm) experiencing stress intensities that increase by nearly 30% compared to shallower cracks. For example, a semi-elliptical crack with an aspect ratio of 0.6 resulted in a 25% reduction in pressure tolerance [20]. Their results suggest that even minor deviations in crack geometry can lead to a marked increase in the likelihood of vessel rupture. These findings underscore the need for strict monitoring of crack morphology in chemical reactors to maintain structural safety. Study uses genetic algorithms alongside FEA to optimize the design of composite cylindrical pressure hulls [21]. They find that optimal configurations increase hull strength by 30% while reducing weight by 15%, beneficial for marine applications. For example, hulls optimized for thickness and layering withstand pressures up to 250 MPa, compared to standard designs which failed at 180 MPa [22]. The research outcomes support sophisticated design strategies for improving structural performance in underwater environments. Internal mixing chamber twin-fluid nozzles can be used as an effective replacement for conventional Y type nozzles in atomizing high viscosity fluids [23]. A study conducted at industrial power plants, focusing on how operating conditions affect the resulting Sauter Mean Diameter (SMD) for a specific fuel oil [24]. Their parametric analysis revealed that the calculated SMD decreases when the fuel oil-to-steam pressure ratio approaches 1. The smallest SMD is achieved when the fuel oil and steam inlet pressures are very close to the power plant's design specifications. Consequently, this nozzle was implemented in a power plant [25].

A study examines the burst strength of chemical reactors with varying wall thicknesses. Their Finite Element Analysis (FEA) results demonstrate that increasing the wall thickness from 10 mm to 15 mm enhances burst strength by about 40%, while a 5 mm reduction in thickness can decrease burst resistance by up to 25%. For thin-walled vessels, burst strength averaged around 200 MPa, while thick-walled vessels withstood up to 350 MPa. These findings help guide vessel design across industries, supporting the need for tailored thickness requirements based on operational pressures [26–28].

The research utilized computational fluid dynamics (CFD) to investigate mixing processes and determine the duration required for mixing in a jet-mixed tank. They conducted three-dimensional simulations using FLUENT 6.2, a CFD software package, to generate data and compare it with experimental findings [29]. In a separate study, examined stress distributions in a horizontal chemical reactor and its saddle supports. The research employed 3D finite element analysis to reveal stress patterns in various components of the saddle, including wear webs, flanges, and base plates. The investigation explored the impact of altering load and geometric parameters, leading to recommendations for optimal ratios [30–33]. These included the proportion of support distance from the vessel's end to the vessel's length, as well as the ratio of vessel length to vessel radius, both aimed at minimizing stresses in the chemical reactor and saddle structure. A review of Finite Element Methodology (FEM) applications in fusion welding, focusing on predictive accuracy in thermal and mechanical outcomes [34]. They find that advanced FEM models predict heat-affected zones within a 5% margin of experimental results, significantly improving process control. Their study also demonstrates that optimized FEM techniques can reduce welding defects by up to 15%, providing a basis for selecting suitable FEM methods for specific welding challenges [35]. The study aimed to evaluate the mixing effectiveness of three Hartridge-Roughton mixer designs with comparable dimensions and identical inlet flow rates. The mixing efficiency of these mixers was assessed using a separation index. The research found that incorporating a distinct mixing chamber before a narrower outlet pipe enhanced mixing efficiency [36]. In the mixer lacking a separate mixing chamber, the flow

exhibited a double spiral pattern. All three mixers achieved mixing times under minutes, with the mixer featuring a narrowing end achieving times below 1 min. The researchers suggested using a mixer with conical narrowing due to its high mixing efficiency. A separate study examined crack propagation and burst pressure in pipelines with longitudinal cracks using an advanced FEA method. Their results show that increasing crack length from 10 mm to 20 mm reduces burst pressure by approximately 35% [37–39]. For instance, pipelines with 20 mm cracks failed at pressures around 180 MPa, while those with shorter cracks-maintained integrity up to 240 MPa. This study highlights the critical role of early crack detection to prevent catastrophic pipeline failure.

A study explores the impact of stress concentration elements, such as notches, on chemical reactor failure. Their FEA results show that these elements increase localized stress by as much as 50%, leading to earlier failure in tested vessels. For example, a vessel with a notch of 1.5 mm depth failed at 175 MPa, while a similar vessel without a notch sustained pressure up to 260 MPa [40]. These findings highlight the importance of minimizing stress concentration elements in vessel design to enhance durability, particularly in applications with high cyclic loads. The study performed a transient dynamic analysis on the tube sheet, which functions as a filter in filter tubes. The analysis yielded maximum stress and deformation values, which were then utilized to determine the infinite fatigue life of the tube sheet. This transient dynamic analysis was conducted to obtain the highest stress and deformation in the tube sheet, with the resulting maximum stress values being used to calculate its fatigue life [41]. A study executed a transient finite element analysis on a balanced stiffness valve to assess time-varying displacements, stresses, strains, and forces in valve components. The study observed the performance of the Balanced Stiffness Valve, specifically the movement of pressure plates [42]. As the supply pressure is applied to the pressure plate, the plate area is immediately exposed to fluid flow, necessitating an examination of the valve's time-dependent dynamic response. The analysis revealed that the maximum stress developed remained within acceptable safety limits, and the deformation was sufficient for valve performance. The research conducted a finite element analysis of a pressurized vessel nozzle interaction with wall thinning damage [43]. They investigated the impact of a specific tee joint on the stress concentration factor of varying wall thinning damage. The study found that the largest force occurred at the crotch corner for tee joints both with and without wall thinning damage [44]. The research performed an experiment to investigate the effects of various parameters, including nozzle diameter, angle of inclination, jet position, and jet velocity, on mixing time. The results showed that increasing the nozzle diameter reduced mixing time at a given level of power consumption and improved energy efficiency. This experiment was analyzed using CFD. A study carried out a nonlinear finite element analysis of a chemical reactor. A study designed and analyzed a pressure vessel in accordance with ASME code. Their finite element analysis of individual models using different materials demonstrated that the stress and deformation values of the modified model were superior to those of the actual model. Consequently, they concluded that the pressure vessel design using SA516GR65 material could be employed with modifications. A study focuses on how semi-elliptical cracks affect the structural integrity of pressure vessels [45]. Using FEA, they show that vessels with larger cracks (aspect ratios of 0.5 or more) have significantly reduced durability, with failure occurring at pressures 40% lower than in vessels with smaller cracks. For instance, a vessel with a semi-elliptical crack at an aspect ratio of 0.7 failed at pressures of only 150 MPa, whereas those without cracks withstood pressures up to 250 MPa. This study reveals the critical impact of crack geometry on vessel resilience, emphasizing the importance of early detection and crack repair in industrial applications [46]. Recent studies highlight the effectiveness of Plasma Transferred Arc Welding (PTAW) in depositing wear-resistant coatings, optimizing process parameters and enhancing high-temperature performance alongside applications in failure analysis and advanced manufacturing.

## INFERENCES FROM LITERATURE SURVEY

The literature review highlights the advancements in the design and analysis of chemical reactors, particularly in the chemical industry, where mixing chambers play a crucial role in facilitating chemical reactions. The operational conditions, such as varying incoming pressures and temperatures, induce deformation in mixing chambers, resulting in localized high-stress regions. To address these challenges,

transient dynamic stress analysis is employed to gain deeper insights into stress distribution and to predict the maximum stress values critical for estimating the fatigue life of mixing chambers [47]. Finite Element Analysis (FEA) has proven to be a valuable tool for predicting burst pressure, crack initiation, and propagation, which significantly impact the fatigue life of chemical reactors. This approach helps mitigate failures by enabling effective design improvements.

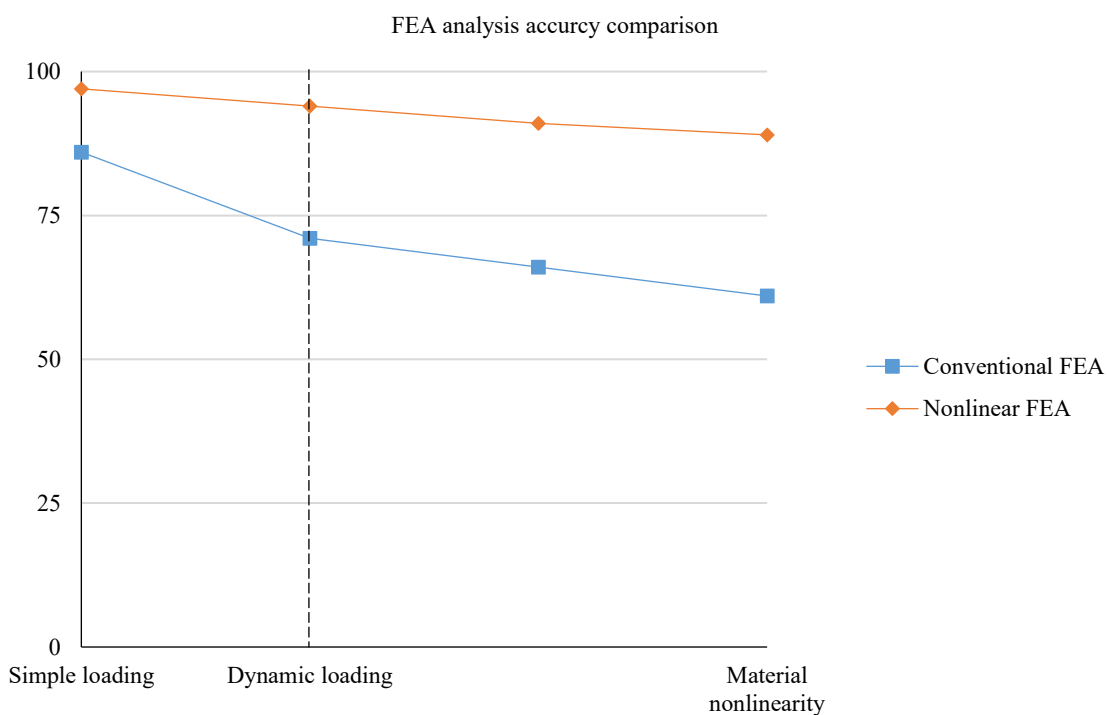
Advanced computational techniques such as computational fluid dynamics (CFD) and nonlinear FEA have revolutionized the study of fluid behavior and structural integrity. For instance, CFD studies on mixing chamber geometries, including the Hartridge-Roughton mixer, reveal that a conical narrowing and separate upstream mixing chambers enhance mixing efficiency compared to double-spiral structures. Similarly, transient FEA has been utilized to evaluate the dynamic response of balanced stiffness valves under time-dependent pressures, ensuring deformation and stress remain within safe limits. Research on twin-fluid nozzles has shown that optimizing nozzle geometry minimizes spray-related issues and improves performance. Moreover, CFD analyses have demonstrated the critical role of jet injection angles and nozzle diameters in reducing mixing times and improving energy efficiency [23]. Nonlinear FEA has further proven to provide more accurate results than conventional methods, particularly for non-routine problems like crack propagation under dynamic loads as shown in Figure 1. These computational approaches not only enable precise predictions of failure modes but also optimize designs for improved safety, reliability, and performance, paving the way for more efficient and resilient chemical reactor systems.

### Mixing Efficiency by Design Type

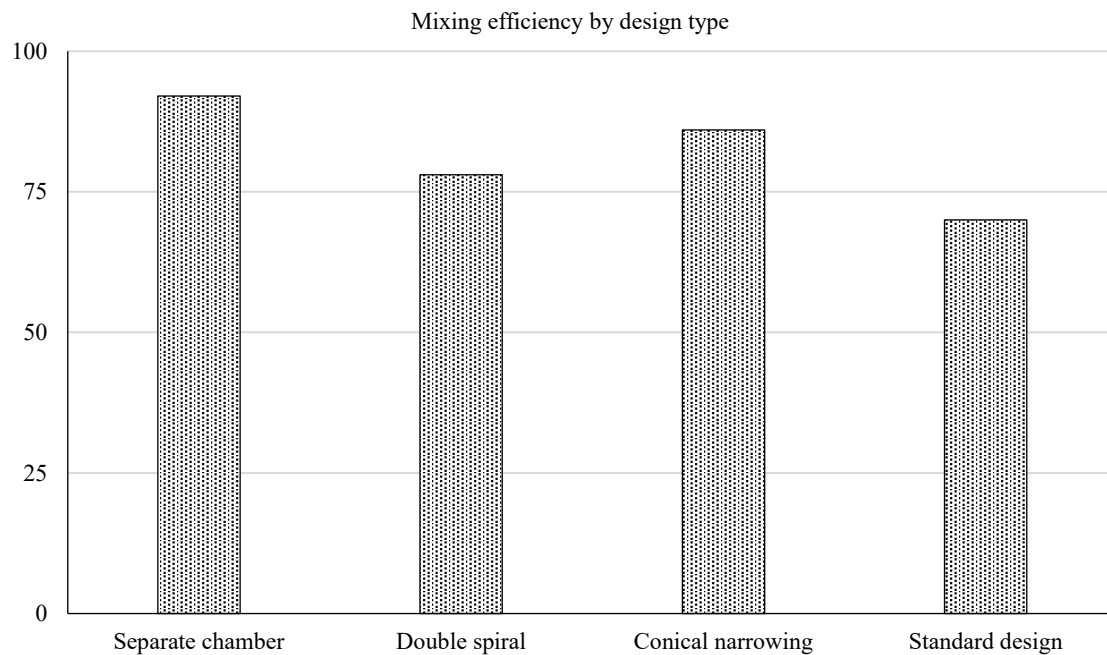
A bar chart shown in Figure 2, represent the relative mixing efficiency of different mixer designs, highlighting the advantages of separate chamber configurations.

### Failure Prevention Method Distribution

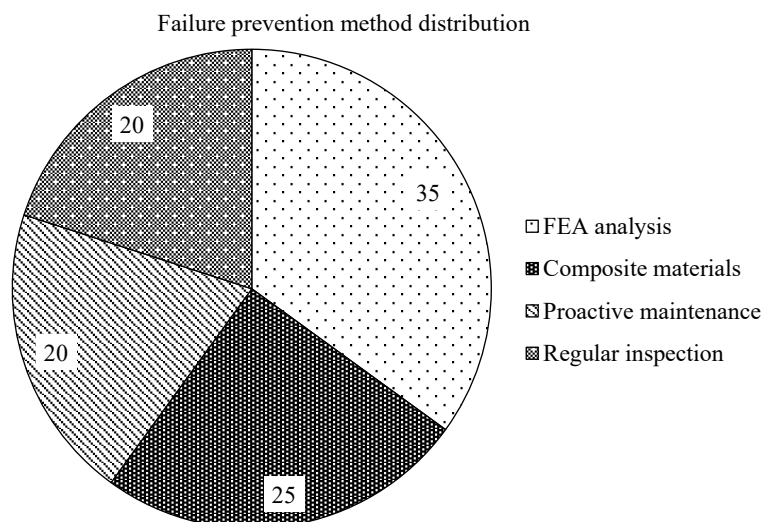
A pie chart shown in Figure 3, illustrating the relative importance of different approaches to failure prevention in chemical reactor design and maintenance.



**Figure 1.** FEA analysis accuracy comparison.



**Figure 2.** Mixing efficiency by design type.



**Figure 3.** Failure prevention method distribution.

## METHODOLOGY

Finite element analysis (FEA) stands out as a prevalent example of engineering analysis and is a powerful feature in CAD software. The FEA process involves dividing an object into a finite number of small elements, typically rectangular or triangular in shape, creating an interconnected network of concentrated nodes. This analysis is often performed using ANSYS software. FEA is essentially a mathematical representation of a physical system, encompassing a model (part or assembly), material properties, and applicable boundary conditions [18]. This process, known as pre-processing, is followed by solving the mathematical representation and examining the results, referred to as post-processing. FEA utilizes computers to solve complex engineering problems, particularly those involving structures with intricate geometries and loads that are challenging or impossible to analyze through theoretical methods. The FEA software provides comprehensive solutions, including information on deflections, stresses, and reactions. Proper modeling techniques, accurate boundary conditions, and an understanding of the procedure's limitations are crucial for effective analysis. FEA is particularly useful

for analysing complex structures such as bridges, aircraft wings, high-rise buildings, and mechanical components, which are difficult to assess using classical theory [17–21].

In the FEA technique, the structure is broken down into very small but finite-sized elements, hence the name "Finite Element Analysis." This process of dividing the structure into smaller elements is called the Discretization Method. By employing this approach, FEA facilitates a more straightforward and precise analysis of complex engineering structures.

### **FEA is Used to Determine Following Structural Properties**

The following aspects can be analyzed:

- a. Stationary displacement and stress.
- b. Eigen frequencies and vibration modes.
- c. Amplitude of forced harmonic response and dynamic stress.
- d. Dynamic response over time and associated stress.
- e. Response to random forces and resulting dynamic stress.

Finite Element Analysis (FEA) involves three main stages for determining deformations and stresses within a structure:

1. Structural modeling or pre-processing.
2. Computational analysis.
3. Results interpretation or post-processing.

### **FEM Steps**

#### ***Step 1: Pre-processing***

The initial phase involves creating a model of the structure, choosing the element type, generating a mesh, defining material properties, and applying boundary conditions and loads. The Finite Element Analysis (FEA) model is composed of numerous elements that collectively represent the entire structure. During this stage, the geometry, constraints, loads, and mechanical properties of the structure are specified [33]. The complete structure is defined by the geometric model, with the mesh representing the structure through nodes and elements.

#### **Step 2: Analysis**

The processing stage encompasses the creation of element stiffness matrices and the global stiffness matrix, solving simultaneous equations, and determining nodal displacements, stresses, and strains. The fundamental equation for both individual elements and the entire structure is:

$$\{F\} = [K]\{u\}$$

Where:

- {F} = External force matrix
- [K] = Global stiffness matrix
- {u} = Displacement matrix

This equation is solved to obtain deflections, which are then used to calculate strain, stress, and reactions. All results are stored for use in creating graphic plots and charts during post-analysis.

#### **Step 3: Post-processing**

The final stage of finite element analysis involves interpreting the raw data obtained in step 2. A CAD program is used to manipulate the data, generating the deflected shape of the structure, creating stress plots, and producing animations. Visual representations of the results are crucial for understanding the structure's behavior.

Structural analysis, the most common application of the Finite Element Method (FEM), is a mathematical process that determines a structure's response to specified loads and actions. This response

is evaluated by calculating internal forces or stress resultants and displacements or deformations throughout the structure.

### Types of Structural Analysis

1. *Static analysis*: This technique evaluates displacements, stresses, and other factors under static loading conditions. It can account for various nonlinearities, including plasticity, stress stiffening, large deflection, large strain, hyper elasticity, contact surfaces, and creep.
2. *Modal analysis*: This method calculates a structure's natural frequencies and mode shapes.
3. *Harmonic analysis*: This approach determines how a structure responds to loads that vary harmonically over time.
4. *Transient dynamic analysis*: This technique assesses a structure's response to loads that change arbitrarily over time.
5. *Spectrum analysis*: An advanced form of modal analysis, this method calculates stresses and strains resulting from a response spectrum.
6. *Buckling analysis*: This approach computes buckling loads and identifies buckling mode shapes. Both linear (Eigen value) and nonlinear buckling analyses can be performed.

In structural analysis, various structural loads are applied to generate different structural outcomes. By default, structural simulations are conducted in 3D. Static analysis is employed when loads remain constant for specific sets of results. A typical application involves determining safety factors, stresses, and deformation for a body or assembly subjected to structural loading.

### CONCLUSIONS

This review highlights the critical role of chemical reactors, particularly mixing chambers, in chemical industries where extreme operational conditions can lead to structural deformation and reduced fatigue life. The advancements in material science, finite element analysis (FEA), and computational modeling have significantly improved the understanding and optimization of chemical reactor performance. Transient dynamic stress analysis has emerged as a valuable tool for predicting stress distribution and fatigue failure, enabling design modifications to enhance longevity and reliability. The application of composite materials, optimized nozzle geometries, and advanced welding techniques has contributed to better performance under fluctuating pressures and temperatures. Finite element simulations have demonstrated their effectiveness in predicting crack propagation, burst pressures, and structural weaknesses, allowing industries to take proactive measures in design improvements. Furthermore, computational fluid dynamics (CFD) studies have proven instrumental in optimizing mixing efficiency, particularly in nozzle and chamber designs. Future research should focus on integrating real-time monitoring systems with predictive modeling techniques to enhance the accuracy of failure predictions and extend the operational lifespan of chemical reactors. Additionally, experimental validation of simulation results will further improve the reliability of computational methodologies. By leveraging these advancements, industries can achieve safer, more efficient, and cost-effective chemical reactor operations, reducing the risk of unexpected failures and enhancing process reliability.

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