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## Mechanical models and simulations of PEMFCs: A comprehensive review

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### ABSTRACT

In recent years, there has been considerable progress in developing models concerning the electrochemical, thermal, and mass transport processes of the Proton Exchange Membrane Fuel Cell (PEMFC). This advancement has resulted in numerous models being documented in the literature, alongside several review articles that aim to categorise them. However, this extensive body of literature does not have a clear definition or a dedicated review to help identify and classify mechanical models of PEMFCs. This article first focuses on identifying key characteristics that define mechanical models for PEMFCs. It then provides a comprehensive classification of these models for each component and more complex structures. To achieve this, an original representation highlights essential model information and traces their chronological evolution. This approach clearly articulates what has been accomplished and what still needs to be addressed, serving as a valuable resource for PEMFC simulation and future research.

### 1. Introduction

Proton Exchange Membrane Fuel Cells (PEMFCs) have recently garnered significant attention as a leading clean energy conversion technology [1]. PEMFCs are characterised by their high efficiency and low environmental impact, making them well-suited for various applications. These include stationary power plants, portable electronic devices, and electric vehicles [2]. The growing demand for sustainable and environmentally friendly energy solutions has driven extensive research and development in PEMFCs, highlighting their potential to replace conventional fossil fuel-based energy systems [3–5].

PEMFCs operate by converting the chemical energy of hydrogen and oxygen into electrical energy, with water and heat as the only by-products. This process ensures zero emissions of pollutants and achieves higher energy conversion efficiencies than traditional combustion engines.

Several technical challenges need to be addressed to realise PEMFCs' potential fully. These include developing durable and cost-effective materials, efficient water and thermal management strategies, and

robust system integration techniques. Extensive research efforts are focused on overcoming these barriers, with numerous studies investigating the optimisation of catalyst materials, membrane properties, and fuel cell design configurations [6].

Significant progress has been achieved in modelling the electrochemical, thermal, and mass transport mechanisms in PEMFCs [2,7–13] and several models have been developed to understand and predict the degradation processes within PEMFCs [14–17]. They have been classified in various ways in the cited reviews, depending on their approach [10–12], whether they operate under steady-state or transient conditions and the scale and dimension they address [7]. These classifications help tailor the models to specific research needs and allow for more targeted improvements and innovations in PEMFC technology. However, despite a growing interest in studying the mechanical behaviour of these systems and their components [18–20], driven by recognising their critical importance in ensuring system reliability and durability [21,22], there is a distinct lack of comprehensive reviews that specifically categorise and analyse models dedicated to mechanical aspects. While some mechanical models are mentioned in reviews related to

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stack assembly and performance [18–20] and published during the last decades [23], to the authors' knowledge, no single article provides a detailed classification and discussion.

Combining the experience accumulated in modelling physical phenomena such as electrochemical reactions, fluid dynamics, thermal management, and mass transport is essential for a thorough mechanical study of PEMFCs. Integrating mechanical modelling with these fields is critical for understanding how mechanical stresses interact with other operational factors, ultimately influencing the efficiency, durability, and overall performance of a fuel cell system. This systematic approach will allow researchers and engineers to develop more robust PEMFC designs, ensuring optimal performance under diverse and challenging operating conditions.

To achieve this, it is crucial to define common points or keywords that help distinguish and classify mechanical models from non-mechanical ones. In Fig. 1, several keywords are presented to provide a clearer understanding of what constitutes a mechanical model, demonstrating that it is possible to classify vastly different models (e.g., a constitutive model of a single component during PEMFC operation and the simulation of the forming process of a BiPolar Plate (BPP)) within the same framework. It is possible to categorise these models based on the component or phenomenon they address, the modelling approach employed, the scale of the analysis, and other critical criteria, such as chronological development and interactions between components, as this article will demonstrate.

The present review is structured to provide a detailed examination of mechanical models in PEMFCs, categorising them according to the

specific component of interest. Whether it be the Proton Exchange Membrane (PEM), Catalyst Layers (CLs), Gas Diffusion Layers (GDLs), BPPs, gaskets, End Plates (EPs), Membrane Electrode Assembly (MEA), or the entire cell or stack (see Fig. 2). How different models capture mechanical stresses, deformations, and overall structural integrity for each component under various operating conditions is reviewed. Additionally, the models will be classified by the used approach (e.g., Finite Element Models (FEMs), Equivalent Stiffness Models (ESMs), etc.), scale (macroscopic, microscopic, or multi-scale), and other relevant criteria. This classification will offer a comprehensive overview of the current state of mechanical modelling in PEMFCs and identify areas where further research is needed to improve understanding and performance.

This article targets a broad audience interested in the mechanical behaviour of PEMFCs, including researchers studying the mechanical properties of individual components using constitutive models, as well as those developing FEMs of the entire structure or coupling mechanical behaviour with other physical phenomena. This review aims to support advancements in understanding, designing, and optimising PEMFC systems from a mechanical perspective by offering a comprehensive classification and discussion of mechanical models.

## 2. Components scale

### 2.1. Proton Exchange Membrane

The PEM is one of the most critical components of a PEMFC. It serves as the electrolyte, facilitating the transport of protons from the anode to

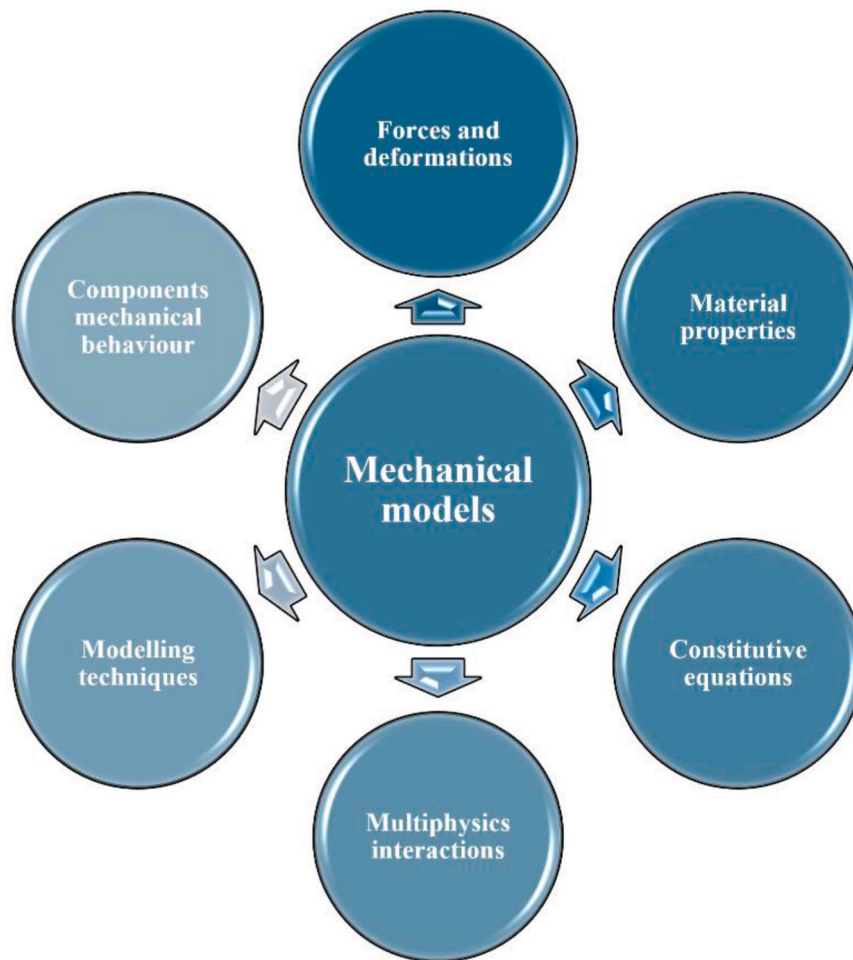


Fig. 1. Keywords to define the mechanical models.

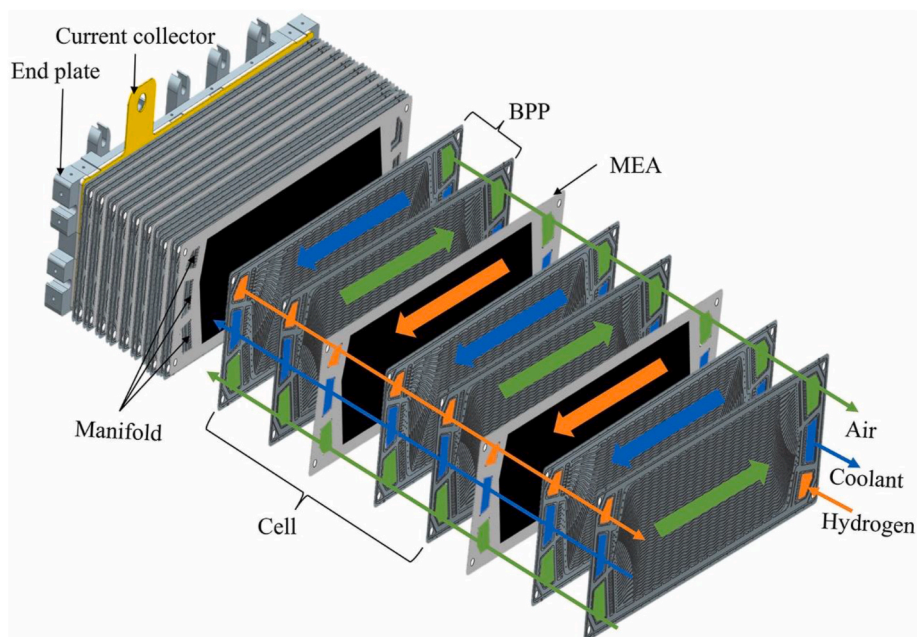


Fig. 2. A PEMFC stack (Permission from Ref. [19], copyright Elsevier).

the cathode while acting as a barrier to electrons and preventing the direct mixing of hydrogen and oxygen gases. This selective proton conduction is essential for the electrochemical reactions that generate electrical energy within the fuel cell. The performance, efficiency, and durability of PEMFCs are heavily dependent on the properties and behaviour of the PEM, making it a focal point of research and development efforts [24,25].

The material used for the PEM must possess several key characteristics: high proton conductivity, excellent chemical and thermal stability, low permeability to gases, and mechanical robustness [26]. Historically, perfluorosulfonic acid (PFSA) membranes, such as Nafion, have been the benchmark in PEM technology due to their high proton conductivity and stability under fuel cell operating conditions. However, the limitations of PFSA membranes, including their high cost, dehydration at elevated temperatures, reduced conductivity at lower humidity, and environmental concerns related to their production and disposal, have prompted extensive research into alternative materials [27]. Recent review articles have extensively discussed the development of new PEM materials, exploring various avenues such as hydrocarbon-based membranes, composite membranes, and incorporating inorganic fillers to enhance membrane performance [2,6,26–28].

Modelling the behaviour of PEMs within fuel cells is crucial for understanding the complex interactions between the membrane and other cell components under various operating conditions. Models have been developed to simulate proton transport, water management, and the thermal stresses that affect membrane performance and durability [7, 29]. However, the literature concerning the mechanical modelling of the PEM is relatively less reviewed [22].

As outlined in the review article by Qiu et al. [30], some constitutive models are developed for membranes to simulate their material behaviours. They are generally categorised into physical and phenomenological models. The first ones are typically grounded in the underlying physical laws and material properties, while phenomenological models are based on empirical observations and data-fitting techniques to capture the observed behaviours of membranes under various conditions. The authors also reported several mechanical models considering the component's mechanical failure for the entire lifespan.

Other review articles consider mechanical degradation models [16, 28]. Some of these studies extend their analysis to incorporate chemical degradation, recognising the interconnected nature of mechanical and

chemical processes in the long-term performance of membrane materials [31]. The combined approach of considering both mechanical and chemical degradation provides a more comprehensive understanding of how membranes behave and degrade under different operating conditions. It is crucial for predicting their lifespan and ensuring their reliability in practical applications.

In this article, an original approach is adopted to classify the mechanical models of the PEMs. We have meticulously categorised and analysed various models through a comprehensive diagram, which serves as the cornerstone of our classification system, as reported in Fig. 3. Coloured circles represent the articles. Each colour indicates the primary phenomenon studied and linked to the mechanical behaviour of the component. Inside the circles, the first author, the year of publication and some notes are reported. These latter regard the model scale, such as  $m$  for the microscopic scale,  $Mm$  for the multiscale models and respective dimensions ( $1D$ ,  $2D$  and  $3D$ ) where this information is available. Normally, the model is macroscopic if there are no notes for the model scale. The articles are positioned in several regions of the diagram as a function of the used approach (e.g., FEM, Analytical Model (AM), etc.) and chronologically following the publication order with the respective time axis. If they are in contact or linked by arrows, they are published by the same team of research or collaborating authors. This diagram allows a precise classification of the existing mechanical models of the PEM. It highlights the models' development trends and is a helpful tool. The same kind of diagram has been done for the other components of the PEMFC. The references shown in Fig. 3 are also reported and classified in the Supplementary Material (Table S1, Section: PEM).

### 2.1.1. First decade: 2004–2014. Mechanical behaviour and operating conditions

The earliest mechanical model, developed by Weber and Newman in 2004 [32], explored the effect of mechanical constraints on the swelling behaviour of PEMs. This work pioneered the incorporation of mechanical effects into a macrohomogeneous model, where membrane constraints during operation build stress that affects water transport and the membrane's properties. It sets the stage for subsequent models by illustrating the importance of considering mechanical constraints in experimental and modelling approaches.

Lai et al. [33] introduced a linear viscoelastic stress model, incorporating the effects of temperature, hydration, and time. The model

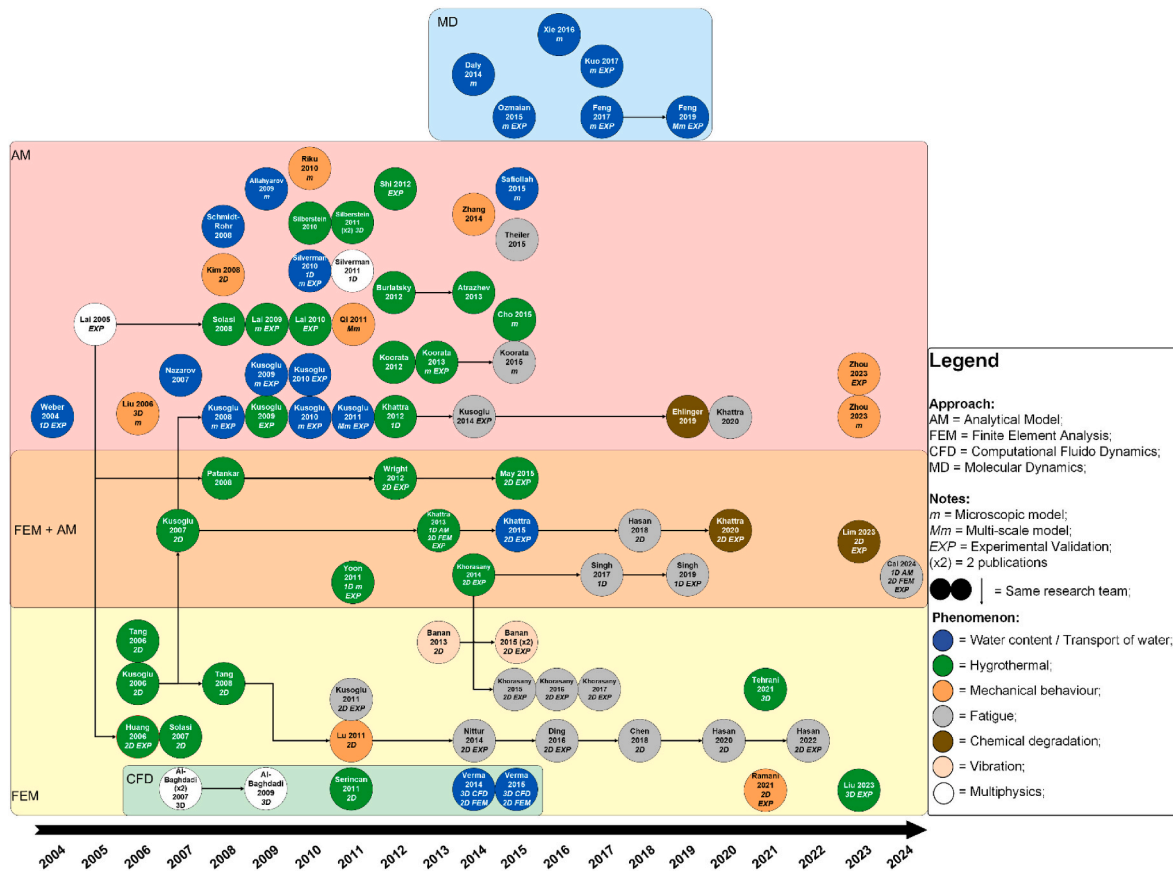


Fig. 3. – PEM mechanical models' classification.

helped quantify the mechanical stress accumulated during the hydration-dehydration cycles and highlighted the role of viscoelastic properties in membrane degradation. Researchers from the same group further advanced their work by integrating more complex viscoelastic and viscoplastic models, refining the stress analysis under real operating conditions. They worked on models for Nafion, including creep compliance, swelling anisotropy, long-term durability, and mesoscale morphological effects [34–39]. They were among the first to use FEM highlighting the significance of delayed mechanical failures in PEMFCs due to long-term stress accumulation [40–42]. In Ref. [40], they introduced FEM modelling to simulate membrane stress during real operational conditions, offering a life prediction method for PEMs. In Ref. [41], Solasi et al. developed a FEM model to analyse the in-plane stresses in PEM membranes, which are constrained and subjected to hydration and temperature fluctuations. This study was pivotal in describing how environmental factors influence mechanical degradation. Their work continued in Ref. [42], incorporating viscoplasticity and accounting for stress relaxation and strain accumulation under different hydration conditions. This was a major step forward in accurately predicting the behaviours of PEMs under operational stress.

In parallel, also Tang et al. [43] used FEM to investigate in-situ stresses in PEMs under hygro-thermal loading. The model revealed how mechanical damage could be driven by thermal and hydration cycles, affecting the longevity and durability of PEM fuel cells. Following this foundational work, the same research collaboration expanded their FEM-based investigations, refining their models in several subsequent studies [44–47] and extending the study to develop microscopic models [48–50], and constitutive models [51–53]. They incorporated more complex stress-strain relationships and extended their focus to other membrane materials and configurations under similar hygro-thermal conditions. Later, applied FEM to a broader range of operating conditions, analysing how various design and

environmental factors influence membrane stress distribution. This series of works laid a strong foundation for subsequent research into the mechanical durability of fuel cell membranes, offering valuable insights into failure mechanisms and the conditions leading to crack formation and membrane rupture.

Through tensile testing, Liu et al. [54] explored the mechanical behaviour of Nafion and other PEM materials. They developed stress-strain models and proposed a bundle-cluster model to correlate the mechanical response to the polymer morphology, providing insights into how molecular structure affects mechanical properties. Al-Baghdadi et al. [55] incorporated Computational Fluid Dynamics (CFD) with three-dimensional models to investigate the distribution of hygro-thermal stresses in PEMs. Their model combined electrochemical, transport phenomena, and stress analysis, offering a more comprehensive look at fuel cell performance. They developed an evolution of the previous work in Ref. [56], integrating gas and liquid phases within the same computational domain and introducing phase change dynamics inside the gas diffusion layers, which wasn't part of their earlier studies. In Ref. [57], they refined the CFD approach and added more detailed stress, displacement, and deformation analyses throughout the fuel cell.

Nazarov et al. [58] developed a non-equilibrium force-balance model for water transport within Nafion-type PEMs. It explored how mechanical compression of the membrane affects water distribution, leading to a more uniform water profile across the membrane thickness. The key insight is that mechanical compression reduces water content and decreases back-diffusion of water within the membrane. Schmidt-Rohr et al. [59] challenged the traditional understanding of Nafion's microstructure by proposing a parallel cylindrical water nanochannels model. This model quantitatively simulated small-angle scattering data and showed that water channels in Nafion are long and cylindrical, surrounded by partially hydrophilic side branches. The findings provided a more accurate picture of water and proton transport

through Nafion, emphasising the role of these nanochannels in maintaining mechanical integrity and facilitating fast water and proton diffusion.

Kim et al. [60] developed a two-dimensional anisotropic model to investigate how localised interfacial delamination between the PEM, CL, and GDL affects the performance of PEMFC. Allahyarov et al. [61] investigated through a coarse-grained simulation how the uniaxial stretching of Nafion membranes affects their internal structure and proton conductivity. Silberstein et al. [62–64] developed a micro-mechanical constitutive model that captures the relationship between intermolecular resistance and elastic network resistance. This model successfully predicts the behaviour of Nafion under different hydration and temperature conditions, including cyclic stress recovery, and can reproduce the nonlinear reloading behaviour observed in experiments. In Ref. [65], the authors develop a nonaffine molecular chain network model to describe the mechanical behaviours of PEM, specifically focusing on how these membranes deform under mechanical stress. Traditional affine network models assume that the molecular chains deform uniformly with the macroscopic material. However, this model allows for a more realistic representation where individual molecular chains can deform nonuniformly, leading to heterogeneous strain distributions within the material. Silverman et al. developed two models [66,67]. Both of them focus on the effects of water uptake and swelling in PEMs, but the first model emphasises the water transport and localised stress gradients due to swelling, primarily in a manufacturing context. The second one takes a more dynamic approach, incorporating thermal effects and hydration cycles to predict fatigue and long-term mechanical failure in operational conditions.

Serincan et al. [68] developed a computational modelling framework to represent the constrained swelling, anisotropic mechanical properties, and the integration of operational factors to predict mechanical degradation and performance of PEMs during real fuel cell operation. The article [69] presents a phenomenological constitutive model for ionomer membranes. This model differs from traditional approaches (elastoplastic, viscoelastic, and viscoplastic models) by incorporating micromechanisms of polymer deformation to better predict the large deformation behaviour of the membrane under different conditions, such as uniaxial loading. It has been validated using FEM simulations, demonstrating strong predictive capabilities for the large deformation behaviour of Nafion membranes across a wide range of temperatures and humidity levels. Shi et al. [70] focused on developing a constitutive model that describes the nonlinear viscoelastic-plastic behaviour of PEM when immersed in water, particularly at 30 °C and 70 °C. The study validated the model through experimental tests and showed good agreement at 30 °C. However, at 70 °C, the model required modifications to account for the more complex behaviour of PEMs at elevated temperatures.

### 2.1.2. Second decade: 2014–2024. Effect of the operating conditions on mechanical degradation

Khattra et al.'s network model [71] introduced a viscoelastic-plastic constitutive approach to model the mechanical behaviours of PEM fuel cell membranes under humidity cycling. The model captures stress redistribution and residual tensile stresses, predicting mechanical degradation over time. This work laid the foundation for further exploration of fuel cell membranes' mechanical fatigue and durability, as demonstrated by its continued enhancement in recent studies [72–76]. The same research collaboration, already cited in Section 2.1.1 [43–53], is also involved in modelling the influence of water transport [77], mechanical fatigue [78–85], and methods for mitigating membrane degradation [86]. The articles published by Koorata et al. [87–90] present a consistent evolution in modelling the mechanical behaviour of fuel cell membranes and electrodes. Starting from the thermomechanical response of fuel cell electrodes in 2013, the authors continued to explore mechanical degradation modes in later works, applying micro-mechanically motivated models. These models progressively became

more detailed, particularly focusing on the coupling between mechanical and chemical degradation processes and the influence of external stressors, such as hygrothermal cycles and structural anisotropy. Each article builds on previous work, advancing the understanding of how different operational conditions affect fuel cell membrane durability and contributing to a broader framework for predicting membrane failure and enhancing mechanical endurance.

The models developed by Banan et al. [91–93] revolve around modelling mechanical damage in PEMFCs, focusing on crack propagation and delamination due to various stressors, such as vibrations, humidity, and temperature changes. They use FEM simulations and cohesive zone theory to understand how mechanical and environmental conditions contribute to damage in the fuel cell membrane. These studies progressively refine the model, addressing different aspects of mechanical degradation, making them interconnected to predict and mitigate damage in PEM fuel cells.

Burlatsky et al. developed a mathematical model that predicts the lifetime of PEM by evaluating the stress induced by repeated hydration and dehydration cycles [94] and stress distribution under operating conditions [95]. The model is also used in Ref. [96]. Khorasany et al. have significantly contributed to understanding the mechanical behaviour and fatigue properties of PEMs and Catalyst-Coated Membranes (CCMs) in fuel cells. Their research spans from developing constitutive models for CCMs [97] to advanced fatigue and crack propagation studies, integrating both in-situ and ex-situ characterisation and focusing on the durability of these key components under operational stress [98–102]. Verma and Pitchumani [103] explored the effects of cyclic changes in the operating potential of the fuel cell on the membrane. Using two-dimensional Finite Element Analysis (FEA) based on water content obtained from CFD simulations, they predicted the membrane's stress and plastic deformation evolution. This research aimed to identify the potential for mechanical failure by analysing plastic strain localisation and stress distributions at various cathode inlet humidity levels. Their model laid the groundwork for future work [104], providing detailed insights into the effects of dynamic loading on the membrane's structural integrity. Some researchers use Molecular Dynamics (MD) simulations to understand how hydration, mechanical stress, and chemical degradation impact the properties and performance of Nafion membranes in fuel cells [105–110].

In [111], the authors use an inverse procedure that matches experimental force-displacement data from uniaxial tension tests with simulation results. This process involves a two-layer viscoplastic constitutive model that describes Nafion's behaviour. The key viscoplastic constants are varied iteratively using an Intergeneration Projection Genetic Algorithm (IP-GA). Safiollah et al. [112] described a simulation model extending the poroelectroelastic water sorption model in PEMs. This model links the water sorption process to the evolution of the pore size distribution, the charge density on pore surfaces, and the shear modulus of the polymeric pore walls. It considers different deformation modes of the polymeric pore walls to derive stress-strain relationships, which determine the swelling law of the membrane. The model is then applied to water sorption data for membranes subjected to hygrothermal ageing or chemical degradation. This application connects the macroscopic swelling behaviour to the statistical distribution of the pore size, fluid pressures, and elastic pressures within the membrane structure. It further evaluates how degradation impacts surface charge density and elastic pressure at the pore walls, providing insights into the degradation mechanisms and their impact on the structural integrity of PEMs.

The article by Tehrani et al. [113] focuses on understanding the mechanical behaviour of Sulfonated Poly(Ether Ether Ketone) (SPEEK) membranes in fuel cells. The authors developed a FEM model to simulate the effects of different operating conditions on the membrane's mechanical properties, such as hydration, temperature, and clamping pressure. In Ref. [114], the authors focus on the numerical and experimental analysis of gas permeation in PEMs. The study incorporates the effects of mechanical degradation on membrane gas permeability. A

numerical model is developed and validated through experimental blister and gas permeation tests. The same research team developed a viscoelastic-viscoplastic (VE-VP) constitutive model for glassy polymers like PFSA membranes [115]. The model considers the non-uniform length distribution of entangled molecular chains and the activation of short chains under mechanical and thermal stress. In Ref. [116], the study systematically analyses the nonuniform mechanical degradation of PEMs by considering the effects of temperature and relative humidity. Using a comprehensive 3D model, the research investigates how nonuniform temperature and water profiles impact stress and strain distribution across the membrane. Lim et al. developed one of the last mechanical models focused on the PEMs [117]. This work models the chemo-mechanical behaviour of Nafion 212 membranes, considering the effects of chemical and mechanical degradation on fuel cell performance. A key aspect of the study is the relationship between fluoride release, a measure of chemical degradation, and the membrane's mechanical properties. A continuum-based pinhole growth model is employed, which predicts the onset of mechanical damage due to stress during fuel cell operation. The study includes experimental validation, correlating membrane degradation with fluoride release and developing pinholes that compromise the membrane's structural integrity.

The detailed diagram in Fig. 3 and the relative classification serve as a tool for classification and a window into the evolving trends in developing mechanical models for PEMs. By providing a clear, organised, and visual representation, we aim to facilitate a deeper understanding of the landscape of mechanical modelling within the context of PEMFCs. While applied here to the mechanical models of PEMs, this methodology mirrors the approach taken for other components of the PEMFC, underscoring our commitment to a holistic and rigorous analysis of the state-of-the-art in this field.

Research on PEMs has evolved significantly since the early models introduced in 2004. Initial studies primarily examined the mechanical constraints and stresses affecting the component, while subsequent research began to incorporate critical factors such as hydration and temperature. As the field progressed, advanced modelling techniques emerged to explore stress distribution, fatigue, and failure mechanisms in greater detail. Furthermore, researchers have enhanced this understanding by integrating mechanical degradation with chemical interactions, leading to a more holistic view of how these membranes behave under various operational conditions.

## 2.2. Gas diffusion layers

The GDL facilitates gas transport, water management, and mechanical support. It connects the CLs to the BPPs, ensuring both physical and electrical contact. Typically, the GDL comprises a macroporous substrate (MPS) for structural integrity and a microporous layer (MPL) that helps manage water and gas diffusion. These layers optimise performance by balancing gas flow, water removal, and supporting mechanical stability [118].

Several recent reviews have focused on the materials and fabrication methods. These studies highlight the evolution of GDL materials, such as carbon-based and composite materials, to improve performance and durability. Key advancements in manufacturing techniques have been explored to enhance the component's structural and functional properties. They underscore the importance of optimising porosity, hydrophobicity, and electrical conductivity for better fuel cell performance [119–121].

As with the membrane in PEMFCs, some reviews emphasise the importance of degradation [122] and mechanical stress [123] in the GDL. However, despite these concerns, there is a notable gap in the literature regarding the classification of mechanical models for the GDL. While mechanical behaviour is critical to the overall performance and durability of the GDL, few studies focus on systematically categorising mechanical models. The same classification was used for this component as for the mechanical models of the PEM, as shown in Fig. 4 and Table S1

(Section: GDL).

### 2.2.1. First decade: 2004–2014. Electrical, thermal and transport properties

In 2004, to the authors' knowledge, Mishra et al. [124] were the first to address the critical issue of electrical contact resistance between GDLs and BPP, using a fractal asperity-based model to predict resistance as a function of pressure, material properties, and surface geometry. Their work established subsequent studies, demonstrating its accuracy under various pressure conditions.

In the following few years, several models have been developed to investigate the contact resistance between the BPP and GDL. L. Zhang et al. [125] developed two FEM-based methods for contact resistance estimation, allowing for accurate contact area and pressure distribution modelling, with experimental validation confirming the results. Meanwhile, P. Zhou et al. [126] focused on the effect of clamping force and rib shape on GDL porosity and contact resistance, identifying an optimal rib design to balance mechanical compression and minimise contact resistance. Y. Zhou et al. [127] introduced a microscale model to simulate the topological interactions between GDLs and BPPs, considering surface roughness and its effect on macroscopic electrical performances. Later, Wu et al. [128] presented an improved model version incorporating carbon fibres' bending behaviour and anisotropic properties and an analytical model incorporating both macroscopic and microscopic factors, such as GDL deformation and roughness [129].

In parallel, some mechanical models focusing on the thermal properties of the GDL have been published. Hottinen et al. [130] investigated how compression impacts the mechanical and thermal properties of GDLs, showing that thermal contact resistance decreases with increased compression pressure. Two studies followed, in which Nitta et al. [131, 132] expanded their model to include inhomogeneous compression of the GDL. In the work of Sadeghi's team [133], a compact analytical model has been developed to evaluate the effective thermal conductivity of fibrous GDLs. This model considers conduction in both the solid fibrous matrix and the gas phase, while also accounting for the spreading resistance at the contact area between overlapping fibres and gas rarefaction effects in microgaps. Subsequent collaborations of the same group of researchers [134–137] expanded on this foundation. They extended the early model by applying them to the specific case of compressed GDLs, examining the role of deformation on thermal and electrical contact resistance. Norouzifar et al. [138,139] further advanced the research by developing more sophisticated models that combined mechanical and thermal aspects, addressing both in-plane and through-plane thermal resistances and integrating these findings into overall PEMFC performance simulations.

Xinmin Lai et al., already cited in the previous sections [19,30,115, 116], are very active in developing mechanical models for GDLs and general mechanical study of PEMFCs. The evolution of their work initially focused on analysing the geometric effects of BPP on contact resistance, using FEM models to identify how the BPP corner radius impacts GDL performance [140]. Subsequently, they developed numerical and analytical models to predict GDL failure and contact pressure distribution, emphasising the importance of BPP geometric imperfections and consistency during assembly [141,142] including an application of the Monte Carlo approach to improve prediction accuracy of contact interactions [143]. The research then evolved with a multi-scale model for contact resistance [144], analyses of the size effect on contact behaviours [145], an integrated model of water transport in nonuniform compressed GDL [146] verified through FEM and CFD approaches and culminating in the recent model that integrates thermo-electrical aspects using graph theory to optimise conductivity and improve GDL design [147]. The graph theory approach is also used by R. Zhang et al. to study the component conductivity [148,149].

Y. H. Lai et al. [150] presented an investigation on the channel intrusion of Gas Diffusion Media (GDM) and its effect on fuel cell performance. The study characterised the mechanical properties of various

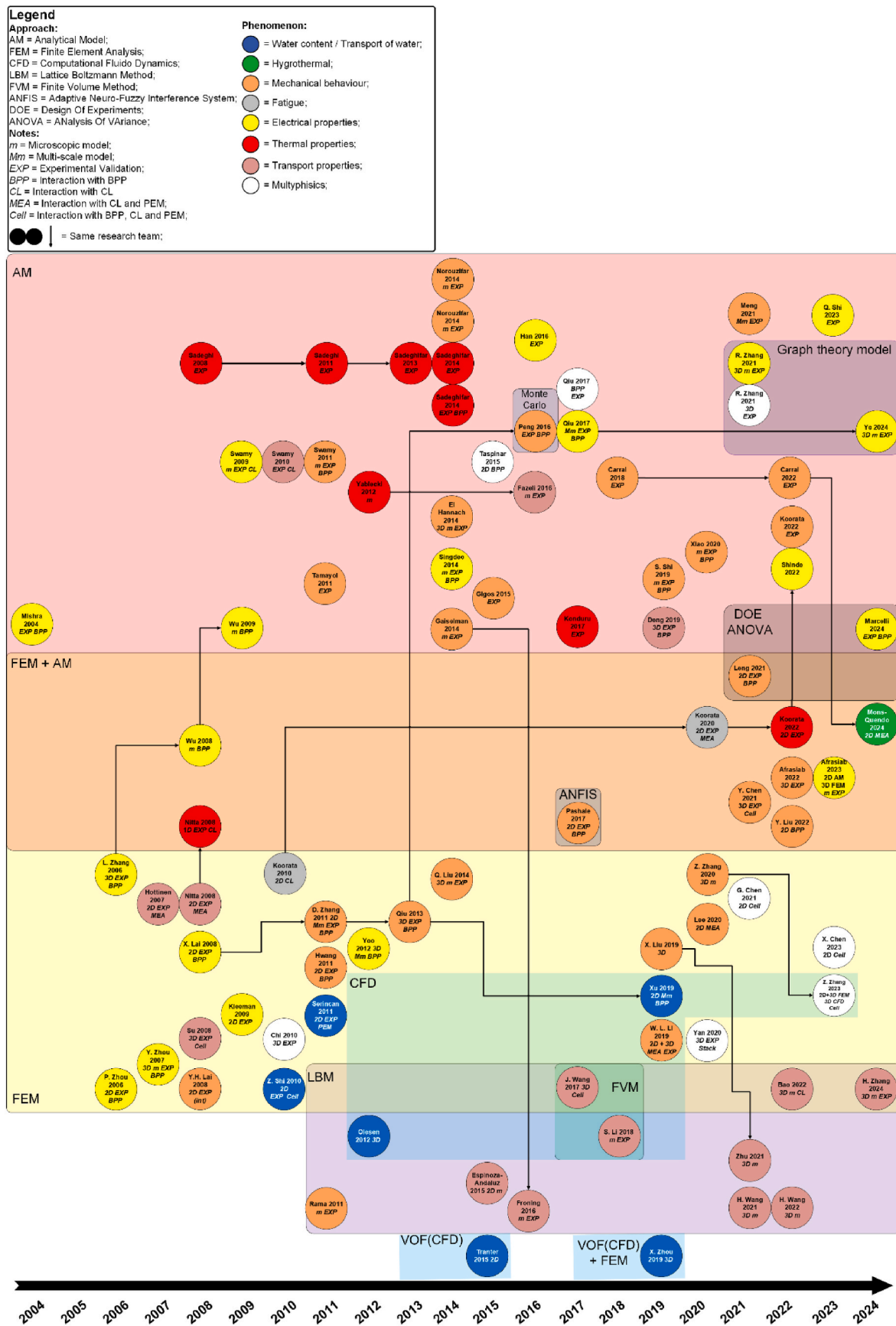


Fig. 4. GDL mechanical models' classification.

GDMs through compression, bending, and shear tests, which were then used in a numerical model to calculate GDM intrusion. A 3D model has been used by Su et al. [151] to simulate the effects of compression on GDL porosity and permeability, revealing that non-uniform compression could significantly impact local current density distribution and overall cell performance. While Kleeman et al. [152] used FEM to simulate the deformation behaviour of GDLs and predict coupled electrical properties under different compression levels. Swamy et al. [153,154] investigated the impact of interfacial morphology between MPL and CL on ohmic and mass transport losses, revealing that surface roughness and elasticity of components significantly influence contact resistance and water storage capacity. In 2011, the focus shifted to the BPP, where Swamy et al. incorporated dynamic changes in interfacial morphology under varying operational conditions [155]. This allowed for a better understanding of the BPP-GDL interactions. Later, Taspinar et al. [156] extended this work on the BPP by integrating a thermal-electrical coupling aspect, providing a comprehensive understanding of the thermal effects on contact resistance in PEMFC interfaces.

Z. Shi et al. [157] used both experimental analysis and modelling to understand how varying levels of compression influence water retention and removal. Results indicated that increased compression leads to reduced porosity, which in turn affects the water management capabilities of the component. Proper management of water content is crucial to maintaining optimal fuel cell performance and avoiding flooding or dehydration issues. In Ref. [158], Chi et al. employed a three-dimensional simulation of the fuel cell, highlighting the oscillatory nature of temperature, heat flux, species concentration, current density, and saturation distributions between the rib and channel locations, emphasising that higher compression ratios generally improved performance but also led to increased fluctuations and challenges in maintaining uniform conditions. The temperature fluctuations are due to differences in heat generation and removal between rib and channel regions, where higher compression under the ribs affects heat dissipation. Maintaining uniform conditions is crucial to avoid localised stress, material degradation, and uneven performance, ensuring optimal efficiency and durability of the fuel cell.

Koorata et al. [159] highlighted the effects of geometrical heterogeneities of the gas-diffusion electrode, specifically the GDL and CL, on mechanical damage evolution and propagation. A Cohesive Zone Model (CZM) was used to investigate damage propagation throughout the interfaces, providing insights into the stress transfer and the influence of material inhomogeneity on modulus, hardness, contact stiffness, and electrical resistance. Subsequent work by the same team continued to build on this foundation. In 2020, they studied the compressive cyclic response of GDLs, providing insights into the mechanical fatigue behaviour under operational conditions [160]. This was followed by their study on thermomechanical stability and inelastic energy dissipation as durability criteria for GDLs, where they investigated the effects of pre-assembly on GDL durability, highlighting critical factors influencing the long-term mechanical stability of the component [161]. In 2022, they introduced a phase-dependent constitutive model to predict the cyclic electrical conductivity in GDLs, emphasising the importance of considering the mechanical-electrical coupling during cyclic loading and developed a deformation mechanics model to describe the cyclic response and constitutive behaviour of GDLs, offering a more comprehensive understanding of the mechanical properties under repeated compression cycles [162,163].

Serincan et al. [164] investigated the effect of GDL anisotropy on mechanical stresses in a PEM through a FEM, particularly highlighting that the through-plane stresses induced in the membrane are negligible compared to the in-plane stresses due to the significantly lower Young's modulus in the through-plane direction. Anisotropy has also been integrated into the permeability tensor of compressed carbon cloth GDLs by Rama et al. [165], who conducted a numerical study to study the effects of compression on structural integrity and gas flow. Using X-ray micro-tomography for 3D reconstruction and the Lattice Boltzmann

Method (LBM) for numerical modelling, they determined that increasing compression significantly reduces mean pore diameter and through-plane permeability while anisotropy peaks at moderate pressures. This approach is also used in Ref. [166] by Espinoza-Andaluz et al. to study the effect of compression on the transport properties of the GDL.

Hwang et al. [167] presented a nonlinear orthotropic model of the inhomogeneous assembly compression of GDLs, highlighting the limitations of linear isotropic models, which tend to overestimate the porosity and partial intrusion of the GDL in the channel region. The experimental and model approach of Tamayol et al. [168] revealed a reverse relationship between PTFE content, mechanical compression, and single-phase through-plane permeability. Yoo et al. [169] developed a multiscale numerical model that combines the micro mechanical-electrical response of the GDL fibres and the macro contact pressure distribution between BPP and GDL.

Olesen et al. [170], using a three-dimensional, multicomponent, two-fluid CFD model, explored the consequences of varying GDL compression on water distribution and gas transport. The model incorporated capillary pressure gradients, Darcy-Forchheimer momentum losses, and nonequilibrium phase changes to represent the behaviour of water within the GDL.

Yablecki and Bazylak [171] developed an analytical model to determine the effective thermal conductivity of compressed GDLs, using microscale computed tomography to capture the heterogeneity and anisotropy of the material. Bazylak also contributed in Ref. [172], where the authors employed pore network modelling to study the effects of compression on multiphase transport in the component. They simulated liquid water transport and oxygen diffusion using synchrotron-based micro-computed tomography images of GDLs under various compression pressures.

A novel microstructural modelling approach has been introduced by El Hannach et al. [173] to generate a realistic 3D carbon fibre paper-based GDM structure employing a stochastic structure generator to create full-length, non-overlapping fibres, carbonised binder, and PTFE as distinct phases, closely simulating the carbon paper manufacturing process. Singdeo et al. [174] developed a model to estimate contact resistance between a graphite BPP and a carbon fibre-based GDL at various temperatures, emphasising the importance of optimal compression conditions to minimise resistive losses. In Ref. [175], the authors' study involved fabricating an inorganic fibrous material and using experimental characterisation to construct a numerical model. The compressive behaviour of this material was simulated using the FEM method, with fibre-fibre contacts realised through contact springs. The study provided insights into the influence of porosity on elastic modulus and compressive strength, and SEM observations verified the predicted failure mechanism.

Gaiselmann's team has been very active in investigating the mechanical response and the transport properties of GDLs under compression [176]. Their work initially focused on introducing a 3D microstructural model that allowed for virtually generating compressed fibre-based GDL structures to study the effects of compression on the material. This model was validated using experimental synchrotron tomography data and showed good agreement between virtually compressed and experimentally compressed structures. In a subsequent work [177], the authors utilised the LBM to explore the effects of compression on gas transport in non-woven GDLs, particularly focusing on High Temperature-PEMFCs.

### 2.2.2. Second decade: 2014–2024. Different approaches: LBM, CFD, graph theory model and DoE

In 2015, Tranter et al. [178] conducted a study on the effects of compression on single and multiphase flow in an idealised 2D lattice model of fibres representing the GDL, and they subjected it to through-plane compression. They employed Volume of Fluid (VOF) simulations for both single-phase and multiphase flows to observe the impact of compression on permeability and capillary flow, which

dominates liquid transport. This latter approach is also used in Ref. [179] by X. Zhou.

Gigos et al. focused on mechanical characterisation and analytical modelling of GDLs under cyclic compression to describe the deformation [180]. The model was specifically developed to simultaneously address nonlinear behaviour and high-pressure cyclic loading. Han et al. [181] measured some polarisation curves at four different GDL compression ratios and decomposed them into an open circuit voltage and three over-voltages resulting from activation, ohmic, and mass-transport losses, respectively. The model fitting showed excellent accuracy, allowing its use in subsequent analysis of the GDL compression effect. The study of Konduru et al. [182] developed an analytical model to evaluate the effective thermal conductivity of the GDL under varying compression conditions accounting for the morphological characteristics of the GDL, including porosity, fibre orientation, and contact resistance. Pashaie et al. [183] developed an Adaptive Neuro-Fuzzy Inference System (ANFIS) to predict contact pressure distribution based on FEM simulation results. The model used dimensional errors as inputs and was validated with experimental data, demonstrating its effectiveness in reducing computational cost while maintaining acceptable accuracy. S. Li et al. [184] developed a three-dimensional, non-isothermal, two-phase flow mathematical model to analyse the impact of GDL compression on various transport parameters through the Finite Volume Method (FVM). This approach was used also in Ref. [185] by J. Wang et al.

In 2018, Carral and Melé [186] developed a constitutive law to predict the compression behaviour of GDLs based on material relative density, providing a better understanding of GDL mechanical properties under different stress levels. Later, they expanded their research by modelling the cyclic compression behaviour of non-woven GDLs, accounting for influences like the presence of a microporous layer and hydrophobic treatments [187]. Finally, they also collaborated with Mons-Quendo et al. [188], who proposed an elastoplastic model to describe the irreversible strain in the GDL after compression and was implemented in a FEM framework to simulate the impact of hygro-thermal cycles.

Liu et al. [189] conducted a solid mechanics simulation of reconstructed GDLs using a novel approach that involved stochastic reconstruction and a FEM solution procedure. The study analysed stress and strain distributions at the fibre scale of GDLs under various conditions, including dynamic contact, frictional motion, and extruding deformation. The same team further developed a model in Ref. [190], where a detailed pore-scale simulation approach is used to understand how compression impacts the microstructure, porosity, and permeability of GDLs.

The impact of assembly pressure on the mass transport of a GDL of a direct methanol fuel cell, a specific type of PEMFC, is investigated through a two-phase model by Deng et al. [191]. They used 3D imaging technology to observe that the transport resistance was exacerbated by inhomogeneous compression and suggested that lowering PTFE content could alleviate CO<sub>2</sub> blockage in the cell. The study of W. Z. Li et al. [192] emphasised the influence of assembly pressure on non-uniform geometric deformation and the resulting effects on transport properties, flow behaviour, local oxygen and current density distributions, polarisation curves, and net power densities coupling a two-dimensional GDL mechanical deformation model using FEA with a three-dimensional two-phase PEMFC model.

S. Shi et al. [193] proposed a logarithmic-type constitutive model that accounts for the effects of contact between carbon fibres and utilises a Hertzian contact framework to describe the GDL deformation characteristics under compression. Z. Zhang et al. [194] used X-ray micro-computed tomography to reconstruct the GDL microstructure and then performed FEM simulations revealing that the mechanical behaviour of the component is highly dependent on its microstructural characteristics, such as fibre orientation, fibre content, and pore size distribution.

In 2020, Lee et al. [195] conducted a parametric study on the deformation of GDL using a three-dimensional FEM model to investigate the effects of various parameters, such as compression pressure, GDL thickness, and material properties, on GDL deformation. Yan et al. [196] demonstrated through a numerical simulation that increased clamping pressure led to significant variations in GDL thickness, affecting local mass transport properties and cell performance. Furthermore, inhomogeneous compression could lead to uneven current density distribution, potentially resulting in hot spots and reduced overall stack performance.

Concerning the constitutive models, Xiao et al. [197] introduced a refined analytical model that accounts for the nonlinear stress-strain behaviour of GDLs under compression. It was validated using experimental data and showed a high correlation between predicted and measured mechanical properties. An original nonlinear constitutive model was also proposed in Ref. [198] by Meng et al., which incorporated the bending of carbon fibres to describe the mechanical properties during both initial and repeated compression stages. Y. Chen et al. [199] investigated the mechanical properties of a carbon paper GDL through a 3D nonlinear and orthotropic constitutive model. The study aimed to represent the material stiffness matrix by incorporating compressive, tensile, and shear properties of the GDL.

Leng et al. [200] examined two kinds of GDL material models with different parameters using the FEM. Taguchi orthogonal experiments and analysis of variance (ANOVA) were conducted to determine the effects of these parameters on GDL deformation. Our previous work also uses the Design of the Experiment and ANOVA approaches to predict the contact resistance variation between the GDL and BPP [201].

H. Wang et al. [202,203], through pore-scale models, focused on how adding a binder and varying levels of compression influenced the transport properties, such as permeability and electrical conductivity, of the GDL. The FEM analysis of G. Chen et al. [204] showed that non-uniform compression significantly affected the transport properties, such as porosity and permeability, leading to variations in current density distribution. Y. Liu et al. [205] presented an analytical method for optimising the BPP rib structure, focusing on reducing stress distribution and deformation within the GDL. They proposed a parabolic rib geometry, significantly reducing the maximum normal and shear stresses.

Afrasiab et al. [206] introduced a novel constitutive stress-strain law for compressive deformation of the GDL starting from the analytical model developed by Carral and Melé [186], which accounts for changes in Young's modulus and Poisson's ratio during compression. Their model, validated using FEM simulations, provides an accurate prediction of GDL deformation and is a useful tool for optimising its mechanical design. Additionally, they conducted electrical and mechanical characterisation of the GDL during compression, constructing an equivalent resistance circuit to describe electrical contact resistance [207].

The numerical investigation conducted by Bao et al. [208] highlighted that compressive stress significantly impacts the permeability and water management capabilities of the GDL wettability plays a crucial role in determining the liquid distribution. Q. Shi et al. [209] investigated the deformation behaviour and fibre fracture in paper-type GDLs through a deformation model based on bending theory and fracture analysis, establishing the maximum allowable pressure criterion. Their study utilised experimental techniques to assess how compressive forces lead to deformation and the eventual fracture of fibres within the GDL structure. The study of Z. Zhang et al. [210], obtained by integrating a non-linear constitutive model into a 2D compression model, suggests an optimal range of assembly pressure to balance these factors for improved fuel cell efficiency. X. Chen et al. [211] focused on how GDL deformation affects fuel cell performance using numerical and experimental methods. More recently, H. Zhang et al. [212] conducted a numerical investigation using a pore-scale model, confirming that compression significantly alters the permeability and gas transport pathways within the MPL, leading to increased resistance and uneven

gas distribution.

The classification and the relative diagram (see Fig. 4 and Table S1, Section: GDL) show that the membrane and GDL are the most mechanically modelled components of the PEMFC. The diagram also reveals the research trends and approaches used for the GDL compared to the PEM. One notable difference is the greater number of techniques used for the GDL, including LBM, various CFD model approaches, graph theory models, and DOE. Additionally, there are interactions with adjacent components, such as BPP for electrical and thermal contact resistances, and the CL to study delamination between them. These differences are also attributed to the structural composition of the material and their roles in the MEA for the fuel cell operation.

### 2.3. Catalyst Layers

The CL is highlighted as a critical component in determining PEMFC performance, durability, and cost. It is essential for driving the electrochemical reactions that generate electricity. On the anode side, hydrogen gas enters the fuel cell and diffuses through the GDL to reach the CL. The hydrogen molecules split into protons and electrons at the catalyst surface, which is typically platinum-based. The protons pass through the PEM to the cathode, while the electrons are diverted through an external circuit, producing an electric current. On the cathode side, oxygen gas also diffuses through the GDL to the CL. Here, oxygen molecules react with the incoming protons and electrons to form water. This process occurs at the triple-phase boundary, where the catalyst, ionomer, and reactants meet. Efficient removal of the produced water is crucial to prevent water flooding, which can block reactants from accessing the catalyst sites and reduce the fuel cell performance. The structure and composition of the CL, including the distribution of the platinum catalyst, the ionomer, and its porous nature, influence the transport of gases, protons, and electrons and water management. These factors directly impact the efficiency and durability of the PEMFC. The catalyst layer thus acts as the central component that facilitates the key reactions, converting hydrogen and oxygen into water while producing electricity [2,6].

This component is widely reviewed in the literature, such as in the recent article review of Zhao et al. [213]. The authors emphasise the challenges associated with understanding the inhomogeneous structure of CLs, which affects their physicochemical and electrochemical properties, operating performance, and long-term degradation. The review explores the relationship between the CL microstructure and its performance, such as pore distribution and material composition. Techniques for visualising and characterising the CL structure, such as

microscopy and tomography, are thoroughly discussed. In addition, theoretical models are presented to elucidate how the CL structure impacts fuel cell performance and durability. The review also addresses the ongoing research on optimising catalyst loading and improving mass transport properties to enhance PEMFC efficiency. Regarding mechanical properties and modelling, the article briefly touches on parameters like Young’s modulus and stress but focuses more on electrochemical performance rather than mechanical models specifically for the CL. The article does not dive into mechanical modelling or properties of the CL in detail, as the primary focus is on the structure’s impact on performance and durability from an electrochemical and physicochemical perspective.

The already mentioned review by Dafalla et al. discusses various mechanical degradation models concerning the CLs [16]. However, the thin structure of the CL and the minimal impact on the mechanical aspect of the cell results in a lower number of mechanical models and the absence of classification for them. The mechanical models’ classification of these components is reported in Fig. 5 and Table S1 (Section: CL), along with the following text, to solve this gap.

In the previous Sections (2.1 and 2.2), some models concerning the interactions between the CL and PEM [60,91–93] or GDL [153,154,208] have already been reported.

One of the first developments of a mechanical model of a CL, aimed at PEMFC application, was published in 2008 by Rong et al. [214,215]. In the first part of their work, they employed a rate-dependent isotropic plasticity model combined with the CZM and a contact model, all implemented through FEM analysis. This approach aimed to describe the viscoplastic behaviour of the component under varying temperature and humidity and explore degradation mechanisms such as crack initiation and delamination caused by load cycling [214]. Additionally, they extended their analysis to simulate the CL microstructure as a random three-phase system based on experimental images, further investigating the impact of start-up and shutdown cycling on mechanical performance [215].

The CZM approach is widely used for the mechanical models of the CL. L. Ma et al. [216] proposed a model based on capillary condensation theory and Kelvin’s equation to understand particle agglomeration in high humidity conditions. This model, applied to Pt/C particles, utilises FEM simulations to assess stresses in Nafion thin films, showing that capillary forces can cause micro-cracks and agglomeration. Additionally, the CZM is employed to examine the Nafion-Pt/C particle interface, shedding light on mechanical failure due to dynamic capillary forces under varying humidity. Chang et al. [217] employed a mathematical model integrating the FEM and a CZM to study the impact of clamping

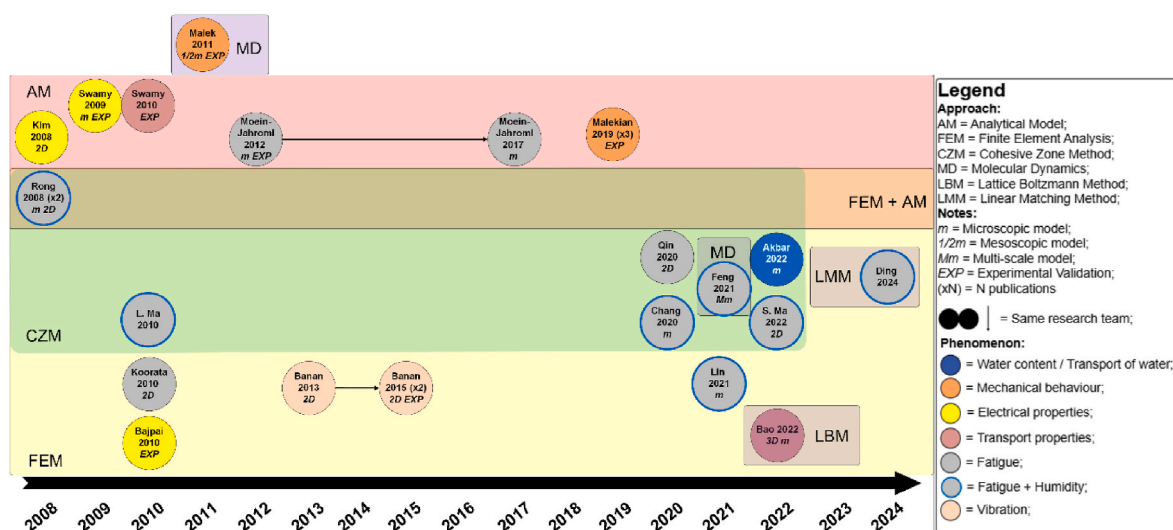


Fig. 5. CL mechanical models’ classification.

force, temperature, and humidity on the microstructure of the CL. They focused on analysing delamination and crack formation, uncovering that relative humidity significantly influences delamination due to the ionomer's expansion and contraction with water content, and this latter propagated with increasing startup and shutdown cycles. The research team of Feng et al., previously recognised for their mechanical models of the PEM using the MD simulation approach [109,110], investigated the mechanical behaviour of the CL under tensile and humidity cyclic loading. They conducted a study that combined MD simulation with CZM modelling [218]. Using a 2D FEM model based on the CZM method, S. Ma et al. analysed the effects of asymmetric RH cycling on the PEM-CL interface delamination process [219]. Akbar et al. conducted a study on the mechanical response of CL under different loading conditions, focusing on tensile and compression effects combined with humidity variations [220]. Their model, which integrated FEM with CZM, revealed that the interplay between mechanical loading and environmental conditions significantly influences the mechanical integrity of the CL.

Concerning the electrical aspects of the interfacial morphology of the CL, Bajpai et al. [221] developed a two-dimensional, non-isothermal, anisotropic numerical model to examine the broader impact of interfacial morphology between the MPL and the CL.

Malek et al. used a mesoscopic model to study the self-organisation processes that define the structure of CL [222]. Their coarse-grained molecular dynamics approach provided insights into the agglomeration of Pt-decorated carbon particles, the formation of ionomer domains, and the porous network within the CL. The study challenged traditional views by showing that ionomer forms a thin adhesive film partially covering Pt/carbon agglomerates instead of following the classical electrolyte-flooded agglomerate model. The model of Moein-Jahromi et al. [223] combined two approaches: calculating the electrochemical surface area and agglomerate size of the CL under cyclic loading and using an existing model [224] to estimate catalyst performance with fixed parameters.

Malekian et al., from the already cited research collaboration of Bahrami and Djilali [133–139,168], conducted three key studies on the CLs compressive behaviour and mechanical properties [225–227]. In the first study, they experimentally investigated the deformation and porosity of CLs under compression, showing that the component exhibits both elastic and plastic deformation depending on the applied pressure [225]. In their second study, Malekian et al. developed an analytical model using effective medium theory to predict CL deformation under compression. The model utilised a representative unit cell based on microstructural properties to simplify the complex CL structure, such as porosity and ionomer-to-carbon ratio. The model was validated against experimental results, successfully predicting the non-linear compressive behaviour of CLs, and was also used to estimate other properties like thermal conductivity and gas diffusivity [226]. The third study focused on the impact of compression on pore size distribution and porosity in CLs. The authors found that larger pores experienced the most significant reduction in size under compression, leading to an increase in the volume fraction of smaller pores. This change in pore structure has critical implications for mass transport within the CL, affecting overall fuel cell performance [227].

In the last few years, Qin et al. [228] developed a 2D FEM model to explore how relative humidity cycling affects interfacial behaviour during startup and shutdown, focusing on PEM-CL delamination exacerbated by cracks in the CL. J. Liu et al. observed Pt/C agglomerate growth under similar conditions, using a FEM model to illustrate microstructural changes leading to interfacial delamination. [229]. Ding et al. conducted a study on the mechanical behaviour of CL using the Linear Matching Method (LMM) to analyse the effects of cyclic loading and humidity variation [230]. Their approach enabled a detailed assessment of the accumulated plastic strain and the progressive damage in the CL under operational conditions.

From its intricate structure, which supports the transport of gases,

protons, electrons, and water, to its delicate balance of materials, the CL must be meticulously optimised to overcome challenges such as mass transport limitations, catalyst degradation, and mechanical failure. The reported models and experimental techniques have highlighted how the mechanical and electrochemical environments interact, underscoring the importance of humidity, temperature, and mechanical loading on the CL performance. Mechanical modelling efforts, particularly those using FEM and CZM, reveal that humidity and mechanical loading significantly influence CL integrity. Early works laid the foundation by simulating stress and degradation within the CL, focusing on interface behaviour and crack propagation. Subsequent studies have built on this, incorporating MD simulations, such as capillary condensation and particle agglomeration under varying environmental conditions. These models also emphasise the importance of humidity cycling in promoting delamination at the PEM-CL interface.

Recent experimental and modelling studies also demonstrate that compression can alter the CL porosity and pore size distribution, impacting its capacity for mass transport and fuel cell efficiency. Further, probabilistic and optimisation models are emerging as valuable tools for fine-tuning CL composition and thickness to improve mechanical resilience while optimising electrochemical performance.

By understanding and mitigating the mechanical stresses and degradation mechanisms affecting the CL, researchers and engineers can enhance PEMFC performance and durability, ultimately contributing to more efficient and reliable fuel cell technologies.

#### 2.4. Gaskets

Gaskets are essential in ensuring the operational integrity of PEMFCs, particularly given the challenges posed by variable humidity, temperature fluctuations, and exposure to aggressive electrochemical environments [231]. While the literature contains extensive information on gasket materials and their mechanical properties due to their broad use in various applications, PEMFCs present a unique set of conditions that require specific attention [232]. This work aligns with the classification of mechanical models for other PEMFC components. The main focus of this Section is to compile and categorise all the mechanical models relevant to gaskets used in PEMFCs (some of them reported in Ref. [233]), providing a coherent approach consistent with the rest of the review (see Fig. 6 and Table S1, Section: Gasket).

Liang et al., whose team has been cited numerous in the previous sections [19,30,114–116,142–147], also investigated the structure failure of sealing in the assembly process through FEM simulations and experiments. They focused on the influence of gasket parameters, sealing groove shape, and gas pressure and compared risks when using metallic versus graphite BPPs [234]. Later, part of the same research team developed an analytical model for gas leakage through the contact interface in PEMFCs. This model incorporated microscale contact modelling and fractal porous structure theory to predict leakage paths at the interface, considering both convection and diffusion mechanisms [235].

In 2020, a study by J. Zhang et al. explored how temperature affects the stress and strain in sealing systems of fuel cells using FEM simulations [236]. Several mechanical models of the gaskets have been developed to study the leakage phenomenon, such as in Ref. [237], where Huang et al. developed a theoretical model combining the LBM for rough wall interfacial gaps, a numerical 3D rough-surface generation technique, and FEA for micro-contact mechanics. The model allowed for assessing the influence of surface roughness, gasket thickness, and strain level on leakage rate, providing insights useful for designing metal-BPP PEMFC sealing structures. Building on this, the same author collaborated in Ref. [238] to explore the interfacial leakage characteristics of rubber sealing under temperature cycling conditions. Q. Xu et al. used helium mass spectrometry leak measurement and FEM calculations to distinguish between interfacial leaks and gas permeation, highlighting gas permeation as the main leak path [239]. Chen et al. proposed a

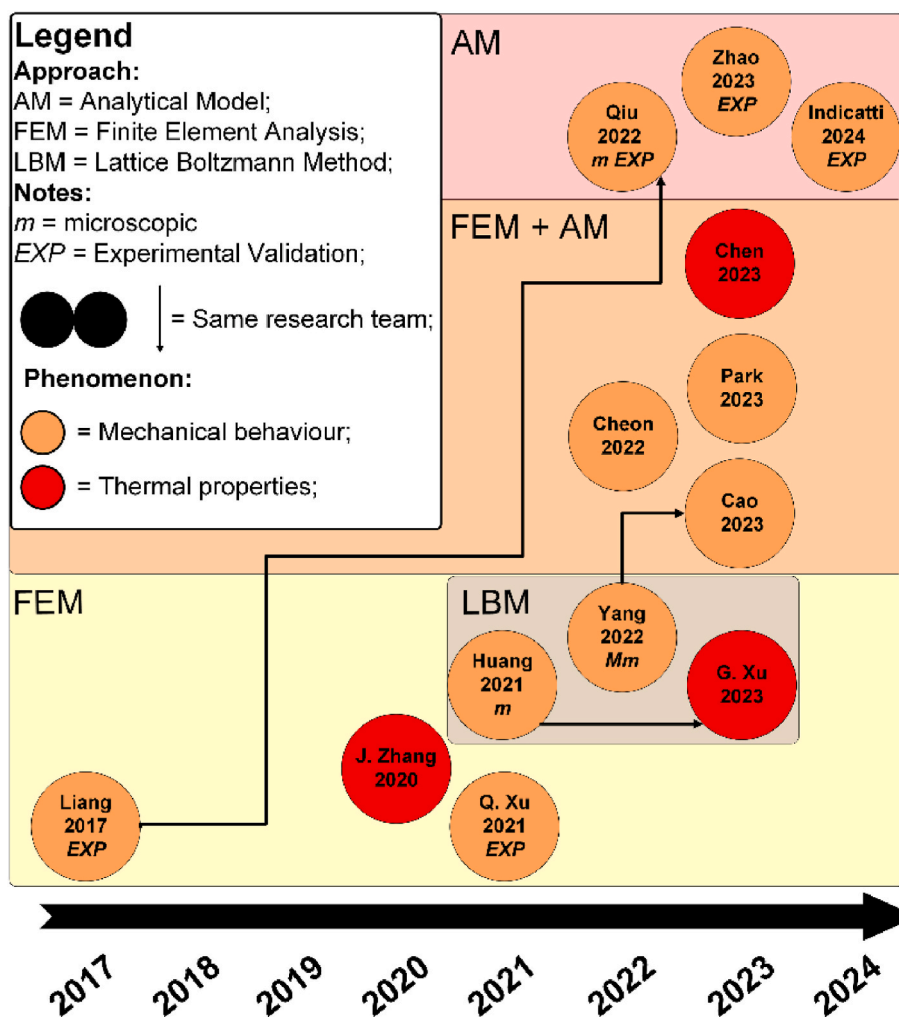


Fig. 6. Gasket mechanical models' classification.

leakage rate prediction model for PEMFC sealing systems, incorporating thermal coupling effects. Their study used FEM simulations and the Greenwood-Williamson model to improve the parallel plate leakage model, accounting for variable channel cross-section heights [240]. Yang et al. also studied the leakage phenomenon using FEM and the LBM to analyse nonlinear contact and microscopic gas flow behaviour. They developed a multi-scale dimensionless model of PEMFC interface leakage, which provided a more accurate prediction of the leakage rate under different gasket compression rates [241]. The same team then advanced to the study described in Ref. [242], focusing on optimising the sealing performance of PEMFCs under 3D stack-up assembly tolerance conditions. Their work used a semi-analytical modelling approach and numerical simulations to evaluate the impact of manufacturing tolerances, such as deviation size, direction, and rotation angle, on sealing behaviour.

Following this, several studies have focused on constitutive models for gasket materials. Cheon et al. employed FEA to determine optimal strain energy density functions for various rubber-like gasket materials, including hyperelastic models such as Mooney-Rivlin, Ogden, and Yeoh [243]. Park et al. also used FEA to assess the suitability of gasket materials, specifically focusing on the effects of ageing and tensile stress. They introduced a comprehensive "dual degradation framework" to evaluate the performance of Liquid Silicone Rubber (LSR) and Ethylene Propylene Diene Monomer (EPDM) materials, concluding that LSR exhibited superior performance in terms of both ageing resistance and tensile conditions [244]. Finally, Zhao et al. investigated the sealing

performance of large metal BPP systems, proposing an innovative double-peak sealing gasket structure. Their study used the Mooney-Rivlin constitutive model to analyse the impact of material hardness, friction coefficient, and compression ratio on sealing effectiveness, showing that the double-peak structure improved contact pressure distribution and optimised the overall sealing performance of PEMFCs [245].

Indicatti et al. investigated using stencil printing to produce fuel cell sealings with reliable layer thickness. They employed supervised machine learning models, including binary logistic regression, to predict printability based on various factors such as surface tension, viscosity, and aspect ratio [246].

In conclusion, this section has provided a comprehensive overview of the various mechanical models and constitutive studies of gaskets used in PEMFCs. The reviewed works highlight the diversity of approaches employed, from FEM and LBM simulations to advanced machine learning techniques, each contributing unique insights into gasket performance under different operational conditions.

## 2.5. Bipolar plates

The BPPs are crucial components that perform multiple functions, such as distributing reactant gases uniformly across the cell, collecting and conducting electrical current, providing mechanical support, and managing water and thermal transport [247]. Typically made from graphite, metal, or composite materials, BPPs are essential for

maintaining effective cell performance and durability while contributing significantly to the overall weight and cost of the fuel cell stack. Various reviews in the literature highlight the design challenges and advancements in materials aimed at optimising their mechanical properties and enhancing their long-term reliability [248,249].

CFD models for BPPs are discussed in Ref. [250], but to the best of the authors' knowledge, a comprehensive review specifically focused on mechanical models for BPPs does not exist in the literature. Therefore, this work presents the mechanical models for BPPs, similar to what has been done for other components (see Fig. 7 and Table S1, Section: BPP).

Since many mechanical models of the BPP focus on electrical contact resistance at the interface with GDL [124–129,140,144,167,169,174,201], or the mechanical interaction with it [136,142–145,155,156,183,205], they are already cited in Section 2.2.

Additionally, two articles describing detailed mechanical models for the BPP can be included to provide further insights [251,252]. The first article, by D. Liu et al. [251], focuses on the effects of assembly errors in the BPP using FEA, Least Squares-Support Vector Machine (LS-SVM) simulation, and statistical analysis to understand how these parameters influence pressure distribution and stress failure in the MEA. The second one, by Li et al. [252], employs 3D laser scanning to assess the similarity of BPPs and combines these measurements with numerical analysis of contact pressure to understand the effects of plate deformation on pressure distribution, offering insights for optimising the assembly process of PEMFCs.

Furthermore, some models belong to a specific category focused on describing the manufacturing process of the component, which offers valuable perspectives on optimising BPP fabrication. The first of them, from the earlier mentioned collaboration of Peng et al. [19,30,114–116,142–147,234,252], was published in 2008 [253]. It presents a comprehensive study that utilises a hydroforming model, DOE, and an Adaptive Simulated Annealing (ASA) optimisation method to optimise the flow channel shape of metallic BPPs. The model considers various forming process parameters, such as geometry and material characteristics, to predict their effects on the final quality and mechanical performance of the BPPs. The same research group has also published a detailed investigation with numerical simulations to predict and mitigate welding-induced distortions [254], a forming limit model for thin metallic BPPs to optimise the channel design for improved formability and reduced material failure [255], and a numerical simulation with a surrogate model for the forming process of a BPP [256].

Hu et al. [257] developed a detailed FEM to simulate the stamping process of metallic BPPs, focusing on reducing defects and improving dimensional accuracy. The model evaluates the influence of forming speed, pressure, and material thickness, providing crucial insights into optimising process parameters for high-quality BPP production. Huang et al. [258] introduced a Genetic Programming (GP) based model to determine the optimal forming conditions by analysing the relationships between process parameters, such as forming pressure and material flow, thus significantly minimising defects and enhancing the mechanical properties of the BPPs. Kolahdooz et al. [259] developed a model using DOE and FEA to systematically investigate the influence of critical factors in the rubber pad-forming process of metallic BPPs, providing a statistical framework. Modanloo et al. [260] introduced a FEM model based on Response Surface Methodology (RSM) to optimise the stamping process of titanium BPPs. This approach helped in analysing the interaction effects of die clearance, stamping speed, and friction coefficient, enabling the identification of optimal conditions to enhance formability and minimise defects. Talebi-Ghadikolaee et al. introduced several models focused on understanding the deformation mechanics and forming limits of thin-walled metallic BPPs (see Fig. 8) [261–263]. These approaches combined numerical simulations with experimental methods to evaluate the effects of key forming parameters on material behaviour during the stamping and rubber pad forming processes. Lastly, P. Zhang et al. [264] introduced a model focusing on the micro-stamping process of metallic BPPs, combining experimental observations with numerical simulations to better understand material failure mechanisms. The model specifically addressed strain distribution and deformation patterns during the stamping process.

In conclusion, the mechanical modelling of BPPs encompasses a variety of approaches, each providing significant contributions to the understanding and optimisation of these critical components. Most mechanical models focus on two key areas: the interaction between the BPP and the GDL and simulations related to the manufacturing processes. From analysing contact resistance and assembly errors at the BPP-GDL interface to optimising forming processes such as stamping and hydroforming, the models presented in this work highlight the complexities involved in BPP manufacturing and performance. Having these references alongside the rest of the review provides a comprehensive perspective on the mechanical behaviour of PEMFCs. Moreover, integrating these mechanical approaches with non-mechanical models, such as the models reported in Ref. [7], could be highly beneficial for

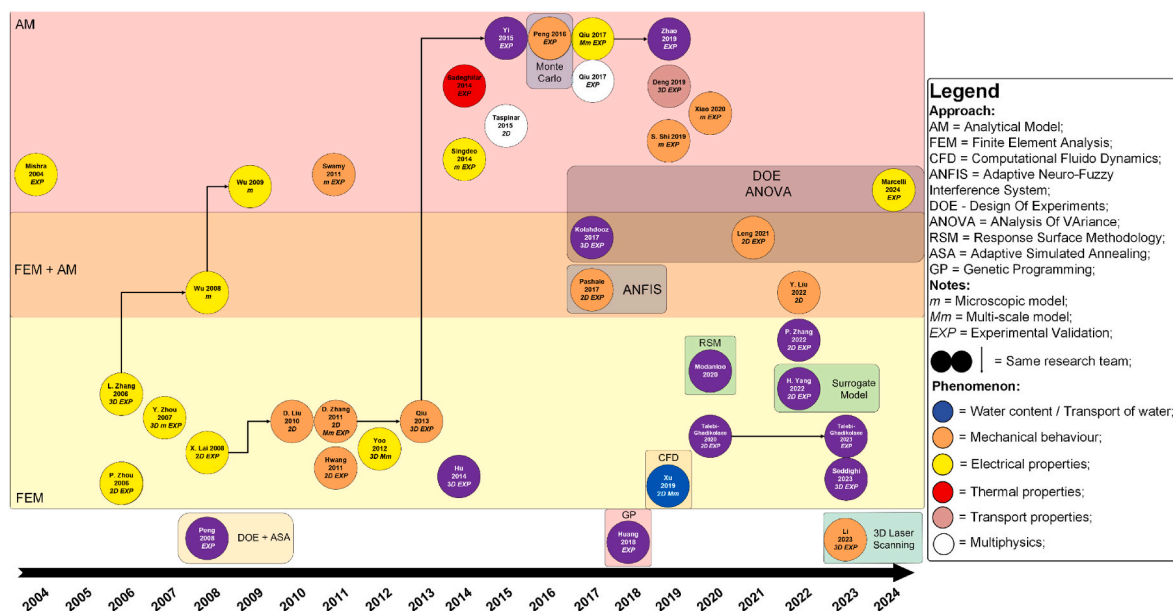


Fig. 7. BPP mechanical models' classification.

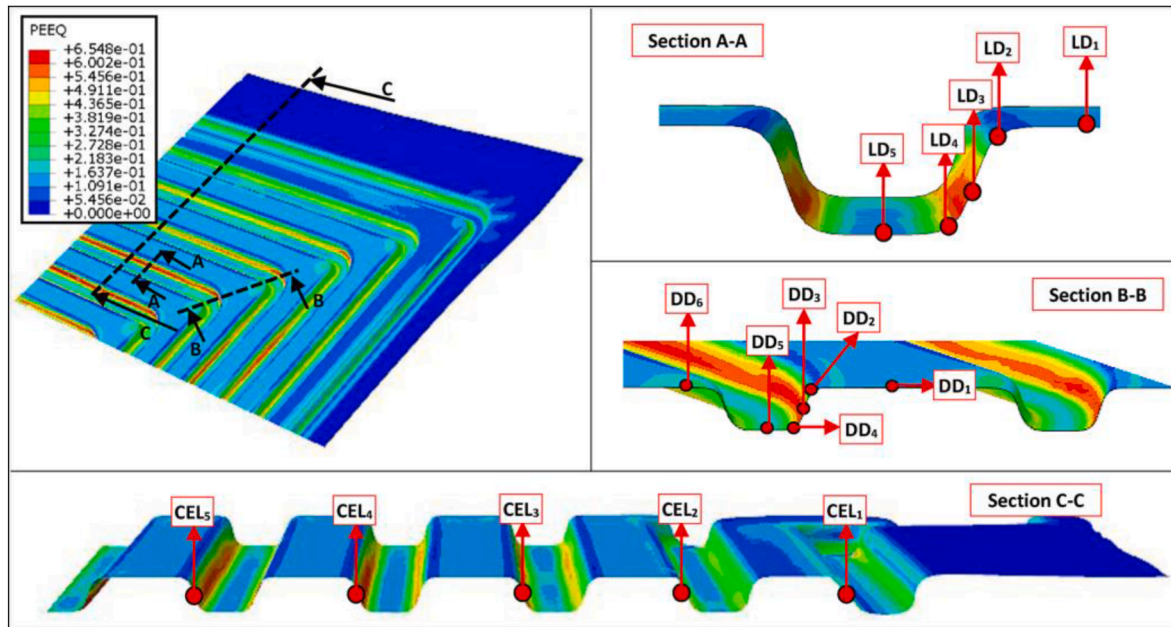


Fig. 8. Numerical simulation of the forming process of a metallic BPP (Permission from Ref. [262], copyright Elsevier).

advancing the holistic understanding and optimisation of PEMFC systems.

### 2.6. End plates

The EPs provide mechanical stability to the entire stack by maintaining the necessary compression on the fuel cell assembly, ensuring proper contact between the various layers, and minimising performance losses due to gas leakage or poor electrical connectivity. They must also manage the distribution of mechanical stresses to avoid localised damage to other components, such as the PEM or CLs. Some articles reviewed the assembly methods and the impact of clamping forces on end plates, discussing how proper assembly can mitigate performance degradation due to uneven compression [18,19]. Wu et al. [20] provided a systematic review focusing on the optimisation design of the EPs, describing the structure performance requirements, the material

selection criteria, and shape and topology optimisation.

Given the primarily mechanical function of the component, all models in the literature can be classified as mechanical and are characterised by FEM analysis, as well as shape and topology optimisation (see Fig. 9 and Table S1, Section: EP).

Karvonen et al. [265], from the same team mentioned in Section 2.2 [130,132], presented a study that used a FEM approach to analyse the compression pressure distribution on GDLs with different EP structures. The results showed that ribbed-plate structures led to more uniform pressure distributions compared to traditional flat plates, and the results were validated with pressure-sensitive film experiments. Yu et al. [266] investigated a design of asymmetric composite sandwich EPs made of carbon fibre and glass fibre composites, utilising pre-curvature generated by residual thermal deformation to achieve the desired pressure distribution. Asghari et al. [267] employed FEM analysis to determine the optimal thickness and material selection for the EPs of a 5 kW

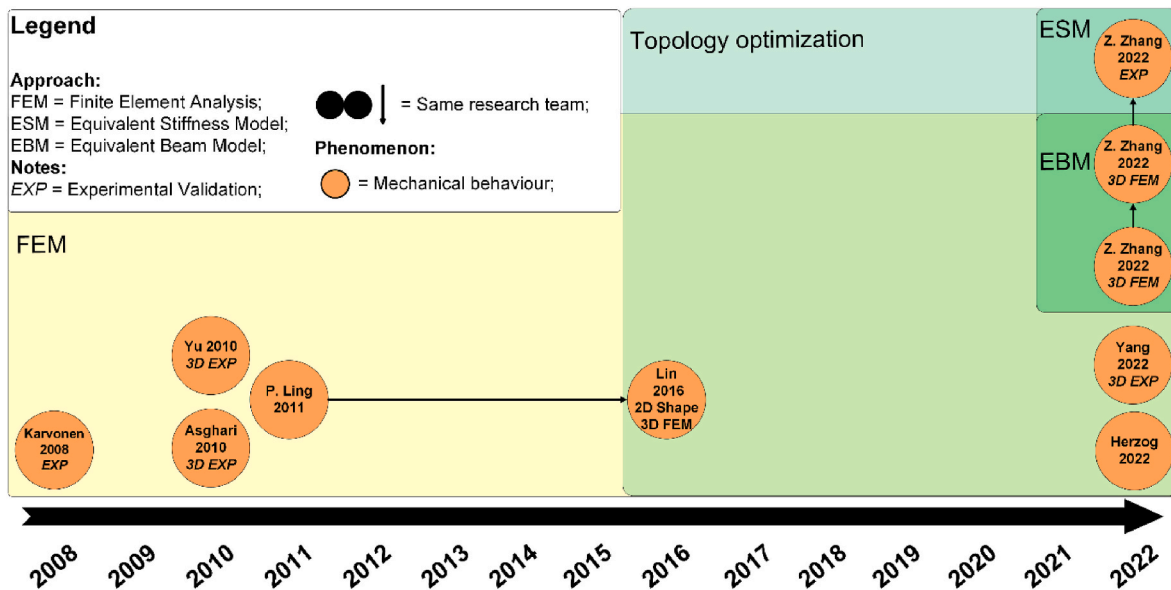


Fig. 9. EP mechanical models' classification.

PEMFC, followed by experimental validation using Electrochemical Impedance Spectroscopy (EIS). The results indicated that the designed components provided a uniform pressure distribution, which was critical for enhancing the stack's overall performance.

The remaining articles showcase a topological optimisation of the component, carried out by four distinct research teams. The first team, already cited in previous chapters [20,126], developed a multi-objective topology optimisation model for the EPs using nonlinear contact boundary conditions to achieve an improved structural design that was both lightweight and manufacturable [268]. Later, they proposed a stepwise approach for the EPs clamped with steel belts, focusing on shape and topology to improve pressure distribution and reduce the mass of the component [269]. Z. Zhang et al. presented three articles that contributed significantly to the understanding and optimisation of EPs in PEMFCs through the FEM approach [270–272]. In the first publication [270], they explored the design of lightweight EPs using topology optimisation to minimise compliance and achieve a uniform stress distribution. The second study focused on optimising cross-sectional shapes to enhance stiffness and reduce deflection under clamping forces [271]. Lastly, they presented an innovative approach integrating Belleville springs into EPs to ensure smoother assembly forces and reduce deformation, optimising their number and placement [272]. The team of Herzog et al. [273] developed a model for improving the EP design using FEM combined with experimental validation. Their work focused on reducing deformation under clamping forces and ensuring uniform pressure distribution, highlighting the importance of structural rigidity in the overall performance of the PEMFC stack. Lastly, Yang et al. [274] also performed numerical simulations to develop a lightweight EP.

In conclusion, the mechanical modelling of EPs for PEMFC stacks is critical in ensuring proper pressure distribution, structural rigidity, and overall stack performance. The cited models provide valuable insights

for optimising the design and ensuring the durability of PEMFC stacks.

### 3. Membrane Electrode Assembly and cell scale

In this article section, mechanical models are classified according to the complex structural interactions within PEMFCs rather than by individual components (see Fig. 10 and Table S1, Section: MEA). Specifically, the focus is on the MEA, which typically includes the PEM, GDLs, and CLs. The single cell, including BPPs and gaskets, is also considered. It is important to note that definitions in the literature often overlap; for instance, some MEA models incorporate BPPs, while some single-cell models may not. Both structures are, therefore, addressed and classified in this section. While some FEM models discussed previously may encompass the entire MEA or cell structure, they often concentrate on the study of a single component that plays a central role in the simulation. In contrast, this section elevates the importance of the MEA or cell structure, although some models may fit into both categories, such as [40,43–47,68,72,77,87,88,103] in Section 2.1 and [130,132,151,157,159,164,185,192,195,204,210,211] in Section 2.2.

Additionally, as described in the following sections, several authors and collaborations mentioned in previous classifications are cited here too. It highlights that the mechanical study of individual components and the structure in which they are used is closely related.

Solasi et al. [275] model can be considered one of the first simulations of the MEA. They conducted experimental tests and incorporated the data into a constitutive model implemented in a FEM to study stress and strain distributions in a three-layer MEA. From the same collaboration, Huang et al. [276] developed a 2D FEM using a CZM and fractional contact model to simulate interface changes caused by hygrothermal cycles. The stress-strain simulations highlighted stress distribution within the MEA, focusing on areas prone to interface changes and membrane thinning. Bograchev et al. developed a linear

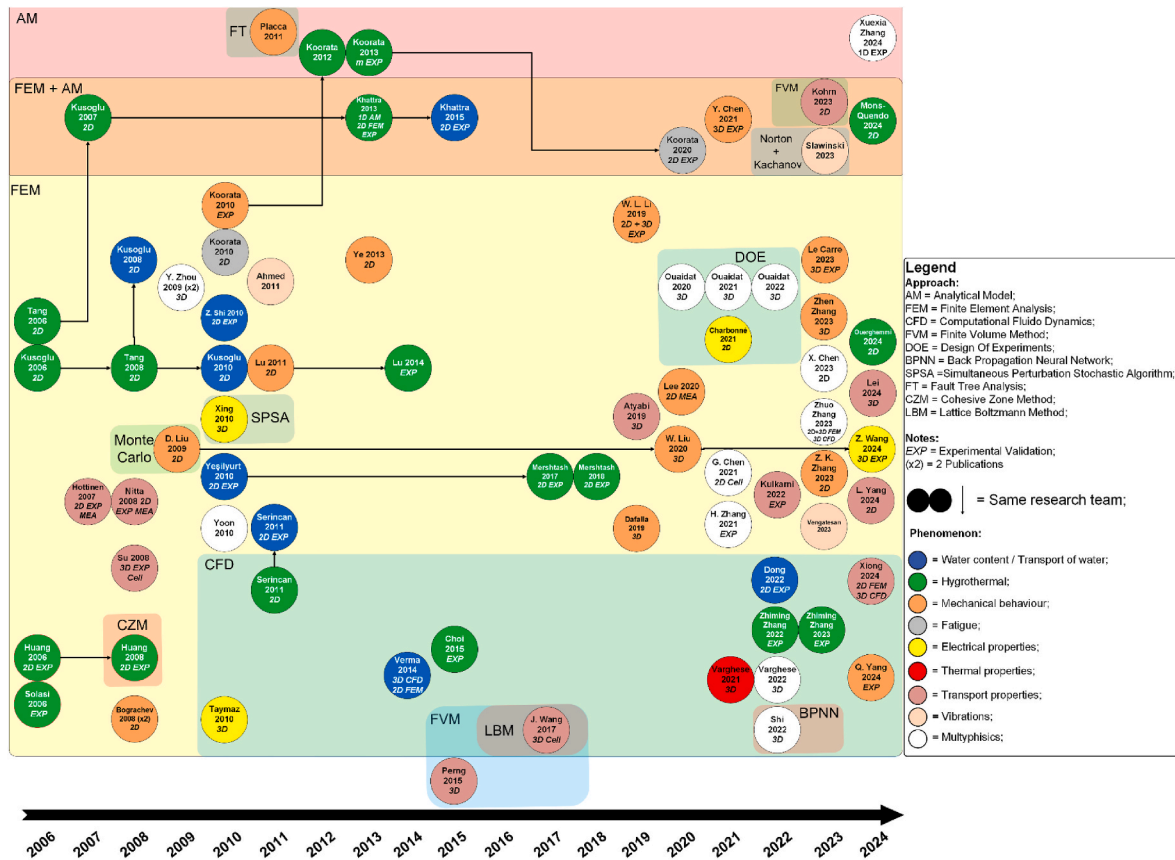


Fig. 10. MEA mechanical models' classification.

elastic-plastic 2D model incorporating hardening effects to analyse mechanical stresses in the MEA during cell assembly and providing insights into the stress distributions at both tooth/channel and global scales. The results are validated through experimental data [277,278].

Kusoglu et al. used the same FEM model cited in Section 2.1 [43–47] to investigate the stress and water distribution in the MEA during operation [279,280]. The same team collaborated in Ref. [281], where they used an experimental-numerical hybrid technique to characterise the mechanical behaviour of electrodes employing reverse analysis through FEMs. In the article of Liu et al. [282], the FEM revealed the impact of dimensional errors on membrane swelling, contact resistance, and performance variation, while the Monte Carlo simulation provided insights into the variability of pressure distributions due to assembly imperfections. In 2020, they presented a 3D FEM highlighting that stress concentrations at the gasket and GDL joint increased with misalignment displacement [283]. Lastly, they collaborated in developing a performance prediction model that considered the impact of assembly error on MEA deformation [284]. The multiphysics model of Zhou et al. [285, 286] combined gas mass transfer analysis based on deformed GDL geometry with microscale electrical contact resistance analysis.

Taymaz et al. developed a FEM coupled with a 3D CFD to analyse the influence of pressure on gas mass transfer and performance [287]. The CFD approach is also used in Refs. [288–290], specifically through the Fluid-Structure Interaction (FSI) approach, in Ref. [291], integrating the Back Propagation (BP) neural network prediction model, in Refs. [292–294] to study the transport properties of the system and by Q. Yang et al. to propose a new structure design [295].

Xing et al. [296] developed a 3D model to analyse the impact of clamping pressure on GDL properties and performance. Using the Simultaneous Perturbation Stochastic Algorithm (SPSA) for optimisation. Yeşilyurt et al. [297] used a numerical simulation employing Maxwell-Stefan equations for species transport in GDLs, Biot's poroelasticity and Darcy's law for deformation and water transport in the PEM, and Ohm's law for ionic currents and electric currents respectively in both of them. A 2D model was developed from the same collaboration in Refs. [298,299].

The research team of Koorata et al. published several models that can be considered in this section as the previous ones, such as the already described articles in Section 2.1 [87,88] and in Section 2.2 [159,160]. In 2010, they also developed a FEM model to investigate the effects of material heterogeneities of the gas-diffusion electrode layer [300].

A FEM multiphysics model is developed by Yoon et al. in Ref. [301]. They integrated a micromechanism-inspired viscoelastic model with hygrothermal expansion for the mechanical behaviour of the ionomer membrane and coupling the charge and mass transport, electrochemical reactions and structural response. Ahmed et al. [302] modelled the PEMFC as a composite plate structure using Mindlin's plate theory. The study calculated natural frequencies and mode shapes, conducting a parametric analysis of how each layer's thickness, Young's modulus, and density influenced these frequencies. Vibration analysis are also performed in Refs. [303,304]. Placca et al. [305] used Fault Tree (FT) analysis to model degradation mechanisms in PEMFCs, focusing on causal relationships among degradation events. The FT analysis provided a quantitative approach to assess the probability of component-specific failures and their impact on overall cell reliability. Ye et al. [306] employed a 2D FEM to analyse different frame materials, frame structures, and contact behaviours to determine their effects on stress distribution. Other frame structures investigations are presented in Ref. [307,308]. Using the SIMPLE-C method, Perng et al. [309] analysed the impact of various geometric parameters of the baffles on gas flow, reactant transport, and overall cell performance. Dafalla et al. [310] developed a 3D cold start model for PEMFCs to study the effects of clamping pressure on cold start performance. Atyabi et al. [311] developed a 3D multiphase model focused on electrical and thermal contact resistances between GDLs and BPPs.

Ouaidat et al. [312] employed a probabilistic approach using Gauss's

law to evaluate the effects of uncertainties in mechanical design parameters such as clamping pressure, GDL thickness, and rib geometry. In another study, they developed a 3D FEM that fully coupled thermal, electrical, and mechanical processes [313]. This multiphysics model was used to predict the electrical resistance of the fuel cell under different operating conditions, focusing on optimising mechanical parameters through a DOE [314]. Also Charbonné et al. [315] conducted a DOE analysis to investigate the influence of geometric and mechanical properties on PEMFC performance.

H. Zhang et al. [316] developed a comprehensive two-phase model coupling solid mechanics, heat and mass transfer, and electrochemical reactions to understand the effects of mechanical compression on the performance and durability of PEMFCs. Kulkarni et al. [317], using X-ray CT to characterise the MEA under compression, developed a coupled structural and electrochemical model to analyse the impact of non-uniform compression on water management, thermal performance, and current distribution. The study of Le Carre et al. [318] revealed complex GDL behaviour when subjected to rib/channel patterned loading compared to uniform compression. FEM modelling using a strain-dependent elastic law showed that the numerical results could not fully capture the experimentally observed effects. The approach of Kohn et al. [319] utilised a novel analytical model for the mechanical sub-model, which significantly reduced computation time compared to traditional FEM. The electrochemical sub-model used a 2D Finite Volume Method (FVM), and both sub-models were fully parameterised, scalable, and modular, providing adaptability for various use cases.

Xuexia Zhang et al. [320] developed a one-dimensional, two-phase multi-physics model to investigate water and thermal distributions within an anomalous PEMFC. The study focused on parameter distributions along the through-plane direction, validated by experimental data. The study of Xiong et al. [321] used a model coupling mechanics and multiphase non-isothermal electrochemical analysis to evaluate the impact of clamping pressure on mass transfer parameters such as porosity, permeability, and electrical contact resistance. Through numerical simulation, L. Yang et al. investigated the impacts of assembly pressure on reactant inhomogeneity within the GDL [322].

Lei et al. [323] investigated the effects of inhomogeneous GDL properties on the transport phenomena and performance of the system using a three-dimensional FEM and User-Defined Functions (UDFs).

Ouerghemmi et al. employed the Kusoglu model [43–47] to analyse the influence of clamping pressure and relative humidity on the mechanical and electrochemical performance of PEMFCs [324]. The study utilised a detailed multi-physics framework to simulate how variations in clamping force affected the durability of the MEA.

A few key research trends emerge in reviewing mechanical models focusing on the MEA and the single cell. Firstly, FEM remains the primary simulation approach across nearly all models, reflecting its adaptability and precision in capturing stress-strain dynamics, multiphysics interactions, and component deformation under various operational conditions. Pioneering studies, such as those of Solasi et al., laid the groundwork for MEA mechanics research. Recent advancements have expanded on this foundation, enabling detailed analyses of clamping pressure, assembly-induced stress, and interface degradation.

Another notable trend is the integration of hybrid methodologies, blending FEM with CFD, DOE, and experimental validation. This combined approach has enabled researchers to simulate multi-parameter influences on PEMFC performance, ranging from material variability within the GDL to thermal-electrical effects at interfaces. Additionally, probabilistic and optimisation techniques underscore a shift towards predicting PEMFC reliability under real-world conditions, considering both structural and environmental uncertainties.

Research also increasingly emphasises tailored analyses for specific cell components. While traditional models addressed single-component stresses, recent studies are mapping out performance variations across interconnected components (e.g., gaskets and GDLs), reflecting an advanced understanding of PEMFC functionality as an integrated system

rather than isolated parts. These trends illustrate a growing interest in holistic modelling approaches that simulate and predictively enhance PEMFC durability and efficiency under diverse operational conditions.

#### 4. Stack scale

In this section, we explore mechanical models of PEMFC stacks, shifting the focus from individual cells and MEA structures to the stack as a whole (see Fig. 11 and Table S1, Section: Stack). Stack modelling presents unique challenges due to the cumulative effects of mechanical pressure distribution, clamping methods, and component alignment across multiple cells. Unlike models centred on single MEAs, stack models must address larger scales and complex interactions between layers, such as cumulative stress and contact resistance variability across the entire assembly.

The majority of stack models are based on FEM simulations, often integrated with experimental validation and probabilistic approaches to reflect the intricate mechanical behaviour under operational and assembly conditions. Innovative approaches, such as equivalent stiffness modelling and optimisation algorithms, contribute to greater computational efficiency and structural resilience in stack simulations, ensuring robustness against operational stresses.

These models are categorised in the following text, detailing the methodologies and parameters underpinning current advancements in PEMFC stack assembly and reliability.

First of all, some models that can be considered in this classification were already cited in the previous sections, such as [196] in Section 2.2 [239], in Section 2.4 [251], in Section 2.5 [269,272], in Section 2.6, and [277,278] in Section 3.

In 2005, the study of Lee et al. [325] used FEM to simulate the PEMFC with a point stack assembly method. By incorporating all fuel cell components' mechanical properties and geometric dimensions, the authors could simulate the compliance and pressure distribution within the single cell. They validated their FEM results using experimental tests. D. Liu et al. [326] used a robust design approach based on RSM to analyse the influence of various assembly parameters, including assembly pressure and bolt position in the stack. These parameters were considered random variables with probabilistic properties, allowing the

study to account for uncertainties in the assembly process. The same team developed other stack models [327], also through original approaches, such as equivalent models [328,329] and the Monte Carlo approach [330]. The article by Vicky Rouss et al. [331] tested a fuel cell stack on a vibrating platform along all three orthogonal axes to understand the effects of mechanical vibrations. The data collected from these experiments were used to create a three-dimensional, multi-input and multi-output model based on an Artificial Neural Network (ANN) approach. Another model focused on the vibration analysis of the stack was developed by Wu et al. [332]. Mikko Mikkola et al. presented a 3D FEM model to optimise various types of fuel cell structures at different temperatures. The study validated the model using pressure-sensitive film measurements involving components of a PEMFC stack with low rigidity and high deformability [333]. Martemianov et al. [334] used the same model cited earlier by Bograchev et al. [277,278], and it was implemented to simulate stress and plastic deformation at both local (single tooth/channel structure) and global scales (entire cell features, including seal joints).

The articles by P. Lin et al. introduce an equivalent stiffness model for large PEMFC stacks, published in two parts [335,336]. The model considers the stack as a series of elastic elements, effectively representing the structural parameters and the influence of temperature on internal stress and contact resistance at component interfaces (see Fig. 12). The equivalent stiffness model was validated against FEA results, demonstrating good prediction accuracy for component stiffness and clamping load. The authors used the model to determine optimal clamping loads and design parameters for the stack structure. This pioneering approach laid the foundation for all subsequent equivalent stiffness models [337–343], providing a comprehensive methodology for improving PEMFC stack reliability by optimising mechanical assembly and minimising potential issues related to stress concentration and uneven pressure distribution.

In 2011, an article by Sun et al. [344] investigated the thermal transport phenomena and mechanical effects due to thermal inertia loading during start-up and shutdown operations of a 3D PEMFC stack in a subfreezing environment. The study uses a combined FEM and upwind FVM discretisation to model the thermal transport and the mechanical behaviour under these conditions. A similar approach is also used by

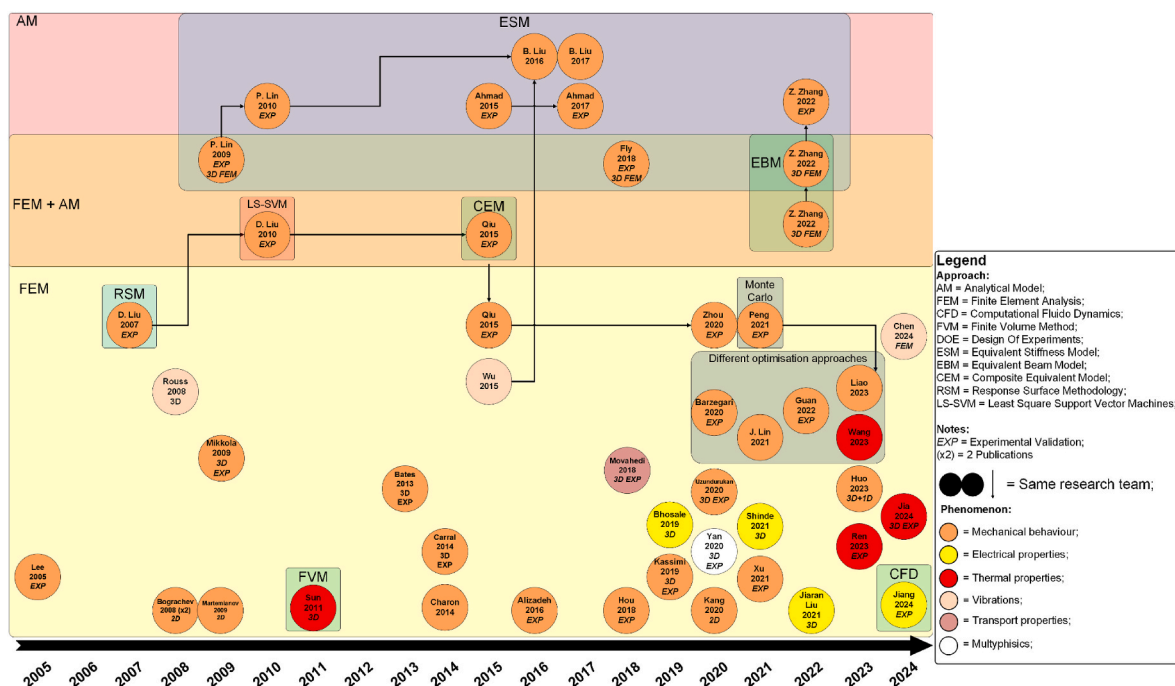


Fig. 11. Stack mechanical models' classification.

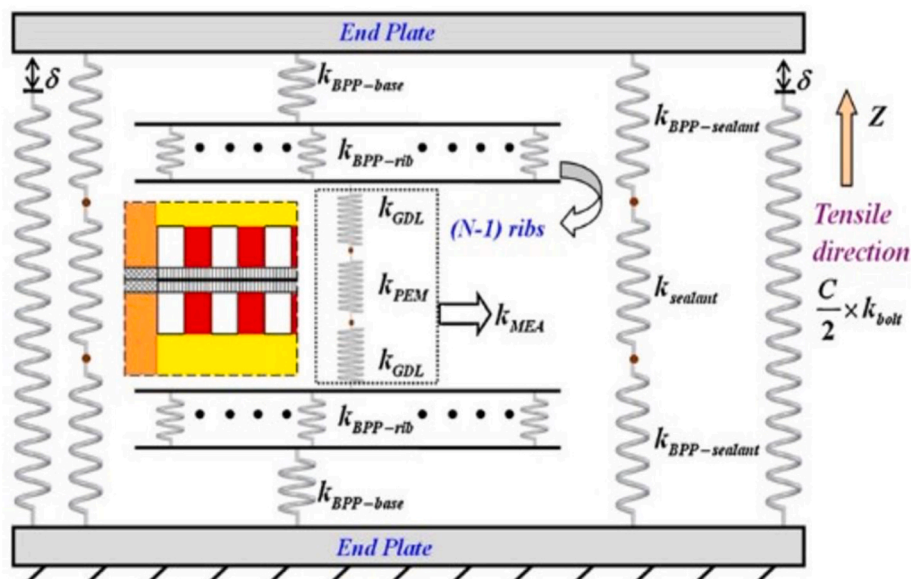


Fig. 12. Equivalent Stiffness Model. (Permission from Ref. [335], copyright Elsevier).

Movahedi et al. [345]. The study of Bates et al. [346] involved numerical simulations and experimental testing to understand the impact of clamping pressure on contact resistance between the GDLs and BPPs. Charon et al. [347] applied a homogenisation technique, replacing complex cell parts with composite finite elements or homogenised Representative Elementary Volumes (REVs) to simplify the model and make it computationally efficient. Carral et al. [23] developed a 3D FEM to investigate how different assembly parameters, such as the number of cells and their position within the stack, affect the uniformity of MEA compression. The model was validated with experimental measurements. The study of Alizadeh et al. [348] develops a model to analyse the effect of parameters such as thickness and material of the EPs, sealant hardness, number of cells in the stack, and cell position on the pressure distribution over the MEA. The model was validated using pressure-sensitive films.

In 2018, Hou et al. [349] developed a simplified FEM consisting of ten cells to investigate the deformation within the stack. The study found that interface slippage occurs when the BPP and MEA are subjected to vertical impact acceleration. The article by Bhosale et al. [350] investigates the optimisation of contact resistance in a unitised regenerative fuel cell stack by using different gasket materials and applying optimal clamping torque through a 3D FEM. Another model with the same dimension is developed by Kassimi et al. [351]. A two-dimensional FEM was developed by Kang et al. for a metal BPP stack to study the stress concentration phenomenon in the MEA in an assembled state, considering factors like assembly load, sealing structure, and sealing material [352]. Uzundurukan et al. [353] investigated the effects of different compression methods on PEMFC performance using numerical and experimental approaches. A three-dimensional FEA model was used to simulate the deformation of the stack components under various clamping methods, including bolt and plate compression. Barzegari et al. [354] employed a central composite design method and finite element simulations to achieve the most uniform contact pressure distribution. The experimental data obtained using pressure mapping systems were used to validate the numerical results.

In 2021, Shinde et al. [355] conducted a numerical investigation to understand the sensitivity of EP design and gas diffusion material models in quantifying localised interface and bulk electrical resistance. The study developed a 3D FEM to simulate the effects of various EP designs and GDL material properties on the contact resistance and overall electrical performance of the stack. Jiaran Liu et al. [356]

considered the possibility of generating uniform contact pressure with a newly designed pneumatic clamping system compared to a traditional clamping mechanism. Based on FEM, two models of the PEMFC were established. J. Lin et al. [357] established bolt-encapsulated stack models at different scales to examine the influence of cell number on contact pressure distribution characteristics in the outermost and innermost GDLs. Using the contact pressure distribution characteristics of a 6-cell stack as a reference, an optimal Latin hypercube design generated 280 data sets with varying clamping conditions. A surrogate model based on Support Vector Regression (SVR) was used to predict contact pressure distribution, which was then optimised using Gray Wolf Optimizer for an 80-cell stack. The study of Guan et al. [358] emphasised that uneven clamping load distribution decreases the durability of PEMFC stacks, making it essential to model the pressure distribution quantitatively and address imbalance issues. A quantitative model was proposed to characterise the pressure distribution on BPPs, using both FEM and experimental measurements with flexible pressure sensors. Furthermore, a nacre-inspired optimisation approach was applied to improve the uneven pressure distributions based on the quantitative model.

In Huo et al. study [359], a large-scale FEM PEMFC model was developed considering realistic assembly using 14 bolts and investigating their impact on key parameters of the GDL. The contact pressure at the interface of GDL and BBP was converted into non-uniform contact resistance, which was incorporated into a self-developed "3D + 1D" full PEMFC multiphase model. The "3D + 1D" model simplified part of the components along the through-plane direction into a 1D model to improve calculation efficiency and stability. Ren et al. [360] model a PEMFC to assess how bolt load, gasket hardness, and size affect contact pressure distribution during assembly. Using thermal-mechanical coupling to simulate operational conditions, a matching relationship among gaskets, GDLs, and seal grooves is proposed. Wang et al. [361] investigated the impact of non-uniform contact pressure on the electrochemical performance of PEMFC stacks. Their study incorporated a heuristic-based optimisation design method to enhance the thermal contact performance of engineering systems. By focusing on the material stiffness of the contact interface, they aimed to reduce thermal contact resistance and improve the contact interface temperature distribution non-uniformity. The paper of Liao et al. [362] proposes a digital twin modelling approach that integrates FEM and ANN to create an efficient design for the stack assembly process. A case study on predicting contact

pressure within the stack validates the digital twin model, demonstrating that the ANN model achieves close to 98% prediction accuracy compared to FEM while enhancing computational efficiency by several orders of magnitude. Jiang et al. [363] employed a combination of structural simulations and experiments to optimise pressure distribution in large-scale PEMFC stacks. They conducted simulations on a single cell and a 40-cell stack under various clamping pressures, comparing these results with experimental data from pressure-sensitive films to assess contact pressure uniformity. Additionally, CFD simulations indicated that the optimal clamping pressure for maximising electrical output performance is approximately 1.33 MPa. Jia et al. [364] conducted experiments measuring pressure distributions between the GDL and flow field and created a validated 3D model combining heat transfer and mechanical responses. Lastly, the Chen et al. article [365] examines the structural integrity of a horizontally mounted fuel cell stack under large impacts, which can cause slippage and bowing, risking performance and leakage. Using FEA, the study analyses a 300 kW stack with 550 unicells, focusing on local vibrations and deformation patterns. The authors enhance the stack's robustness by adding reinforcement bars, demonstrating that proper design can produce a resilient stack for automotive applications.

The review of PEMFC stack models reveals significant research trends in addressing the mechanical complexities of multi-cell assemblies. FEM remains the predominant simulation technique, proving instrumental in capturing stress distribution, clamping effects, and pressure variations across the stack. A clear trend in stack modelling is the focus on probabilistic and optimisation-based approaches, which allow for robust design by accounting for variability in component characteristics and assembly parameters. Furthermore, a noteworthy advancement is the increased use of thermal and vibrational analyses, highlighting the broader scope of stack models to account for both structural and functional aspects. Models that simulate real-world conditions—such as thermal cycling, subfreezing start-up, and mechanical vibrations—reflect the progression towards comprehensive stack simulations that support durability and performance optimisation design.

In summary, these stack models underscore the evolving complexity in PEMFC modelling approaches, moving towards integrated frameworks that combine FEM with multiphysics simulations and probabilistic methods to ensure PEMFC stack reliability and robustness under diverse operational conditions.

## 5. Conclusions

In this work, specific modelling characteristics are defined for the first time and utilised as a guiding framework to group a collection of models focused on the mechanical behaviour and structure of PEMFCs, as well as their interaction with other phenomena occurring during operation.

The classification presented, along with the associated diagrams, represents an original and valuable method that allows the classification of models based on different characteristics within a unified framework. This differs from previous reviews that covered non-mechanical models and classified them separately according to specific attributes such as chronology, scale, component, or modelling approach, often leading to fragmented information. For example, a specific-component model could previously be found in a list dedicated to the used approach or in a list of models focusing on the model scale, which dispersed information across different categories. With this new method, gathering all models of a single component in one environment is possible, considering the publication chronology, applied approach, studied phenomena, model scale, experimental validation, and collaboration between research teams.

The review has classified all PEMFC components and structures, highlighting both the key differences and common features among them. Notably, a similar effort to categorise mechanical models in this way has never been conducted before. This unified approach to classification is

also highly relevant for other research domains and applications, potentially providing a new perspective on categorising and understanding different modelling approaches.

From the review, it was possible to summarise the research trends in the mechanical modelling of PEMFCs, showing similarities and differences across different components. Notably, some research teams and collaborations, such as the one of Linfa Peng et al. [19,30,114–116,142–147,234,235,251–253,282–284,322–326,357] have studied the mechanical behaviour of the complete PEMFC and its different components. Similar approaches would be highly useful and insightful for future studies. There is a clear need for a stronger focus on mechanical modelling, and this work offers a useful and comprehensive resource for researchers looking to gain an overarching view of the state of the art in mechanical modelling of PEMFCs.

In conclusion, the presented classification provides a comprehensive overview of the existing mechanical models and suggests that integrating mechanical modelling with models of other phenomena occurring during PEMFC operation, possibly using non-mechanical models, would be highly beneficial. This holistic approach would help to further advance the understanding and efficiency of PEMFCs.

## CRediT authorship contribution statement

**Luca Marcelli:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Dominique Chamoret:** Writing – review & editing, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Xavier François:** Writing – review & editing, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Yann Meyer:** Writing – review & editing, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Denis Candusso:** Writing – review & editing, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

## Generative AI and AI-assisted technologies

Generative AI and AI-assisted technologies have been used to improve the language and readability of the paper.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2025.03.004>.

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