

Graph Neural Network Modeling of Aggregate Contact Networks for Predicting Stress Distribution in Asphalt Mixtures

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Abstract

Asphalt mixtures are complex particulate systems whose mechanical performance emerges from the arrangement, contact, and load transfer among coarse and fine aggregates, mastic, and voids. Predicting stress distribution within such materials is central to pavement design, durability assessment, and infrastructure sustainability, yet conventional continuum models often smooth over the heterogeneous contact networks that govern localized failure. This paper examines graph neural network modeling of aggregate contact networks as a system-level approach for predicting stress distribution in asphalt mixtures. It frames the mixture as a meso-scale infrastructure in which nodes represent aggregate particles or contact zones and edges encode physical adjacency, contact morphology, and load-transfer capacity. The discussion connects graph representation learning, discrete element modeling, image-based aggregate characterization, and materials informatics. It then analyzes architectural trade-offs involving inductive versus transductive learning, message passing depth, attention mechanisms, interpretability, and computational cost. The paper emphasizes robustness under noisy imaging, uncertain contact parameters, and distribution shift across mix designs and environmental conditions. It also considers deployment pipelines, data governance, fairness in infrastructure decision-making, and policy implications for transportation agencies. The central argument is that graph neural networks can provide a useful bridge between meso-scale contact topology and system-level stress prediction, but only when technical accuracy is coupled with validation, uncertainty quantification, sustainable computational practices, and transparent governance.

Keywords

graph neural networks, asphalt mixtures, aggregate contact networks, stress distribution, meso-scale modeling, infrastructure sustainability, materials informatics, transportation policy.

1. Introduction

Asphalt mixtures are foundational materials of modern transportation infrastructure, yet their mechanical behavior remains difficult to predict because performance emerges from interactions across mineral aggregates, asphalt mastic, air voids, and contact zones. Continuum mechanics offers efficient descriptions of pavement response at the scale of roads and vehicles, but it often treats the material as a homogeneous or statistically averaged medium. That abstraction is useful for design and construction, although it can obscure the localized force chains, contact anisotropies, and meso-scale discontinuities that initiate cracking, rutting, and fatigue damage. The rise of graph neural networks offers a different modeling logic. Instead of representing the mixture primarily as a grid or continuous field, graph neural networks learn from relational structures in which entities and their interactions are explicit. This orientation makes them attractive for asphalt mixtures, where the aggregate skeleton can be understood as a contact network that transmits stress through a finite set of physical connections. The graph neural network model introduced by Scarselli and colleagues provided an early foundation for learning over graph-structured data by propagating information among connected nodes [1]. Since then, graph learning has expanded into a broad family of architectures and applications that can be adapted to particulate and materials systems.

The problem of predicting stress distribution in asphalt mixtures is not merely a computational challenge. It is also an infrastructure challenge with consequences for maintenance scheduling, lifecycle cost, safety, and environmental impact. Pavements are long-lived socio-technical systems embedded in public budgets, procurement rules, technical standards, and political priorities. A model that predicts stress concentrations more accurately could help agencies optimize mix designs, reduce premature failures, and lower material consumption. At the same time, such a model could introduce new dependencies on proprietary data, specialized computation, and opaque inference. The governance of these models therefore matters alongside their accuracy. This paper argues that graph neural network modeling of aggregate contact networks should be developed as a transparent, validated, and policy-aware component of pavement engineering rather than as a purely technical substitute for existing methods. The discussion proceeds from conceptual foundations to architecture, robustness, deployment, governance, and future research.

2. Conceptual Foundations: Asphalt Mixtures as Meso-Scale Networks

Asphalt mixtures can be described as meso-scale infrastructures because their macroscopic properties depend on the arrangement and interaction of discrete constituents. Coarse aggregates form a load-bearing skeleton, fine aggregates and mastic fill voids, and air voids influence compaction, permeability, and damage evolution. Discrete element modeling has long recognized this granular nature by representing particles and contacts explicitly [7]. Early three-dimensional discrete element models of asphalt mixtures demonstrated that particle-level geometry and contact behavior can be used to study mechanical response under loading [8]. Related numerical studies showed that discrete element methods can capture the heterogeneous force transmission that continuum models may miss [9]. Image analysis has further enriched this view by quantifying aggregate shape, angularity, orientation, and distribution within compacted specimens [10]. These developments collectively support the idea that an asphalt mixture is not simply a material volume but a networked assembly of contact relationships.

Within this conceptual frame, nodes may represent aggregate particles, clusters of particles, contact zones, or even mastic bridges. Edges may represent physical contact, proximity, load

transfer, or morphological compatibility. The graph is not a neutral mathematical artifact; it encodes decisions about what matters physically and what can be ignored computationally. If nodes are too coarse, the model may lose the localized stress concentrations that cause damage. If nodes are too fine, the graph may become computationally expensive and sensitive to imaging noise. Edge definitions are equally consequential. A contact edge based only on distance may miss interlocked or angular particles that transmit force through complex surface geometry. An edge weighted by contact area, orientation, or stiffness may better represent load transfer, but it also introduces parameter uncertainty and calibration burden. A recent study on coarse aggregate morphology and asphalt mixture meso-structure using image recognition technology illustrates how aggregate shape and contact arrangement can be extracted and analyzed in ways that inform such graph representations [11]. This line of work is valuable because it links physical imaging to network construction without reducing the mixture to a single averaged descriptor.

The network perspective also reframes damage evolution. Cracking, rutting, and fatigue are not instantaneous global events but progressive changes in contact topology and force transmission. A contact may debond, slide, or rotate; a force chain may intensify; a cluster may reorganize. A graph model can represent these changes as edge removal, edge reweighting, node state updating, or subgraph evolution. This dynamic capability is important because pavement performance is path-dependent. The same initial aggregate gradation can produce different stress distributions depending on compaction, moisture, temperature, and loading history. A purely static graph may provide useful predictions for a given state, but a dynamic or temporal graph is needed to capture damage accumulation. The meso-scale network therefore becomes a bridge between material characterization and lifecycle prediction.

3. Graph Neural Network Architectures for Aggregate Contact Modeling

Graph neural networks are a family of machine learning models designed to learn representations from nodes, edges, and graph-level structure. The graph convolutional network popularized by Kipf and Welling uses localized neighborhood aggregation to learn node representations in a manner analogous to convolution on irregular domains [2]. GraphSAGE introduced inductive learning by sampling and aggregating features from local neighborhoods, which is important when new particles, specimens, or mix designs must be evaluated without retraining the entire model [3]. Graph attention networks extend this logic by learning attention weights that prioritize more relevant neighbors, a mechanism that can be useful when some contacts are more mechanically significant than others [4]. Comprehensive surveys describe the broader landscape of graph neural network methods, including spectral approaches, spatial approaches, recurrent graph models, and autoencoders [5]. Reviews of methods and applications further show how graph learning has moved from citation and social networks into chemistry, physics, transportation, and engineering [6].

For asphalt mixtures, architecture choice involves several trade-offs. A shallow message passing model may generalize well and remain interpretable, but it may fail to capture long-range force chains that span many particles. A deeper model can propagate information across larger neighborhoods, yet it may suffer from oversmoothing, where node representations become too similar and localized distinctions are lost. Attention mechanisms can help identify influential contacts, but attention weights are not automatically causal explanations. A high attention weight may reflect statistical utility rather than physical load transfer. Architecture design must therefore be coupled with mechanical validation. If the model predicts a stress

concentration at a particular contact, engineers need evidence that the prediction corresponds to a plausible force chain, not merely a learned correlation.

Materials informatics provides useful precedents. Graph neural networks have been used to predict properties of molecules and crystals by treating atoms as nodes and bonds as edges [12]. Crystal graph convolutional neural networks demonstrated that graph representations can achieve accurate and interpretable predictions of material properties [13]. Graph networks have also been proposed as a universal machine learning framework for molecules and crystals, enabling transfer across related tasks [14]. Benchmarking studies have clarified where graph neural networks perform well and where data scarcity, feature choice, and target complexity limit performance [15]. Asphalt mixtures differ from molecular crystals because their nodes are not identical atoms, their edges are not fixed bonds, and their properties depend on compaction and temperature. Nevertheless, the core lesson is transferable: graph construction, feature engineering, and validation design are as important as the neural architecture itself.

A practical architecture for aggregate contact networks might combine geometric node features, contact edge features, and global mixture descriptors. Node features could include aggregate size, shape, angularity, orientation, mineralogy, and position within the specimen. Edge features could include contact area, orientation, distance, mastic thickness, and estimated stiffness. Global features could include binder grade, air void content, temperature, loading rate, and compaction method. A message passing network could then predict stress or strain at nodes, edges, or subgraphs. However, the paper avoids reducing this process to a fixed algorithm because the appropriate design depends on available imaging resolution, computational budget, and the engineering question being asked. The system-level challenge is not simply selecting the best neural network but aligning data collection, graph construction, training, validation, and deployment with pavement engineering workflows.

4. Predicting Stress Distribution and Robustness

Stress distribution in asphalt mixtures is spatially heterogeneous. Under traffic loading, some contacts carry disproportionately high forces while others remain relatively unloaded. These force chains can shift as temperature changes, moisture infiltrates, or damage accumulates. A graph neural network can be trained to predict nodal stress, edge force, or global stiffness by learning from discrete element simulations, laboratory tests, or field instrumentation. The advantage of a graph approach is that predictions are conditioned on contact topology. Two mixtures with similar aggregate gradation but different particle arrangements may exhibit different stress distributions, and a graph model can in principle distinguish them. This is a meaningful advance over models that rely only on bulk volumetric properties.

Robustness is a central concern. Imaging pipelines may misidentify particle boundaries, merge adjacent aggregates, or miss fine contacts. Graph construction may then produce spurious edges or omit important load paths. A model trained on clean synthetic data may perform poorly on noisy field specimens. Robustness can be improved through data augmentation, uncertainty-aware training, ensemble methods, and physics-informed constraints, but these strategies introduce trade-offs. Data augmentation may create physically unrealistic graphs. Uncertainty quantification may increase computational cost and complicate user interpretation. Physics-informed constraints may improve extrapolation but can also bias predictions when the underlying physical assumptions are incomplete. Robustness must therefore be evaluated not only by average error but also by performance on edge cases such as highly angular aggregates, high air void contents, and moisture-damaged specimens.

Distribution shift is another challenge. A model trained on one mix design, climate, or compaction method may not generalize to another. Pavement infrastructure is regionally diverse, and material sources vary widely. A graph neural network that learns from a limited set of laboratory specimens may encode local correlations that do not hold elsewhere. Inductive learning methods such as GraphSAGE are attractive because they can generalize to unseen nodes and graphs [3]. Transfer learning, domain adaptation, and meta-learning may further improve cross-domain performance. Yet these methods require careful validation. A model that performs well on a held-out specimen from the same laboratory may fail on a field core from a different climate. Robustness is therefore a socio-technical property: it depends on data diversity, documentation, and the willingness of agencies to test models outside their original training distribution.

Interpretability is also essential for stress prediction. Engineers are unlikely to adopt a model that cannot explain why a particular contact is predicted to fail. Attention weights, saliency maps, and subgraph explanations can provide useful signals, but they must be validated against mechanical reasoning. For example, a model may highlight a contact because it is geometrically unusual rather than because it carries high force. Interpretability should therefore be developed with domain experts, and explanations should be tested against discrete element simulations, photoelastic experiments, or laboratory measurements. The goal is not to make the model transparent in every internal detail but to make its predictions auditable and actionable within engineering practice.

5. Deployment, Infrastructure, and Sustainability

Deploying graph neural networks for asphalt mixture analysis requires more than a trained model. It requires an infrastructure pipeline that connects imaging devices, data storage, graph construction tools, simulation environments, training servers, validation protocols, and user interfaces. Star and Ruhleder argue that infrastructure becomes visible only when it breaks, and that its design is inseparable from the work practices it supports [17]. This insight applies directly to computational materials modeling. If the pipeline is too fragile, too slow, or too dependent on specialized expertise, it will not be used in routine pavement design. If it is too automated, it may produce predictions that engineers cannot interpret or trust. Deployment must therefore balance standardization with flexibility. Standardized graph formats and metadata schemas can improve reproducibility, while modular architecture allows agencies to adapt models to local materials and conditions.

Computational sustainability is another consideration. Training deep graph neural networks can consume significant energy, especially when large ensembles are used for uncertainty quantification. The environmental benefit of better pavement design may outweigh the computational cost if it reduces material use or extends service life, but this trade-off should be measured rather than assumed. Smaller models, efficient message passing, pruning, quantization, and federated learning may reduce energy use. Edge computing could allow some inference to occur near imaging devices, reducing data transfer. However, efficiency gains must not come at the cost of robustness or fairness. A model that is cheap but unreliable may lead to costly failures and erode public trust.

Lifecycle thinking is essential. Asphalt mixtures are already a focus of sustainability efforts because they can incorporate recycled materials, warm-mix technologies, and alternative binders. A graph neural network that predicts stress distribution could help optimize these mixtures by identifying contact arrangements that improve load transfer without increasing brittleness. It could also support digital twins of pavements, where sensor data and periodic

imaging update the graph over time. Such digital twins could inform maintenance decisions, but they require long-term data governance. Who owns the data? Who is responsible for model updates? How are errors handled when they affect public infrastructure? These questions are not peripheral. They determine whether graph neural network modeling becomes a trusted public asset or a proprietary black box.

6. Governance, Fairness, and Policy

The governance of graph neural network models for infrastructure must address accountability, transparency, and equity. Rittel and Webber described many planning problems as wicked problems because they involve contested goals, uncertain knowledge, and irreversible consequences [16]. Pavement management has wicked characteristics. Agencies must balance safety, cost, environmental impact, and political expectations. A model that predicts stress distribution may appear to offer a technical solution, but its outputs must be interpreted within these competing priorities. If the model is trained predominantly on data from wealthy regions with high-quality roads, it may perform poorly in under-resourced areas. That disparity could translate into unequal maintenance outcomes. Fairness in infrastructure modeling therefore requires attention to data representation, model validation across regions, and inclusive decision-making.

Winner argues that artifacts can have political properties because they shape social arrangements [18]. A pavement model that prioritizes certain mix designs, suppliers, or construction practices may reinforce existing power relationships. If the model relies on proprietary imaging equipment or cloud platforms, smaller agencies may be excluded from its benefits. Open standards, public datasets, and collaborative governance can mitigate these risks. Ostrom's work on governing the commons suggests that shared resources can be managed through polycentric institutions, nested rules, and collective choice arrangements [19]. Data and models for public infrastructure can be understood as commons that require similar governance. They should not be enclosed entirely by private interests nor left unmanaged as fragmented local artifacts.

Algorithmic fairness literature provides additional guidance. Barocas, Hardt, and Narayanan emphasize that fairness is not a single metric but a set of contested commitments involving allocation, representation, and accountability [20]. In pavement engineering, fairness may mean equitable distribution of maintenance resources, transparent criteria for model-based prioritization, and accessible channels for appeal when communities disagree with predictions. National and regional policy frameworks increasingly recognize both the promise and risk of artificial intelligence. The National Science and Technology Council outlined strategic directions for artificial intelligence research and development [21]. The European Commission's white paper on artificial intelligence proposed a human-centric approach that balances innovation with trust [22]. These frameworks are not specific to asphalt mixtures, but they establish expectations for transparency, risk management, and public accountability that should inform transportation applications.

Policy implications include procurement standards, model documentation, and liability rules. Agencies may require model cards, validation reports, and uncertainty estimates before accepting graph neural network predictions into design decisions. They may also invest in shared benchmark datasets that represent diverse climates, materials, and traffic conditions. Liability is complex: if a model underestimates stress and a pavement fails prematurely, who is responsible? The model developer, the agency, the contractor, or the inspector? Clear governance can clarify roles while preserving space for engineering judgment. The goal

should be to use graph neural networks as decision support rather than automated authority. Engineers, planners, and communities should retain the ability to question, override, and revise model outputs.

7. Validation, Limitations, and Future Research

Validation of graph neural network models for asphalt mixtures must be multi-level. At the computational level, models can be compared against discrete element simulations and finite element analyses. At the laboratory level, predictions can be tested against mechanical tests, acoustic emission, digital image correlation, and computed tomography. At the field level, predictions can be compared with pavement performance data, distress surveys, and sensor measurements. Each level introduces different uncertainties. Discrete element simulations may themselves rely on calibrated contact models. Laboratory tests may not reproduce field loading. Field data may be sparse and noisy. A robust validation strategy must therefore combine multiple evidence streams and report uncertainty honestly.

Several limitations remain. Graph construction from images is still challenging, especially for fine aggregates and mastic-rich regions. Contact parameters are difficult to measure directly and often must be inferred. Deep graph neural networks can be data-hungry, while high-quality labeled data for asphalt mixtures are scarce. Model interpretability is improving but remains incomplete. Computational cost may limit routine deployment, particularly for large specimens or repeated simulations. Finally, social and institutional barriers may be as significant as technical ones. Engineers may distrust black-box models, agencies may lack data infrastructure, and vendors may resist transparency. Future research should address these barriers through interdisciplinary collaboration involving materials scientists, computer scientists, transportation engineers, policy analysts, and social scientists.

Promising directions include physics-informed graph neural networks that embed conservation laws and contact mechanics, temporal graph networks that model damage evolution, and uncertainty-aware architectures that quantify predictive confidence. Federated learning could allow agencies to share model improvements without centralizing sensitive data. Digital twins could integrate graph models with real-time sensor networks. Standardized benchmarks could accelerate progress and reduce duplication. Yet these advances should be guided by the principles of robustness, sustainability, fairness, and governance. The most successful systems will not be those with the highest benchmark accuracy alone, but those that are trusted, maintainable, and aligned with public infrastructure goals.

8. Conclusion

Graph neural network modeling of aggregate contact networks offers a promising path for predicting stress distribution in asphalt mixtures. By representing aggregates and contacts as nodes and edges, graph models can capture the heterogeneous load paths that continuum approaches often smooth over. They connect naturally with discrete element modeling, image-based aggregate characterization, and materials informatics. They also introduce new challenges in graph construction, architecture design, robustness, interpretability, deployment, and governance. This paper has argued that these challenges should be addressed at the system level rather than treated as isolated technical problems. The value of graph neural networks for pavement engineering depends not only on predictive accuracy but also on their integration into infrastructure workflows, their environmental and computational sustainability, their fairness across regions and communities, and their accountability within public decision-making.

The required reference by Shi and colleagues illustrates how aggregate morphology and meso-structure can be studied through image recognition, providing an important empirical bridge between physical characterization and network modeling [11]. Combined with broader advances in graph learning [1], [2], [3], [4], [5], [6] and materials informatics [12], [13], [14], [15], such work can support more nuanced models of stress distribution. However, the transition from research prototype to routine practice will require open benchmarks, transparent validation, uncertainty quantification, and policy frameworks that protect public interests. Asphalt pavements are long-lived public assets. The models used to design and maintain them should be as durable, equitable, and accountable as the infrastructure they serve.

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