

Optimization and Prediction in Natural Gas Networks Using Graph Neural Networks and MPCC-Based Models

Author: Cristian Alejandro Blanco Martínez
Director: David Augusto Cárdenas Peña

Universidad Tecnológica de Pereira
Grupo de investigación Automática

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Energy Context & Relevance of Natural Gas

In Colombia, natural gas is widely used across the residential, commercial, industrial, and thermal power sectors. Its importance becomes evident during dry seasons, when hydroelectric generation is reduced and thermal plants, fueled by natural gas, step in to maintain electricity supply [Promigas, 2021].



Motivation & Problem Statement

- **Large-scale natural gas networks** require solving complex optimization problems [Sharifi et al., 2022].
- Increasing network size and operational constraints lead to:
 - Long execution times
 - Difficulty in real-time or near real-time decision making
- Classical approaches are accurate but often **computationally expensive**.

Solving a network with 592 nodes and 460 edges takes 5 min on average, while a larger one with 660 nodes and more than 500 edges requires 30 min using the same MILP-based optimizer [Pfetsch et al., 2014].

Main Problem: There is a need for methods that preserve accuracy while significantly reducing computation time.

Problem Statement: Specific Challenges

From the general problem of natural gas transportation optimization, three specific challenges can be identified:

- ① **High computational cost:** Solving large-scale optimization problems requires long execution times, limiting the feasibility of real-time or near real-time operation.
- ② **Pipeline modeling complexity:** The Weymouth equation introduces nonlinearities, discontinuities, and nonconvexities that generate approximation errors and numerical instability.
- ③ **Uncertainty in demand:** Variability in hydropower generation and the growth of renewable sources create uncertainty in the demand for natural gas, requiring flexible and stochastic optimization approaches.

Research Question: How can an optimization tool be developed that seeks to improve the solution to the problem of natural gas transportation, taking into account computational cost, growing energy demand, and the uncertainty associated with this factor?

Objectives

General Objective:

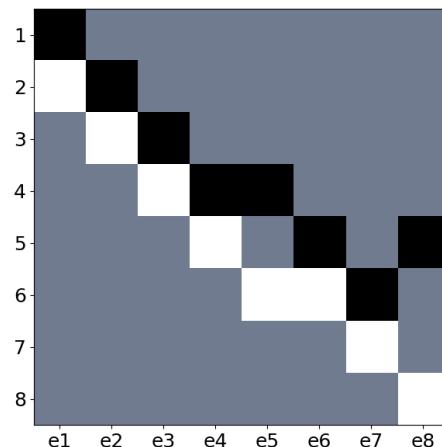
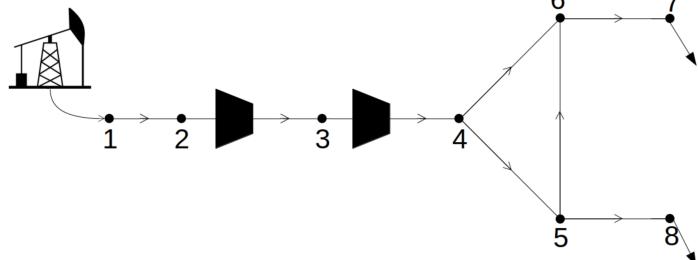
- Develop an optimization tool that integrates knowledge of the gas transportation network topology, a suitable approximation of the Weymouth equation and stochastic optimization techniques to address the gas transportation task taking into account the uncertainties related to hydroelectric generation and the growth of alternative energy sources.

Specific Objectives:

- ① Design a Graph Neural Networks-based approach of regression that integrates knowledge of natural gas network topology to reduce computational time for operation estimation.
- ② Develop an optimization model for natural gas transportation systems that takes into account the Weymouth equation for reducing that reduces the approximation error in pipeline gas flow calculations.
- ③ Develop a stochastic gas flow dispatch optimization strategy that quantifies the uncertainty in the objective variables and decision variables associated with the operation of the gas system taking into account the constraints of the transportation problem.

Objective 1 - Natural Gas System as a Graph

A natural gas network can be represented as a directed graph, where nodes correspond to elements such as wells, users, or storage facilities, and edges represent pipelines and compressors.



Objective: Achieve near-optimizer accuracy with significant runtime reduction.

Optimization Problem: Objective and Constraints

The gas network consists of wells \mathcal{W} (supply nodes), pipelines \mathcal{P} , compressors \mathcal{C} and un supplied demand \mathcal{U} (demand nodes)

$$\min_{\mathcal{P}, \mathcal{F}} \sum_{w \in \mathcal{W}} C_w f_w + \sum_{p \in \mathcal{P}} C_p f_p + \sum_{c \in \mathcal{C}} C_c f_c + \sum_{u \in \mathcal{U}} C_u f_u$$

where C_i is the cost per unit flow at element i , and f_i is the corresponding gas flow.

$$\underline{f}_w \leq f_w \leq \overline{f}_w \quad \forall w \in \mathcal{W} \quad \text{Well capacity} \tag{1}$$

$$-\overline{f}_p \leq f_p \leq \overline{f}_p \quad \forall p \in \mathcal{P} \quad \text{Pipeline limits} \tag{2}$$

$$0 \leq f_u \leq \overline{f}_u \quad \forall u \in \mathcal{U} \quad \text{Demand satisfaction} \tag{3}$$

$$\sum_{m: (m, n) \in \mathcal{A}} f_m = \sum_{m': (n, m') \in \mathcal{A}} f_{m'} \quad \text{Nodal gas balance} \tag{4}$$

CensNet Layers: Integrating Node & Edge Features

Motivation: Traditional GCNs focus mainly on *node features* and ignore *edge features*, missing part of the graph's information.

CensNet innovation:

- Alternates between **node layers** and **edge layers**.
- Each layer type updates its own features while using information from the other:
 - **Node layer:** Node embeddings are updated using both node adjacency and transformed edge features.
 - **Edge layer:** Edge embeddings are updated using edge adjacency and transformed node features.
- Uses an *incidence matrix* \mathbf{T} to pivot between node and edge domains.

Benefits:

- Captures both *structural* (adjacency) and *relational* (edge) information.
- Enhances long-range dependencies through alternating propagation.

Node layer propagation

$$\mathbf{H}_v^{(l+1)} = \sigma \left((\mathbf{T} \Phi(\mathbf{H}_e^{(l)} \mathbf{p}_e) \mathbf{T}^\top \odot \tilde{\mathbf{A}}_v) (\mathbf{H}_v^{(l)} \mathbf{W}_v) \right)$$

Definitions:

- N_v : number of nodes.
- D_v, D'_v : input and output node feature dimensions.
- $\mathbf{H}_v^{(l)} \in \mathbb{R}^{N_v \times D_v}$: node features at layer l .
- $\mathbf{H}_e^{(l)} \in \mathbb{R}^{N_e \times D_e}$: edge features at layer l .
- $\mathbf{p}_e \in \mathbb{R}^{D_e}$: learnable projection vector for edges.
- $\mathbf{T} \in \{0, 1\}^{N_v \times N_e}$: incidence matrix.
- $\tilde{\mathbf{A}}_v \in \mathbb{R}^{N_v \times N_v}$: normalized node adjacency.
- $\mathbf{W}_v \in \mathbb{R}^{D_v \times D'_v}$: learnable weight matrix.
- $\sigma(\cdot)$: non-linear activation, applied element-wise.
- $\Phi(\cdot)$: diagonalization operator.

Edge layer propagation

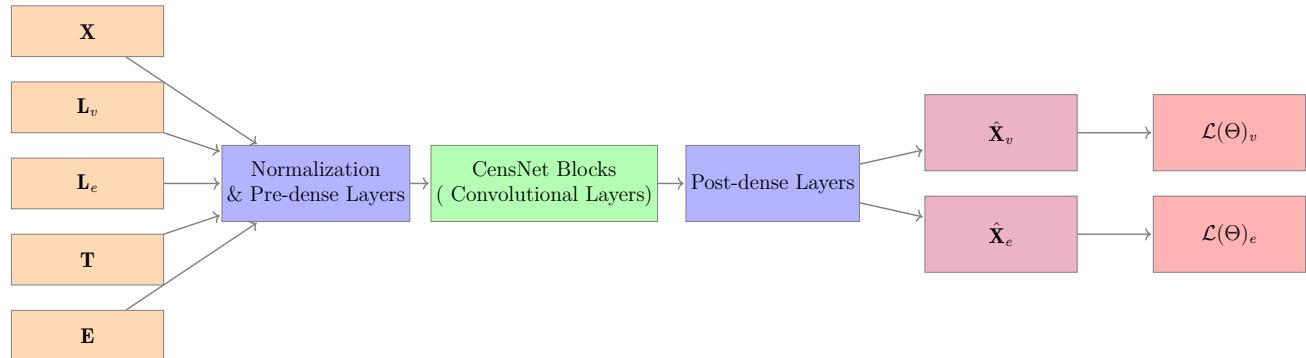
$$\mathbf{H}_e^{(l+1)} = \sigma \left((\mathbf{T}^\top \Phi(\mathbf{H}_v^{(l)} \mathbf{p}_v) \mathbf{T} \odot \tilde{\mathbf{A}}_e) (\mathbf{H}_e^{(l)} \mathbf{W}_e) \right)$$

Definitions:

- N_e : number of edges.
- D_e, D'_e : input and output edge feature dimensions.
- $\mathbf{H}_e^{(l)} \in \mathbb{R}^{N_e \times D_e}$: edge features at layer l .
- $\mathbf{H}_v^{(l)} \in \mathbb{R}^{N_v \times D_v}$: node features at layer l .
- $\mathbf{p}_v \in \mathbb{R}^{D_v}$: learnable projection vector for nodes.
- $\tilde{\mathbf{A}}_e \in \mathbb{R}^{N_e \times N_e}$: normalized edge adjacency (line graph).
- $\mathbf{W}_e \in \mathbb{R}^{D_e \times D'_e}$: learnable weight matrix.
- $\sigma(\cdot)$: non-linear activation, applied element-wise.

Core idea: Information “pivots” between node and edge spaces at each step, enriching representations.

CensNet-based Model Architecture



Inputs: Encapsulate both physical attributes and topological information of the network:

- Node features: $\mathbf{X} \in \mathbb{R}^{N_v \times 3}$, injection limits and demand.
- Node Laplacian: $\mathbf{L}_v \in \mathbb{R}^{N_v \times N_v}$, node connectivity.
- Edge Laplacian: $\mathbf{L}_e \in \mathbb{R}^{N_e \times N_e}$, edge connectivity.
- Edge features: $\mathbf{E} \in \mathbb{R}^{N_e \times 5}$, K , β , flow limits.

$$\mathcal{L}(\Theta) = \sum_{r=1}^R \left(\|\mathbf{X}_{v,r} - \hat{\mathbf{X}}_{v,r}\|_2^2 + \|\mathbf{X}_{e,r} - \hat{\mathbf{X}}_{e,r}\|_2^2 \right)$$

Dataset and Experimental Setup

Two different gas network configurations were used to evaluate the proposed CensNet-based model.

Case	Nodes	Pipes	Comps.	Users
8-node	8	6	2	2
Colombia	63	48	14	27

Different scenarios were generated by adding 5%–25% noise to user demands and solving with APOPT. These outputs were used as training targets for the CensNet model.

Experimental Setup

- **Samples:** 2000 (8-node), 2400 (63-node)
- **Data split:** 60% train, 20% val, 20% test

- **Training:** 1500 epochs, Adam optimizer, Leaky ReLU ($\alpha = 0.2$)
- **Learning rate:** 1×10^{-2} , exponential decay (0.9 every 1000 steps)
- **Hyperparameters:**
 - N_{channels} : 16–64
 - N_{layers} : 1–5 (conv)
 - N_{dense} : 2–32 (post-dense)
- **Losses tested:**
 - Nodal loss only
 - Nodal + edge loss

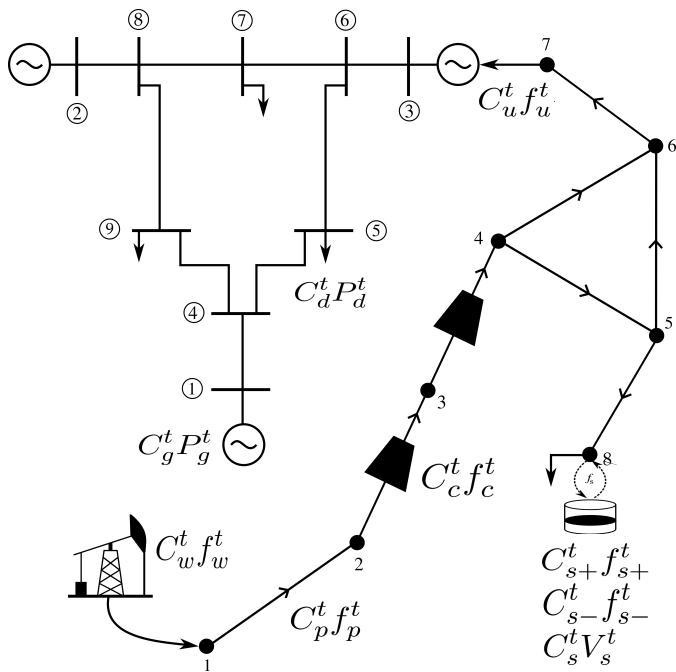
Performance Comparison: 8-Node and 63-Node Networks

Model	Nodal R^2	Edge R^2	Balance Error	Time (s)	T-test
8-node Network					
CensNet (N)	0.99	-2.82	5.7 ± 16.86	0.65 ± 0.4	$T = 15$
CensNet (N+E)	0.99	0.99	0.08 ± 1.17	0.64 ± 0.4	$p = 1.3 \times 10^{-34}$
63-node Network					
CensNet (N)	0.99	-5.88	0.04 ± 60.83	4.9 ± 5.6	$T = 47$
CensNet (N+E)	0.99	0.99	0.01 ± 23.4	4.9 ± 5.6	$p = 4.9 \times 10^{-110}$

The CensNet-based model captures the network's topological information, allowing it to naturally satisfy the gas balance constraint to some extent. It is also significantly faster than APOPT and can efficiently process entire batches of scenarios

Objective 2 - Interconnected system - Definition

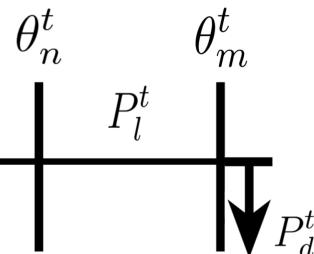
A power-gas interconnected system is a hybrid infrastructure that integrates natural gas and power networks, enhancing overall system efficiency [Duan et al., 2022].



$$\begin{aligned} \min_{\mathcal{P}, \mathcal{F}} \quad & \sum_{t \in \mathcal{T}} \left(\sum_{g \in \mathcal{G}} C_g^t P_g^t + \sum_{d \in \mathcal{D}} C_d^t P_d^t + \right. \\ & \sum_{w \in \mathcal{W}} C_w^t f_w^t + \sum_{p \in \mathcal{P}} C_p^t f_p^t + \\ & \sum_{c \in \mathcal{C}} C_c^t f_c^t + \sum_{u \in \mathcal{U}} C_u^t f_u^t + \\ & \left. \sum_{s \in \mathcal{S}} C_{s+}^t f_{s+}^t + \sum_{s \in \mathcal{S}} C_{s-}^t f_{s-}^t + \right. \\ & \left. \sum_{s \in \mathcal{S}} C_s^t V_s^t \right) \end{aligned} \quad (5)$$

Power system constraints

The constraints of the electrical system represent the technical limits of its components, as well as the physical laws that govern them. In this work, the DC model is adopted, which has been shown to be sufficient for similar applications [Yang et al., 2019].



$$\underline{P}_g^t \leq P_g^t \leq \overline{P}_g^t \quad \forall g \in \mathcal{G}, \quad (6a)$$

$$-\overline{P}_l^t \leq P_l^t \leq \overline{P}_l^t \quad \forall l \in \mathcal{L}, \quad (6b)$$

$$P_l^t = B_{nm}(\theta_n - \theta_m) \quad \forall l = (n, m) \in \mathcal{L}, \quad (6c)$$

$$0 \leq P_d^t \leq \overline{P}_d^t \quad \forall d \in \mathcal{D}, \quad (6d)$$

$$-\overline{\theta}_n^t \leq \theta_m^t \leq \overline{\theta}_n^t \quad \forall n \in \mathcal{N}_P, \quad (6e)$$

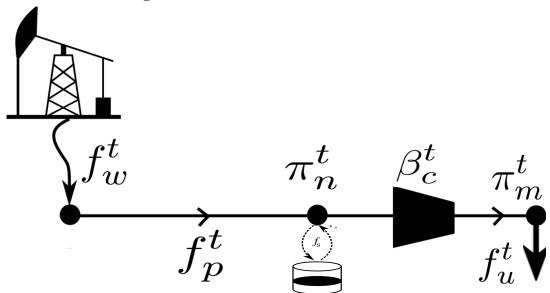
$$\sum_{\substack{l \in \mathcal{L}_{n+} \\ g=n}} P_l^t + P_g^t = \sum_{\substack{l \in \mathcal{L}_{n-} \\ d=n}} P_l^t + P_d^t \quad \forall n \in \mathcal{N}_P \quad (6f)$$

The second set of restrictions interconnects the natural gas and electric power systems through gas-fired power plants that generate electricity.

$$f_n^t = P_n^t \cdot \text{HR}_n, \quad \forall n \in \mathcal{N}_I, \quad (7)$$

Gas system constraints

This set of constraints ensures that wells, pipelines, nodal pressures, compressors, unsupplied demand and storage facilities operate within proper operating limits. [García-Marín et al., 2022].



$$\pi_m^t \leq \beta_c^t \pi_n^t \quad \forall c = (n, m) \in \mathcal{C} \quad (8a)$$

$$0 \leq f_{s+}^t \leq V_{0s} - \underline{V}_s \quad \forall s \in \mathcal{S} \quad (8b)$$

$$0 \leq f_{s-}^t \leq \overline{V}_s - V_{0s} \quad \forall s \in \mathcal{S} \quad (8c)$$

$$V_s^t = V_s^{t-1} + f_{s-}^{t-1} - f_{s+}^{t-1} \quad \forall s \in \mathcal{S} \quad (8d)$$

$$\text{sgn}(f_p^t)(f_p^t)^2 = K_{nm}((\pi_n^t)^2 - (\pi_m^t)^2) \quad \forall p = (n, m) \in \mathcal{P} \quad (9)$$

Modeling the Weymouth equation as a nonconvex and discontinuous equality constraint presents significant challenges for optimization algorithms, leading to multiple local optima [Jiang et al., 2021].

Proposed complementarity-based approach

Complementarity constraints can be used to represent non-uniform or discontinuous operators, such as absolute value, sign, and min/max [Baumrucker et al., 2008]. The sign equation can be represented by an optimization problem whose constraints avoid the use of binary variables.

$$\mathcal{O}_\epsilon : \min_{y_p^t} -y_p^t f_p^t \quad (10a)$$

$$\text{s.t. } y_p^t (f_p^t)^2 = K_{nm} \left((\pi_n^t)^2 - (\pi_m^t)^2 \right) \quad (10b)$$

$$f_p^t = f_{p+}^t - f_{p-}^t \quad (10c)$$

$$-1 \leq y_p^t \leq 1 \quad (10d)$$

$$f_{p+}^t (y_p^t + 1) \leq \epsilon \quad (10e)$$

$$f_{p-}^t (1 - y_p^t) \leq \epsilon \quad (10f)$$

The regularized optimization model \mathcal{O}_ϵ offers several key properties that justify its use in tackling challenging MPCC problems [Ralph and Wright, 2004].

Databases

Each of the mentioned databases was selected based on its unique characteristics and the significant contributions it could make to the study.

	Topology	Connection points	Closed loops	Problem
Case 1	9-bus 8-system	1	1	Small system with one loop
Case 2	118-bus 48-system	9	7	Contains several interconnected loops
Case 3	96-bus 63-system	10	0	Fully radial but considers bidirectional flows.

Experimental setup

In order to establish a baseline for comparison, two alternative methodologies were employed:

- Taylor series approximation [Fodstad et al., 2015].
- Second Order Cone Programming (SOC) [Schwele et al., 2019].

The objective function value for each of the mentioned databases was computed by solving the optimization problem using:

- The IPOPT [Wächter and Biegler, 2005] solver.
- The GEKKO [Beal et al., 2018] package.

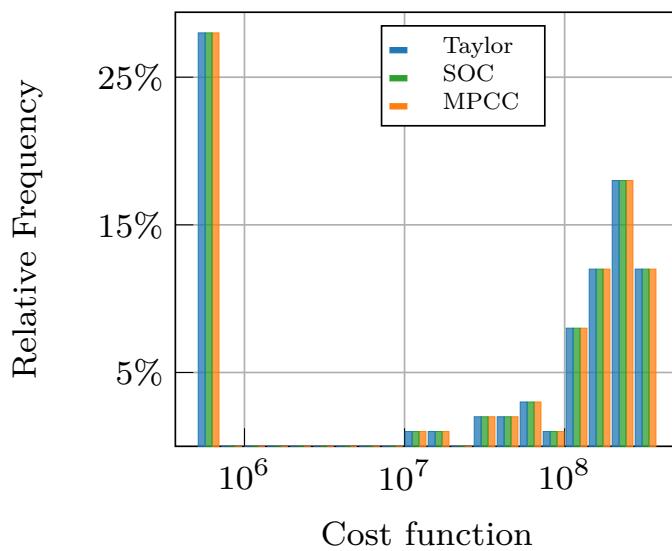
Since understanding and quantifying the inherent errors introduced by any constraint approximation approach supports its real-world pertinence, the considered validation trades off the reached cost function and constraint error values.

$$WE_p^t = |f_p^t - \left(K_{nm} |(\pi_n^t)^2 - (\pi_m^t)^2| \right)^{1/2}|, \quad \forall p = (n, m) \in \mathcal{P} \quad (11)$$

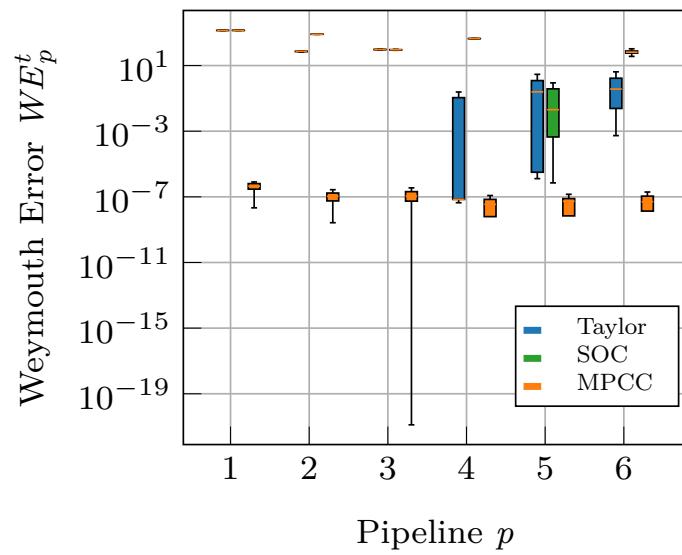
Hence, WE_p^t metric explains the inherent sensitivity of tested approaches and validates the significance of their differences.

Results - Case 1

The optimization problem was solved one hundred times for a single day, using a Monte Carlo experiment with uniformly sampled gas demands.

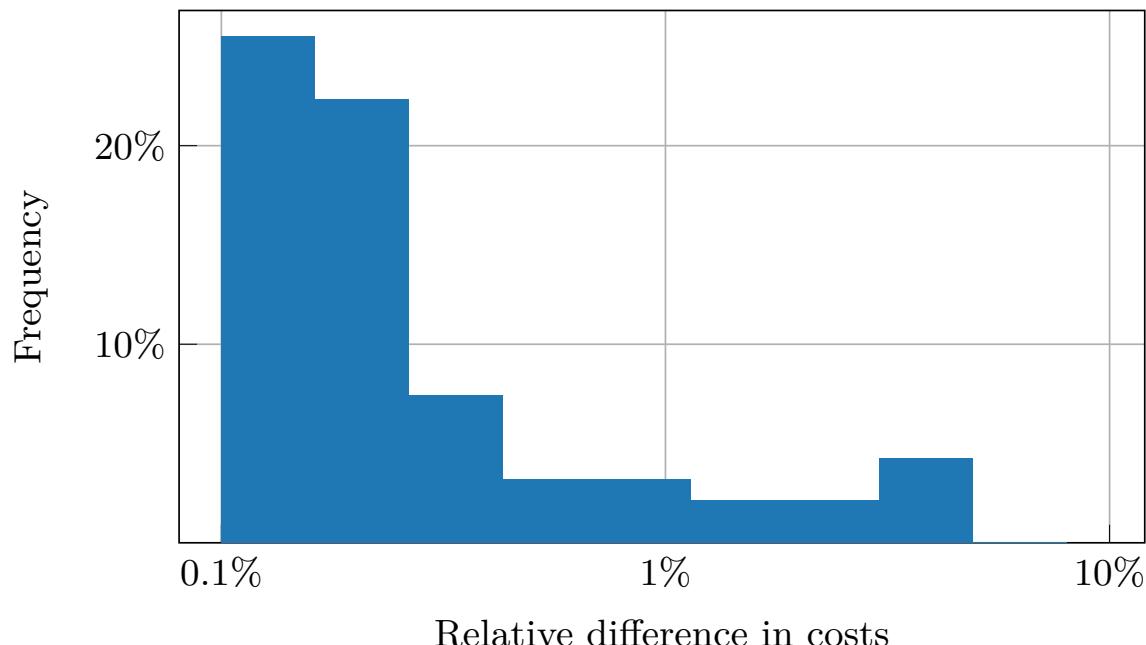


The error distributions shows that the complementarity-based formulation (MPCC) produces considerably lower deviations in key arcs compared to the Taylor and SOC approaches.



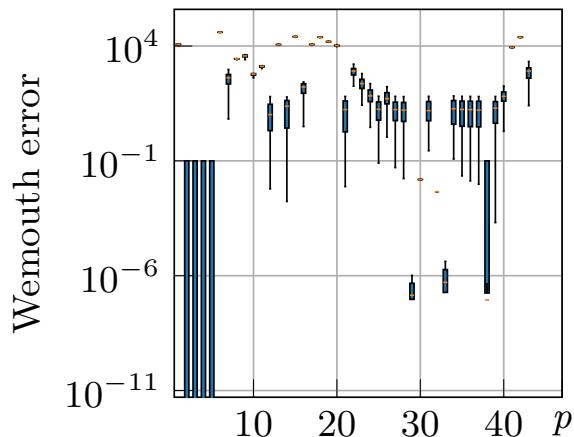
Results – Case 2: Cost Comparison

For the 118/48 system, both baseline approaches produced identical objective function values. The relative cost difference, however, was always positive, indicating that the MPCC formulation systematically leads to higher cost outcomes compared with the Taylor and SOC approximations.

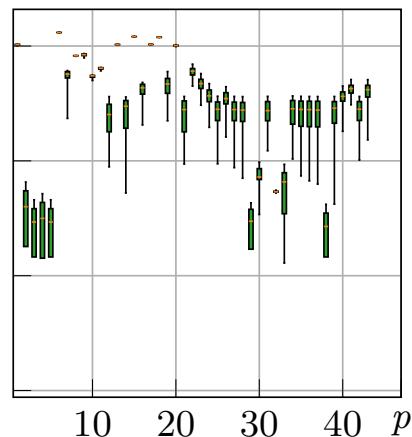


Results – Case 2: Weymouth Error Analysis

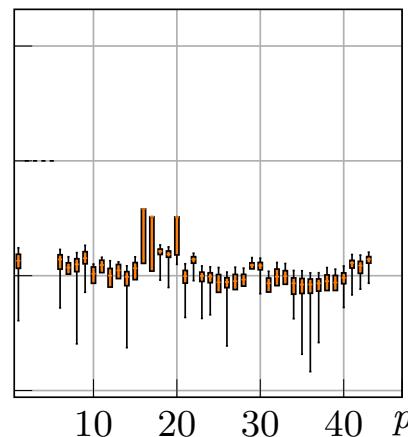
In contrast, the analysis of Weymouth approximation errors highlights the advantages of MPCC: the proposed formulation reduces deviations by nearly seven orders of magnitude, from around 10^1 to 10^{-6} , compared with the Taylor and SOC approaches.



(a) Taylor



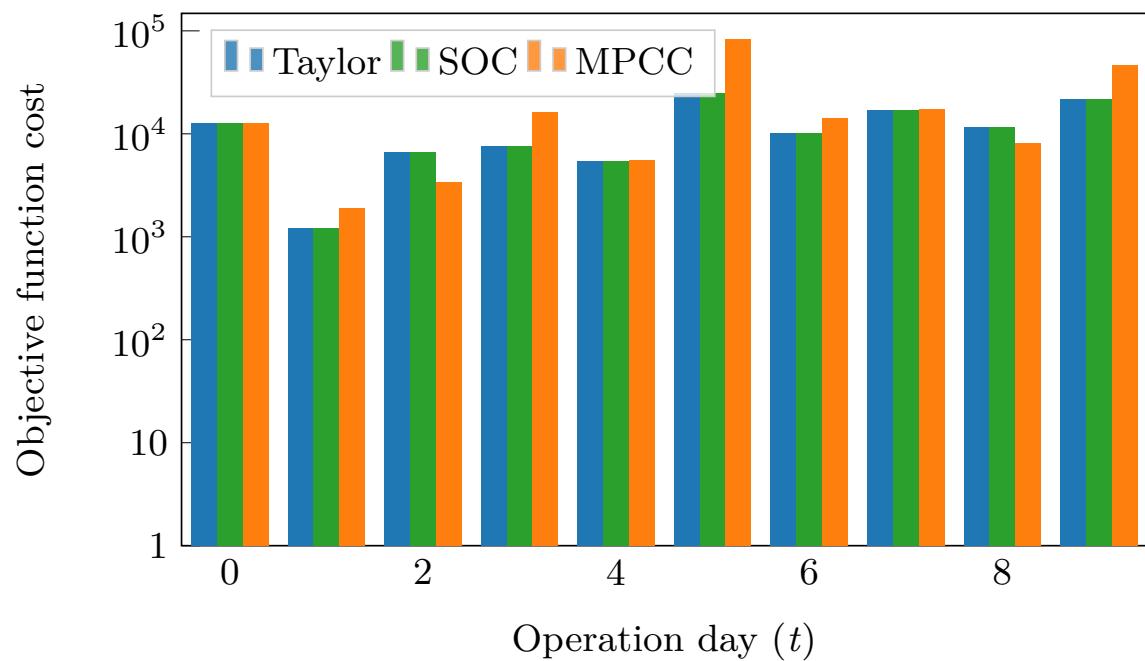
(b) SOC



(c) MPCC

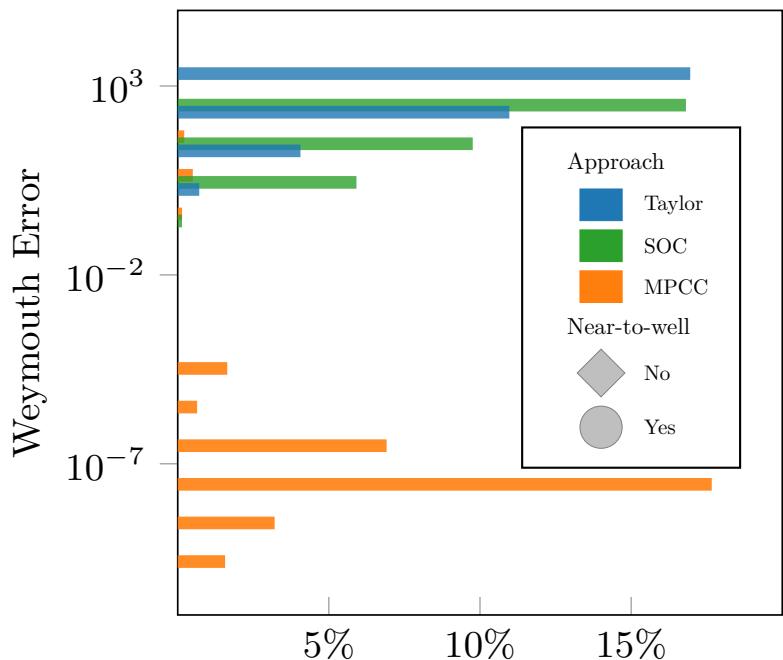
Results - Case 3 (Part 1)

For the 96/63 system, the evaluation differs from the previous cases. The Weymouth approximations were tested in an operational setting covering ten consecutive days ($|\mathcal{T}| = 10$), with gas extraction costs varying randomly each day.

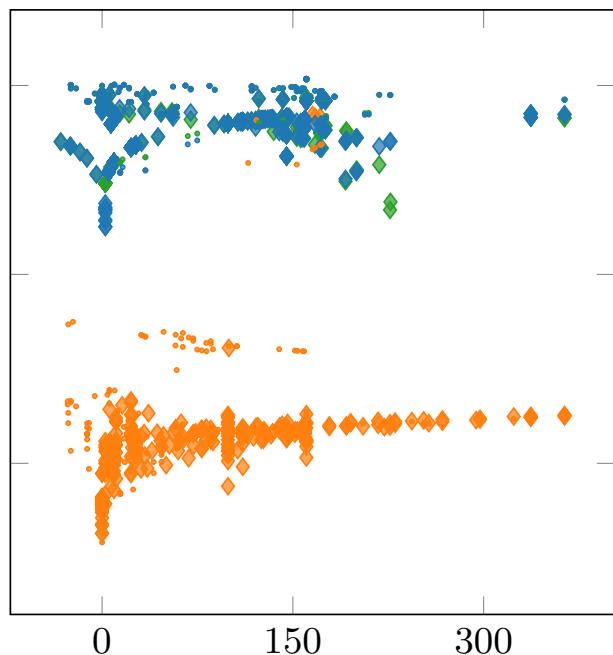


Results - Case 3 (Part 2)

Throughout the three experiments, the proposed MPCC-based approach consistently achieved significantly lower errors, demonstrating its superior accuracy in representing the physical behavior of the gas network.



(a) Relative frequency



(b) Pipeline flow (f_m^t)

Objective 3 - Physics-Guided Neural Networks

Traditional neural networks fit patterns in data but ignore system physics, which increases the risk of producing unrealistic or infeasible predictions when faced with uncertain scenarios.

Physics-Informed Neural Networks (PINNs):

- Integrate *physical laws* directly into the training process.
- Loss function penalizes violations of:
 - **Gas balance constraint** – nodal mass conservation.
 - **Weymouth equation** – pressure–flow relation in pipelines.
- Act as a *regularizer*, enhancing generalization under stochastic conditions.

Methodology: Physics-Guided CensNet

Overall loss function:

$$\mathcal{J}(\Theta) = \mathcal{J}_{\text{data}} + \mathcal{J}_{\text{balance}} + \mathcal{J}_{\text{weymouth}}$$

Gas balance loss:

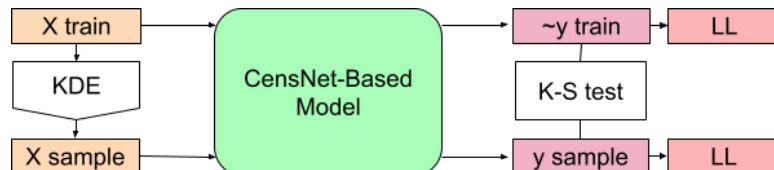
$$\mathcal{J}_{\text{balance}} = \mathbf{T} \cdot \hat{\mathbf{f}}_e - \mathbf{d} + \hat{\mathbf{f}}_n$$

Weymouth loss:

$$\mathcal{J}_{\text{weymouth}} = \mathbf{M}_{\mathcal{P}} \left(\hat{\mathbf{f}}_e^{\circ 2} - \mathbf{K} \circ (\mathbf{T} \cdot \hat{\boldsymbol{\pi}}^{\circ 2}) \right)$$

Stochastic analysis:

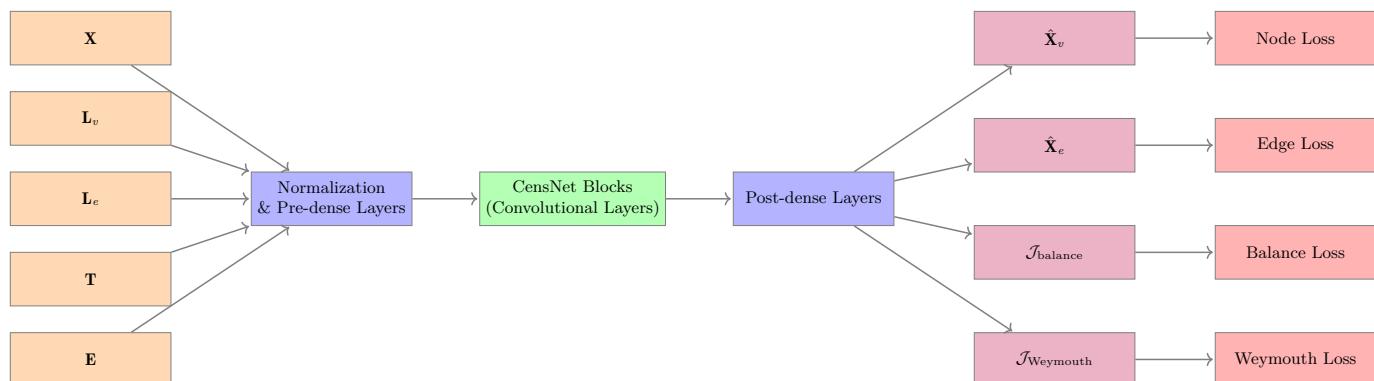
- KDE fitted to training inputs to generate synthetic samples.
- Samples propagated through CensNet to obtain outputs.
- Log-likelihoods and K-S tests used to assess distributional similarity.



Methodology: Physics-Guided CensNet

Implementation:

- Built on CensNet architecture from deterministic setup.
- Training data from nonlinear gas network optimization (MPCC).
- Noise (5%–25%) injected to emulate operating uncertainty.



Two additional loss terms were introduced to guide the training process using physical constraints from the gas balance and Weymouth equations.

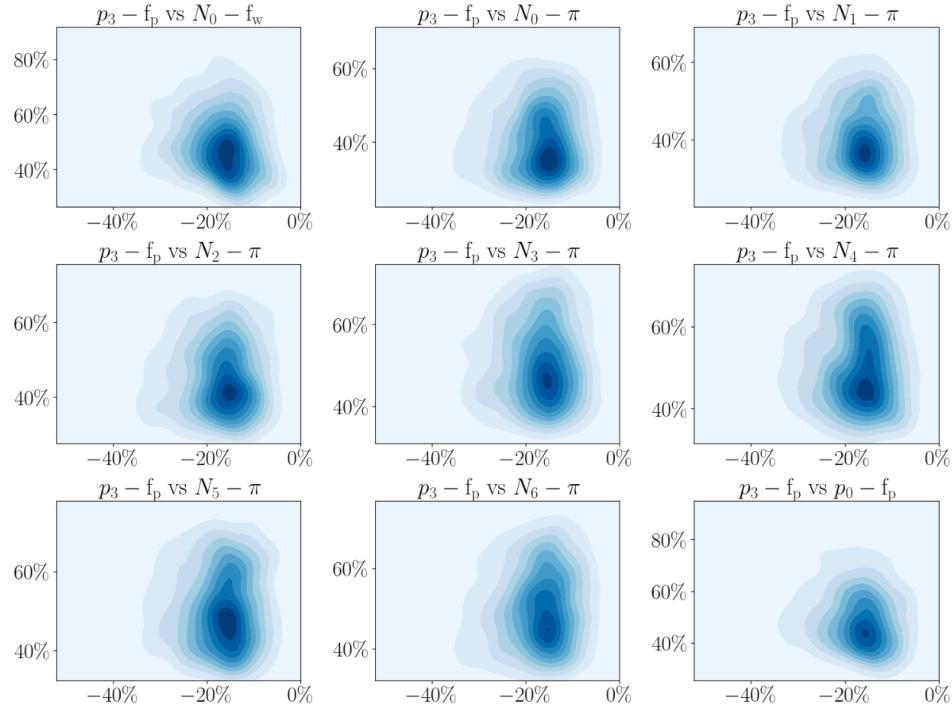
Case Study I: 8-Node Network – Performance Comparison

Method	Node Error	Edge Error	Balance Error	Time (s)
CensNet (N)	0.00 ± 17.99	22.76 ± 15.43	-0.01 ± 17.45	0.86 ± 0.50
CensNet (N+E)	-0.11 ± 18.27	0.22 ± 21.65	-0.12 ± 1.70	0.85 ± 0.50
CensNet (N+E+B)	-0.02 ± 18.00	-0.02 ± 21.30	-0.03 ± 0.90	0.85 ± 0.50
CensNet (N+E+W)	-0.07 ± 17.56	2.60 ± 20.03	-0.07 ± 2.21	0.86 ± 0.50
CensNet (N+E+B+W)	0.05 ± 17.91	0.25 ± 21.14	0.05 ± 1.69	0.85 ± 0.50

- Using only node loss leads to accurate nodal flows but large errors in edge predictions.
- Adding edge loss (**N+E**) reduces edge error from 22.76 to 0.22 and improves global balance.
- Including balance loss (**N+E+B**) further minimizes balance error, achieving best overall consistency.
- Weymouth loss (**N+E+W**) introduces slight trade-offs, slightly increasing edge/balance errors but retaining nodal accuracy.
- All CensNet variants are over an order of magnitude faster than IPOPT, with **N+E+B** offering the best accuracy-speed compromise.

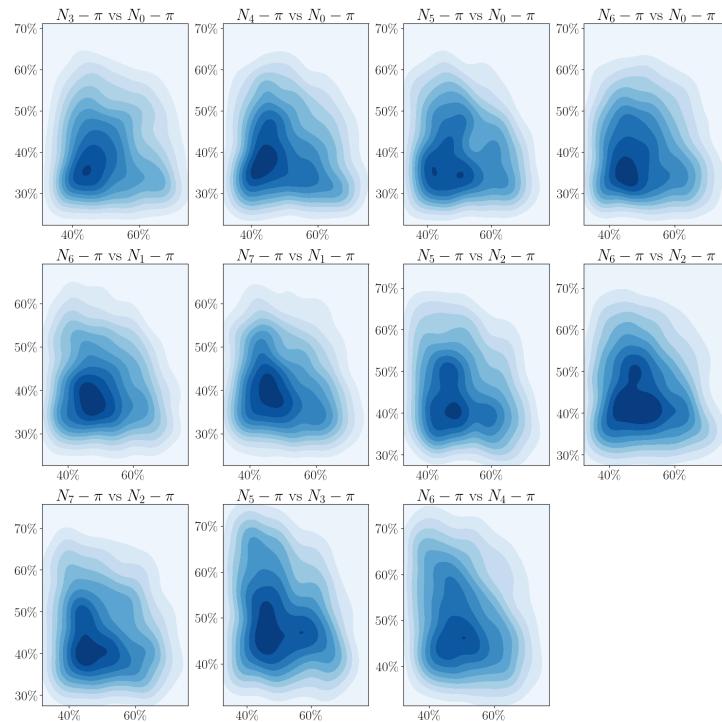
Negative Flows in Pipeline p_3

- Flow in p_3 consistently negative across scenarios and KDE samples.
- Caused by orientation assumption → optimizer adjusts direction.
- Operability unaffected, but p_3 supports cost minimization.



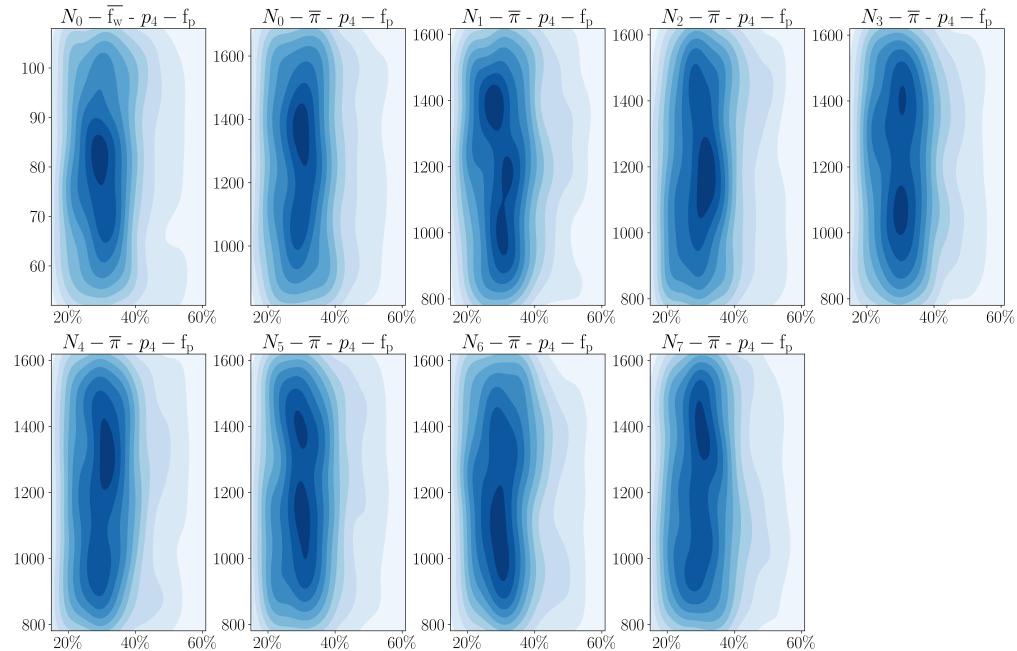
Pressure Concentration in Mid-Range

- Nodal pressures cluster at 30–40% of normalized limits.
- Avoids extremes, ensuring reliable operation.
- Implies optimizer favors efficiency + stability.



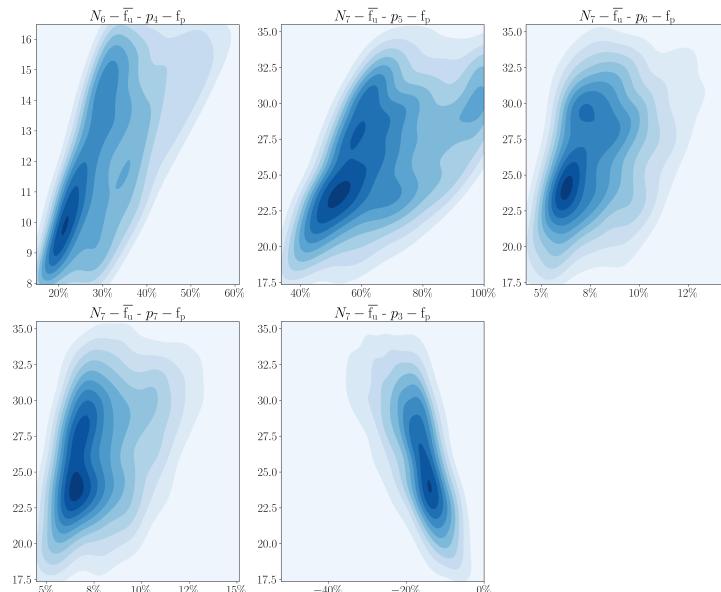
Stable Utilization of Pipeline p_4

- Despite wide dispersion in inputs, p_4 flow remains 20–40%.
- Reflects robustness: optimizer stabilizes this delivery path.
- Behavior consistently learned and reproduced in KDE samples.



Linear Input–Output Relations

- Positive correlation: demand bounds (N_6, N_7) vs. p_4-p_7 flows.
- Negative correlation: N_7 demand bound vs. p_3 flow.
- Shows network internalized optimizer's allocation strategies.



Results:

- Log-likelihoods: $y_{\text{sample}} = -6.696 \times 10^6$, $\bar{y}_{\text{train}} = -6.657 \times 10^6$.
- K–S test: $p > 0.44$ across all alternatives.
- ⇒ Synthetic outputs statistically consistent with training outputs.

Conclusions

- **GNN-based prediction:** CensNet achieved accurate and scalable predictions for natural gas networks, with significant reductions in computation time compared to traditional optimization.
- **Optimization with MPCC:** Proposes a formulation to approximate Weymouth's restrictions, improving accuracy of pressure–flow representation and showing robustness in real-world scheduling tasks.
- **Stochastic modeling:** Physics-guided neural networks preserved structural dependencies and generalized reliably under uncertainty, validated through KDE sampling and K–S testing.
- **Overall:** Integrating physical constraints with GNNs yields efficient, accurate, and robust surrogates for optimization in natural gas systems.

Future Work

- Extend GNN-based models to capture **transient dynamics** and **operational uncertainty**.
- Develop **stochastic MPCC formulations** to handle variability from renewables and uncertain demand.
- Integrate with **climatological forecasting tools** to anticipate gas consumption and interactions with renewable energy sources.

Products

Publications

- **Paper A1:** *Optimization of Interconnected Natural Gas and Power Systems Using Mathematical Programs with Complementarity Constraints.*
Journal: *Mathematics*.
DOI: [10.3390/math12142224](https://doi.org/10.3390/math12142224).
- **Proceedings:** *Approximation of Weymouth Equation Using Mathematical Programs with Complementarity Constraints for Natural Gas Transportation.*
Journal: *Engineering Proceedings*.
DOI: [10.3390/engproc2023039091](https://doi.org/10.3390/engproc2023039091).

Software

- **OPTIGASFLOW:** *Optimizando el Flujo de Gas Natural.*
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