

EMISSION-CONSTRAINED OPTIMIZATION OF GAS SYSTEMS WITH INPUT-CONVEX NEURAL NETWORKS

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ABSTRACT

Planning optimization of gas networks under emission constraints prioritizes gas supply with the smallest emission footprint. As this problem includes complex gas flow physical laws, standard optimization solvers cannot guarantee convergence to a feasible solution, especially under strict emission constraints. To address this issue, we develop an input-convex neural network (ICNN) aided optimization routine which incorporates a set of trained ICNNs approximating the gas flow equations with high precision. Numerical tests on the Belgium gas network demonstrate that the ICNN-aided optimization dominates non-convex and relaxation-based solvers, with larger optimality gains pertaining to stricter emission targets.

1 INTRODUCTION

Energy system operators worldwide introduce carbon reduction measures to control the emission content of energy supply (Liu and Raftery, 2021). Such measures include soft monetary penalties (e.g., carbon tax) or hard emission constraints (e.g., carbon cap or renewable portfolio standard) within operational planning routines. When operation planning is insufficient, more expensive yet effective long-term planning optimizes network design in order to accommodate more environment-friendly supply.

In gas networks, carbon reduction measures can be used to prioritize pipeline-quality gas from renewable suppliers, such as biogas produced from organic matter, syngas produced by steam reforming, or hydrogen produced from electrolysis at large offshore wind sites, like the proposed North Sea hub (NSW, 2022). However, solving such planning optimization problems with emission targets is challenging due to complex gas flow physics.

Contributions. To meet emission targets in gas networks, we develop a new optimization method that substitutes the non-convex Weymouth equation of gas flows with a composition of trained input-convex and input-concave neural networks (ICNNs). Together, they explain the dependency of gas flows on nodal pressures. We embed trained ICNNs into planning optimization problems in a computationally tractable manner. Tests on the Belgium gas network demonstrate that ICNN-aided optimization successfully solves generally intractable optimization problems and facilitates reducing the overall emission footprint of gas networks.

1.1 RELATED WORK

Gas network optimization. Designing optimization methods to aid operation planning dates back to at least 1979 (O’Neill et al., 1979). Since then, solvers based on mixed-integer (Wilson et al., 1988), piece-wise linear (De Wolf and Smeers, 2000), quadratic (Singh and Kekatos, 2019; 2020) and semi-definite (Ojha et al., 2017) programming have been introduced. The CO₂ footprint of

integrated gas and electricity networks has been addressed by integrating renewables (Ordoudis et al., 2019; Ratha et al., 2020; Roald et al., 2020; Dvorkin et al., 2021; 2022) or directly incorporating carbon reduction measures in operational (Piperagkas et al., 2011; Cheng et al., 2019) and long-term expansion planning problems (Degleris et al., 2021; Qiu et al., 2014; Cheng et al., 2018).

Neural networks to aid optimization. Using the mixed-integer neural network (NN) reformulation (Tjeng et al., 2017; Xiao et al., 2018; Grimstad and Andersson, 2019), NNs can be used for approximating complex input-output dependencies within optimization, e.g., in power systems problems (Murzakhanov et al., 2022; Donon et al., 2020; Hu et al., 2020; Kody et al., 2022). The reformulation represents the activation of each ReLU function using linear and binary constraints parameterized by NN weights and biases, which can be computationally challenging at scale (Grimstad and Andersson, 2019). Here, we explore an alternative functional approximation (i.e., neural surrogate) that relies on *input-convex* NNs, whose constrained network weights ensure the output is a convex function of inputs (Amos et al., 2017). Since trained ICNNs can be recast as linear optimization problems (Amos et al., 2017; Duchesne et al., 2021), we leverage them to convert non-convex optimization problems into linear bilevel optimization problems (Pozo et al., 2017).

2 EMISSION-AWARE GAS NETWORK PLANNING PROBLEMS

Operational planning problem. A gas network includes n nodes, representing gas injections and extractions, and ℓ edges, representing pipelines. The operational planning problem identifies the least-cost supply allocation $\vartheta \in \mathbb{R}^n$ satisfying gas demands $\delta \in \mathbb{R}^n$, while ensuring that pressures $\pi \in \mathbb{R}^n$ and gas flows $\varphi \in \mathbb{R}^\ell$ remain within technical limits. This problem is solved using the following optimization (Dvorkin et al., 2021):

$$\min_{\varphi, \vartheta, \pi \in \mathcal{F}} c^\top \vartheta \quad (1a)$$

$$\text{s.t. } A\varphi = \vartheta - \delta, \quad (1b)$$

$$\varphi \circ |\varphi| = \text{diag}[\omega]A^\top \pi, \quad (1c)$$

which minimizes gas supply costs subject to technical constraints. Using admittance matrix $A \in \mathbb{R}^{n \times \ell}$, equation (1b) ensures gas mass balance. Given the fixed friction coefficients $\omega \in \mathbb{R}^\ell$, the steady-state Weymouth equation (1c) enforces the non-convex dependency of gas flows on pressure variables. Finally, a convex set \mathcal{F} is used to respect the technical limits on gas mass and pressures.

Although cost function (1a) typically includes only marginal production costs, it can also internalize an emission (carbon) tax to penalize gas producers with higher environmental impact. Alternatively, emissions can be regulated by carbon cap constraints on the total emission level. Although the equivalence of carbon tax and carbon cap can be shown through the Karush–Kuhn–Tucker conditions (Brown and Reichenberg, 2021), the carbon cap is preferred due to non-convexities in (1c). Indeed, the same emission goal may not be achieved under the carbon tax, since local search algorithms may fail to minimize the penalty term globally; meanwhile, the carbon cap is introduced through the hard constraint, i.e.,

$$e^\top \vartheta \leq \bar{e}, \quad (2)$$

with vector $e \in \mathbb{R}^n$ of carbon intensities and carbon cap \bar{e} .

Long-term planning problem. Since a carbon cap may significantly affect the operating cost in (1a), the long-term planning problem optimizes the network design to enable more economical satisfaction of the emission constraint (2). This problem is especially relevant for the design of future hydrogen gas transport networks which governments are actively considering (Khan et al., 2021). Let the diameter $d \in \mathbb{R}^\ell$ of gas pipelines be the design variable. Since pipeline friction is often modeled as being linearly proportional to diameter (Sundar and Zlotnik, 2019), a constant $\hat{\omega}_i$ can be used to relate friction and diameter via $\omega_i = \hat{\omega}_i d_i$. The diameter enters the operational problem (1) through the Weymouth equation (1c) as

$$\text{diag}[d]^{-1} \varphi \circ |\varphi| = \text{diag}[\hat{\omega}]A^\top \pi, \quad (3)$$

where the right-hand side has no explicit dependence on diameter. By defining a vector $\lambda \in \mathbb{R}^\ell$ of expansion costs, we obtain a long-term planning optimization from problem (1) by augmenting the total cost of expansion $\lambda^\top d$ to (1a) and substituting equation (1c) with its dynamic counterpart in (3).

3 EMISSION-AWARE PLANNING WITH INPUT-CONVEX NEURAL NETWORK

Addressing the non-convex equation (1c), we observe that its left-hand side $f(\varphi_l) = \varphi_l|\varphi_l|$ is convex for $\varphi_l \geq 0$ and concave for $\varphi_l \leq 0$. Hence, $f(\varphi_l)$ can be approximated with a sum $f(\varphi_l) \approx \Phi_+(\varphi_l) + \Phi_-(\varphi_l)$ of one input-convex $\Phi_+(\varphi_l)$ and one input-concave $\Phi_-(\varphi_l)$ neural network. We use the following k -layer architectures under ReLU activation functions:

$$\begin{aligned}\Phi_+(\varphi_l): \quad & z_+^1 = \max(0, W_+^0 \varphi_l + b_+^0), \quad z_+^{i+1} = \max(0, W_+^i z_+^i + b_+^i), \quad \forall i = 1, \dots, k-1, \\ \Phi_-(\varphi_l): \quad & z_-^1 = \max(0, W_-^0 \varphi_l + b_-^0), \quad z_-^{i+1} = \max(0, W_-^i z_-^i + b_-^i), \quad \forall i = 1, \dots, k-1,\end{aligned}$$

with a scalar input φ_l , scalar output z_k , and weights and biases W and b , respectively. In $\Phi_+(\varphi_l)$, the weights $W_+^i, \forall i = 1, \dots, k-1$ are non-negative to render the output a convex function of the input. In $\Phi_-(\varphi_l)$, the weights W_-^i are also non-negative for $i = 1, \dots, k-2$, but they are non-positive for $i = k-1$ to render the output a concave function of the input. With such architectures, we have a piece-wise functional approximation $f(\varphi_l) \rightarrow z_+^k + z_-^k$. From (Amos et al., 2017, Appendix B), we can retrieve the output of the trained ICNNs from the input by solving a linear program, e.g.,

$$\min_{z_+^1, \dots, z_+^k} z_+^k \quad (4a)$$

$$\text{s.t.} \quad z_+^1 \geq W_+^0 \varphi_l + b_+^0, \quad z_+^{i+1} \geq W_+^i z_+^i + b_+^i, \quad z_+^i \geq 0, \quad \forall i = 1, \dots, k-1, \quad (4b)$$

for the $\Phi_+(\varphi_l)$ architecture, and it takes a similar form for the $\Phi_-(\varphi_l)$ architecture. Thus, to approximate the Weymouth equation, we need to embed two linear programs (one convex and one concave) for each pipeline. The computational burden, however, will depend on the number of hidden layers and neurons. To reduce the burden, we note that for $\varphi_l \geq 0$, solution z_+^k is an *outer approximation* of the trained ICNN output, and the number of approximating hyperplanes 2^p is the number of unique combinations of p hidden neurons. For small – yet sufficient to represent a convex function – architectures, we can screen approximating hyperplanes and leave only a set \mathbb{H}_+ of *supporting* hyperplanes, for which there exists an input φ_l which makes such hyperplanes active (binding). Such hyperplane parameters are obtained from the trained ICNN as

$$\prod_{r=k}^0 (s_j^r \circ W_+^r) \varphi_l + \sum_{i=0}^k \prod_{r=k}^i (s_j^r \circ W_+^r) b^i = w_+^j \varphi_l + v_+^j, \quad \forall j \in \mathbb{H}_+,$$

with slope w_+^j and intercept v_+^j . Vector $s_j \in \mathbb{R}^p$ collects a unique combination of ReLU activations (1 if active, and 0 if otherwise) of hyperplane j , and s_j^r is a subset of s_j with hidden neurons of layer r . Similarly, we obtain hyperplanes for the concave part of $f(\varphi_l)$.

We now put forth the bilevel planning optimization with embedded trained ICNNs:

$$\min_{\varphi, \vartheta, \pi \in \mathcal{F}} c^\top \vartheta \quad (5a)$$

$$\text{s.t.} \quad \text{Constraints (1b), (2),} \quad t_+ + t_- = \text{diag}[\omega] A^\top \pi, \quad (5b)$$

$$t_+^l \in \min_{t_+^l} t_+^l, \quad \text{s.t.} \quad w_+^i \varphi_l + v_+^i \leq t_+^l, \quad \forall i \in \mathbb{H}_+, \forall l \in 1, \dots, e \quad (5c)$$

$$t_-^l \in \max_{t_-^l} t_-^l, \quad \text{s.t.} \quad w_-^i \varphi_l + v_-^i \geq t_-^l, \quad \forall i \in \mathbb{H}_-, \forall l \in 1, \dots, e \quad (5d)$$

where (5c) and (5d) are lower-level optimization problems, each including a single auxiliary variable t^l which returns the ICNN output (problem (5c) is a light-weighted version of (4) producing the identical result). Appendix A provides a tractable mixed-integer reformulation of (5) using Karush–Kuhn–Tucker (KKT) conditions of (5c)–(5d). Appendix B shows that the dynamic Weymouth equation (3) can also be approximated by ICNNs.

4 NUMERICAL TESTS ON THE BELGIUM GAS NETWORK

To demonstrate emission-constrained planning, we use a modified Belgium system from (De Wolf and Smeers, 2000), with a meshed topology, tighter pressure bounds, and more distributed gas supply and demand hubs. Using this system, we compare three methods to solve operation planning: 1) an interior point solver IPOPT (Wächter and Biegler, 2006), 2) a mixed-integer quadratic programming (MIQP) relaxation, detailed in Appendix C, and 3) the proposed ICNN-aided optimization. The last two are solved with mixed-integer Gurobi solver (Gurobi Optimization, LLC, 2022). The long-term

planing is solved by the 1st and 3rd methods only, as no convex relaxation of equation (3) is known. The CPU time for all methods does not exceed several minutes. The NN architectures include 1 hidden layer with up to 15 neurons, which was sufficient to approximate convex and concave parts of the Weymouth equation. Test data, details on the training procedure, and codes to replicate our results are available at <https://doi.org/10.5281/zenodo.7606328>

The CO₂ intensity of the gas supply in the test system varies between 0.6 and 2.7 kg/m³, and solving the operational planning problem (1) without emission constraint (2) results in up to 125.9 kT of emitted CO₂ with the IPOPT solver. To limit emissions, we select one moderate emission cap of 100 kT and one extreme cap of 48.9 kT, below which no method returns a feasible solution.

The solutions for operation planning are collected in Table 1. As emission cap reduces, the IPOPT solver becomes more sensitive to initialization and fails to provide a feasible solution with probability up to 39.0%. Although the termination status of the MIQP relaxation is always optimal, it is never feasible with respect to the original, non-relaxed Weymouth equation; using it as a warm start for IPOPT, we observe the gap between the relaxation and the feasible solution of up to $\frac{1,929.2-1,540.8}{1,929.2} \times 100\% = 20.1\%$. The proposed ICNN-aided optimization improves on the MIQP solution and consistently returns the best solution found with IPOPT, regardless of the emission cap value. In the most constrained case, with $\bar{e} = 48.9$ kT, the ICNN-aided optimization solution provides the least-cost operation cost, thus dominating both IPOPT and MIQP solutions.

Table 2 provides the summary of long-term planning cost, which includes both operating cost and adjusted (to a single, peak hour) expansion cost. While the IPOPT solver exhibits a large variance and fails to produce any solution with probability up to 41.4%, the ICNN-aided optimization always returns the best solution discovered with random IPOPT initializations. With respect to the worst case IPOPT outcomes, the ICNN-aided solution yields 3.2%–5.9% cost savings, as it requires less pipeline expansion; e.g., for $\bar{e} = 48.9$ kT, it expands pipelines by 117mm less on average across the network.

Table 1: Cost summary of the emission-constrained operation planning (€1,000).

Emission cap, kT	1,000 random IPOPT initializations				MIQP relaxation		ICNN-aided solution	
	min	mean	max	prob. of failure	optimal	warm start for IPOPT	optimal	warm start for IPOPT
∞	1,923.3	1,927.2	1,929.2	16.6%	1,540.8	1,929.2	1,932.3	1,923.3
100	2,225.1	2,235.1	2,256.2	16.0%	2,137.2	2,225.1	2,241.3	2,225.1
48.9	4,344.6	4,344.6	4,344.6	39.0%	4,200.8	4,344.6	4,290.1	4,291.2

Table 2: Cost summary of the emission-constrained long-term planning (€1,000).

Emission cap, kT	1,000 random IPOPT initializations				ICNN-aided solution	
	min	mean	max	prob. of failure	optimal	warm start for IPOPT
∞	2,671.7	2,701.8	2,829.5	28.6%	2,666.4	2,671.6
100	3,057.8	3,090.2	3,191.9	30.3%	3,056.6	3,057.8
48.9	5,079.1	5,138.7	5,247.9	41.4%	5,079.9	5,079.1

5 CONCLUSION

We developed a new method based on aiding planning optimization with trained input-convex and input-concave neural networks, which allows for accommodating ambitious emission reduction targets in operation and long-term planning of gas networks in a feasible manner. We empirically demonstrated that our method is robust even to the strictest emission targets, for which the non-convex and relaxation-based solvers are often intractable, failing to produce a feasible solution. Our method achieves savings of up to 1.2% in operational costs and 5.9% in costs for long-term emission-constrained planning.

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A REFORMULATION OF ICNN-AIDED OPTIMIZATION VIA KKT CONDITIONS

We consider the lower level problem from (5c) associated with the input convex NN (the concave case is dealt with similarly) for a single line l :

$$\min_{t_+} t_+ \tag{6a}$$

$$\text{s.t. } w_+^i \varphi + v_+^i \leq t_+ : \mu_+^i \in \mathbb{R}^E, \quad \forall i \in \mathbb{H}_+, \tag{6b}$$

where μ_+^i is the Lagrange multiplier associated with the i^{th} inequality constraint. The Lagrangian function Boyd et al. (2004) associated with this linear program is given by

$$L(t_+, \mu_+) = t_+ + \sum_{i \in \mathbb{H}_+} \mu_+^{i\top} (w_+^i \varphi + v_+^i - t_+). \tag{7a}$$

The KKT conditions associated with the linear program (6) may now be derived. Primal and dual feasibility can be directly stated:

$$\begin{aligned} \text{primal feasibility: } & w_+^i \varphi + v_+^i \leq t_+, \quad \forall i \in \mathbb{H}_+ \\ \text{dual feasibility: } & \mu_+^i \geq 0, \quad \forall i \in \mathbb{H}_+. \end{aligned} \quad (8)$$

The stationarity condition can be computed by taking the derivative of the Lagrangian (with respect to the primary variable) and setting it equal to 0:

$$\frac{\partial}{\partial t_+} L(t_+, \mu_+) = 1 - \sum_{i \in \mathbb{H}_+} \mu_+^i \equiv 0. \quad (9)$$

Therefore, stationarity and complementary slackness are given as

$$\begin{aligned} \text{stationarity condition: } & \sum_{i \in \mathbb{H}_+} \mu_+^i = 1, \\ \text{complementary slackness: } & \mu_+^i \cdot (w_+^i \varphi + v_+^i - t_+) = 0, \quad \forall i \in \mathbb{H}_+. \end{aligned} \quad (10)$$

Since only one inequality constraint in (6b) can be active, the dual variables are implicitly constrained to be binary: $\mu_+^i \in \{0, 1\}$, $\forall i \in \mathbb{H}_+$, but only one may take a nonzero value. Since the dual variables are constrained to be binary, the quadratic complimentary slackness constraints can be effectively linearized using Big-M:

$$\mu_+^i (w_+^i \varphi + v_+^i - t_+) = 0 \quad \Leftrightarrow \quad (\mu_+^i - 1)M \leq w_+^i \varphi + v_+^i - t_+ \quad (11)$$

where no upper bound is needed, since $w_+^i \varphi + v_+^i - t_+ \leq 0$ is implied by primal feasibility. The final KKT reformulation of the lower-level problem is:

$$\begin{aligned} & w_+^i \varphi + v_+^i \leq t_+, \quad \forall i \in \mathbb{H}_+ \\ & (\mu_+^i - 1)M \leq w_+^i \varphi + v_+^i - t_+ \leq 0, \quad \forall i \in \mathbb{H}_+ \\ & \sum_{i \in \mathbb{H}_+} \mu_+^i = 1, \quad \mu_+^i \in \{0, 1\}, \quad \forall i \in \mathbb{H}_+. \end{aligned} \quad (12)$$

Similarly, the KKTs of the concave lower-level problem are:

$$\begin{aligned} & w_-^i \varphi + v_-^i \geq t_-, \quad \forall i \in \mathbb{H}_- \\ & 0 \leq w_-^i \varphi + v_-^i - t_- \leq (1 - \mu_-^i)M, \quad \forall i \in \mathbb{H}_- \\ & \sum_{i \in \mathbb{H}_-} \mu_-^i = 1, \quad \mu_-^i \in \{0, 1\}, \quad \forall i \in \mathbb{H}_-. \end{aligned} \quad (13)$$

Both of these formulations are additionally applicable for neural networks which map multiple inputs (rather than just a single input φ) to scalar outputs.

B MODELING DIAMETER-DEPENDENT WEYMOUTH EQUATIONS

The pipeline friction ω_i from (1c) incorporates the fixed pipeline length, diameter, rugosity, as well as gas temperature, compressibility and density relative to air De Wolf and Smeers (2000). There

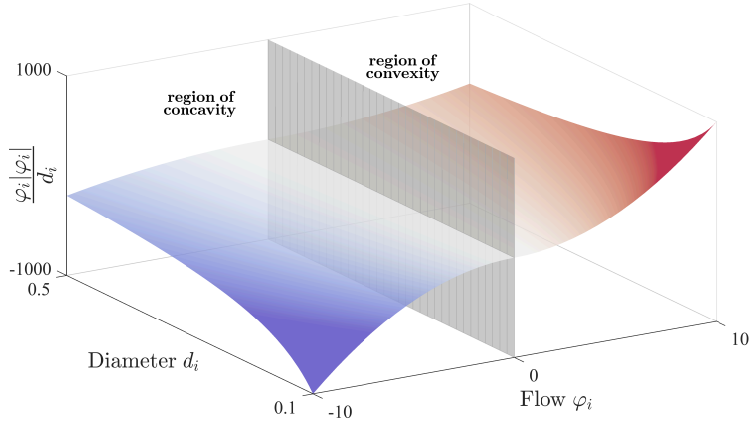


Figure 1: The concave region of the function $\varphi_i |\varphi_i| / d_i$ is depicted on the left (for $\varphi_i \leq 0$) in blue, and the convex region is depicted on the right (for $\varphi_i \geq 0$) in red.

are a spectrum of different methods available for modeling pipeline friction coefficients, but in this paper, we use the simplifying assumption that ω_i is linearly proportional to diameter of the line d_i , as in Sundar and Zlotnik (2019) (i.e., the Darcy—Wiesbach friction factor is assumed constant, regardless of the pipeline’s diameter). From (3), we then seek to use ICNNs to build a surrogate model which mimics the rational expression

$$f(\varphi_i, d_i) = \frac{\varphi_i |\varphi_i|}{d_i}. \quad (14)$$

Despite its nonlinearity, (14) can be expressed as the sum of one convex function (f_+) and one concave function (f_-) across its domain of practical usage: $f(\varphi_i, d_i) = f_+(\varphi_i, d_i) + f_-(\varphi_i, d_i)$. Figure 1 depicts the convex and concave regions of $f(\varphi_i, d_i)$.

C MIQP RELAXATION OF THE OPERATIONAL PLANNING PROBLEM

The quadratic programming relaxation of the static Weymouth equation (1c) is

$$\varphi \circ |\varphi| = \text{diag}[\omega] A^\top \pi \xrightarrow{\text{relax.}} \begin{cases} \pi_i - \pi_j \geq \frac{1}{\omega_l} \varphi_l^2 & \text{if } \varphi \geq 0 \\ \pi_j - \pi_i \geq \frac{1}{\omega_l} \varphi_l^2 & \text{if } \varphi \leq 0 \end{cases} \quad \forall l = (i, j) \in 1, \dots, \ell, \quad (15)$$

which distinguishes between two cases of either positive or negative gas flow in every line l with sending and receiving ends denoted by i and j , respectively. Using a binary variable x_l , this relaxation can be written as

$$(2x_l - 1)\pi_i + (1 - 2x_l)\pi_j \geq \frac{1}{\omega_l} \varphi_l^2, \quad \forall l = (i, j) \in 1, \dots, \ell, \quad (16)$$

such that, when $x_l = 1$, we have $\varphi_l \geq 0$, and when $x_l = 0$, we have $\varphi_l \leq 0$. The bilinear terms $x_l \pi_i$ and $x_l \pi_j$ can be handled using the Big-M method. Using an auxiliary variable $z_{li} = x_l \pi_i$, the first bilinear term can be restated as follows:

$$x_l \underline{\pi}_i \leq z_{li} \leq x_l \bar{\pi}_i, \quad (17a)$$

$$\pi_i + (x_l - 1)\bar{\pi}_i \leq z_{li} \leq \pi_i + (x_l - 1)\underline{\pi}_i, \quad (17b)$$

where $\underline{\pi}_i$ and $\bar{\pi}_i$ respectively denote the lower and upper pressure limits at node i . When $x_l = 1$, $z_{li} = \pi_i$, and when $x_l = 0$, $z_{li} = 0$. Then, the MIQP relaxation of the Weymouth equation is

$$2z_{li} - 2z_{lj} - \pi_i + \pi_j \geq \frac{1}{\omega_l} \varphi_l^2, \quad \forall l = (i, j) \in 1, \dots, \ell, \quad (18a)$$

$$x_l \underline{\pi}_i \leq z_{li} \leq x_l \bar{\pi}_i, \quad \forall i = 1, \dots, n, \quad \forall l = 1, \dots, \ell \quad (18b)$$

$$\pi_i + (x_l - 1)\bar{\pi}_i \leq z_{li} \leq \pi_i + (x_l - 1)\underline{\pi}_i, \quad \forall i \in 1, \dots, n, \quad \forall l = 1, \dots, \ell. \quad (18c)$$

Substituting the Weymouth equation (1c) with equations (18) yields the relaxed planning problem.