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(eds.)

PROCEEDINGS OF THE 7th INTERNATIONAL CONFERENCE ON APPROXIMATION METHODS AND NUMERICAL MODELLING IN ENVIRONMENT AND NATURAL RESOURCES

Oujda, Morocco, May 17-20, 2017

MAMERN'17

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2017

UNIVERSIDAD
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Departamento de
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PROLOGUE

The 7th International Conference on Approximation Methods and Numerical Modeling in Environment and Natural Resources held in Oujda, Morocco, on 17-20 May 2017. This Conference was jointly organized by Numerical Analysis and Optimization Laboratory of the University Mohammed First of Oujda (Morocco), the Department of Applied Mathematics of the University of Granada (Spain), and the Applied Mathematics Laboratory of the University of Pau & CNRS UMR 5142 (France). The term MAMERN comes from the French acronym "Méthode dApproximation et Modélisation Numérique en Environnement et Ressources Naturelles". The first conference MAMERN05 was held in Oujda, Morocco, on May 9-11, 2005, the second one MAMERN07 was held in Granada, Spain, on July 11-13, 2007, the third one MAMERN09 was held in Pau, France, on June 8-11, 2009, the fourth one MAMERN11 was held in Saidia, Morocco, on 23-26 May, 2011, the fifth one MAMERN13 was held in Granada, Spain, on 22-25 April 2013, and the sixth one was held in Pau, France, on 31 May-5 June 2015. This meeting is a biennial international conference co-sponsored by CNRS: Centre National pour la Recherche Scientifique (France), CNRST: Centre National pour la Recherche Scientifique et Technique (Morocco) and IMACS: International Association for Mathematics and Computers in Simulation. Selected papers from each MAMERN conference are published, after a refereeing process, as a special issue of the journal Mathematics and Computers in Simulation.

This volume contains the abstracts of the plenary lectures and contributions presented at MAMERN VII-2017, and the USB key includes the extended abstracts of the contributions. The scientific program of the conference consisted of 7 invited plenary lectures, 4 mini symposiums with about 60 talks and 60 contributed talks and posters.

This conference was attended by participants coming from thirteen different countries: Algeria, Brazil, France, Germany, India, Madagascar, Morocco, Netherlands, Portugal, Saudi Arabia, Spain, Tunisia, and Venezuela.

The aim of the conference was to bring together researchers, scientists, engineers, and students to exchange and share their experiences, new ideas, and research results about approximation, numerical modeling and their applications in the environment sciences and natural resources.

The topics of the conference are

- Approximation and modeling applied to environment sciences and natural resources.
- New applications and developments in approximation methods.
- Mathematics and computation in geosciences.
- Modeling of ecosystems.
- Oceanographic and coastal engineering.
- Numerical modeling of flow and transport in porous media.
- Mathematical analysis of models in porous media.
- Multi-Scale Modeling of Flow and Transport in Porous Media.
- Statistical modeling in geosciences. Uncertainty quantification.
- Stochastic partial differential equations.

The conference could not have been held without the financial support of the organizing institutions. Special acknowledgment is due to the Department of Applied Mathematics of University of Granada (Spain).

We would like to thank all the organizers of the mini symposiums for their active role in the organization.

Last, but not least, we want to acknowledge all participants for their contribution and efforts in making the conference an interesting, pleasant and successful event.

On behalf of the organizing committee

Brahim Amaziane, Domingo Barrera, Driss Sbibih

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LIST OF INVITED PLENARY SPEAKERS

- Alfredo Bermúdez de Castro, Universidade de Santiago de Compostela, A Coruña, Spain.

  Modelling, Simulation and Optimization of Gas Transportation Networks
- Martin Buhmann , University of Giessen, Germany.

  Quasi-Interpolation and Applications with Radial Basis Functions
- Clément Cancès, INRIA Lille - Nord Europe, France.

  Entropy diminishing numerical schemes for parabolic equations
- Holger Class, University of Stuttgart, Germany.

  Flow, transport, and microbial activities in engineered subsurface applications: numerical modeling and experimentation
- Janin Jaeger, University of Giessen, Germany.

  Radial basis function interpolation on spheres with application to electroencephalographic data
- Delfim F. M. Torres, University of Aveiro, Portugal.

  Modeling, Global Stability and Optimal Control of HIV/AIDS through PrEP

- Martin Vohralik, INRIA de Paris, France.

  Flux and potential reconstructions for guaranteed error bounds in numerical approximations of model PDEs

LIST OF MINISYMPOSIA

- *1st MAMERN-FIC Porous Media Day.*

  Organizer: Brahim Amaziane (UPPA and CNRS, Pau, France) and Michel Quintard, Président of the FIC (IMFT, CNRS, Toulouse, France).
- *Approximation and applications.*

  Organizer: María José Ibáñez and Domingo Barrera, University of Granada, Spain.
- *Nonstandard multiphase flows in porous media.*

  Organizers: Mazen Saad, Ecole Centrale de Nantes, Laboratoire de Mathématiques Jean Leray, Nantes, France.
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PLENARY LECTURES

MAMERN VII–2017: 7^{th} International Conference on Approximation Methods
and Numerical Modelling in Environment and Natural Resources
Oujda (Morocco), May 17-20, 2017

Modelling, Simulation and Optimization of Gas Transportation Networks

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Keywords: Gas networks, Mathematical modelling, Numerical methods, Optimization.

Abstract. *The goal of the presentation is to summarize an industrial research project related to mathematical methods for simulation and optimization of gas transportation networks. In the first part, the one-dimensional dynamic gas equations are recalled for a single pipe. Then, the gas network is modelled by a directed graph and a system of equations for steady state simulation are introduced. The existence of a solution to this system is proved and numerical algorithms are given. Next, an optimization problem related to compression stations is stated and numerically solved. Finally, some results for real gas networks are shown.*

1 Introduction

Managing a gas transport network is a complex problem because of the great number of possibilities of routing the gas through the pipes (see Fig. 1). The most important aim in this kind of systems is to fulfill the demand within the pressure bounds, independently of its associated costs. However, some cost drivers are also taken into account by means of different objective functions in

Figure 1: Primary Spanish network.

order to manage the network in an efficient way. This work deals with mathematical modeling and optimization of gas transport networks, where a two-stage procedure is proposed. In the first stage, optimization algorithms based on mathematical programming are applied to make some decisions (whether to activate compressor stations, control valves and other control elements) and gives an initial solution to the second stage. The second stage, which is based on control theory techniques, refines the solution to obtain more accurate results. Due to the reduced complexity in each stage, both can be solved within reasonable runtimes for relatively large gas networks. Based on the mathematical methods involved, a software called GANESO has been developed for the Reganosa company.

Mathematical modelling of gas flow in pipelines is an important subject in planning and operating gas transportation networks (see reference books, [1], [2]). Some recent papers have been devoted to the transient case (see [3], [4]). Usually, they assume isothermal or isentropic flow (see [5]) but in real networks neither temperature nor entropy remain constant because, first, there is heat exchange with the environment (see [6],[7]) and second there is dissipation in the boundary layer near the wall of the pipelines due to viscous

friction. These features complicate the model because they lead to two respective source terms in the physical balance laws (see [8],[9],[10]). However, in the present paper we restrict ourselves to the steady state case because it is the one for which optimization can be done in a reasonable computing time. Unlike other related works focused on the practical part, we are also interested in mathematical analysis to get an existence theorem for the network model.

A gas network basically consists of a number of controllable elements such as compressor stations and control valves that are connected by pipes where the pressure of flowing gas decreases due to the friction on the walls. This pressure loss makes difficult to guarantee the security of supply, that is to meet the demand at the exit points with gas supplied at the entry points within some pressure bounds. Therefore, compressor stations have to be employed to counterbalance the pressure loss, but they consume a fraction of gas flowing through the pipes (the so-called gas self-consumption). Taking this fact into account is very important to manage the gas transport network efficiently, in order to reduce this self-consumption in compressor stations. Thus, mathematical optimization theory is an important tool to handle this problem (see, for instance, [12, 13, 14, 15, 16, 17]).

In this work we present a simplified mathematical model which reproduces the physical behavior of a gas network, including the aforementioned elements. Regarding network optimization we will have to deal with mixed integer nonlinear programming (MINLP) problems. Indeed, there are many nonlinear aspects, mainly due to the pressure loss in the pipes, to the gas consumption formula in compressors and to the operation diagram of them. The model must also account for the binary decisions regarding whether or not a given valve or compressor is active. We propose a two-stage approach to tackle this complex problem. In the first stage, the mathematical model of the gas flow in the network is considered as a set of equations that are part of the constraints for the optimization problem. Then, in the second stage, we employ methods based on optimal control theory. This means that the equations of the model are not included in the set of constraints. On the contrary, they allow us to eliminate implicitly the so-called state variables in terms of the control or decision variables. The optimization problem of the first stage is solved numerically by using a sequential linear programming (SLP) algorithm. Further details can be found in [13] and [18]

2 One-dimensional model for gas flow in a pipe

Firstly, we write models for gas flow in single pipe. The starting point are the conservation principles of thermomechanics:

- *Mass conservation equation*:

$$A\frac{\partial \rho}{\partial t}(x,t) + \frac{\partial q}{\partial x}(x,t) = 0, \tag{1}$$

where

  - A is the area of the cross-sections (m^2).
  - $\rho(x,t)$ is the average density on section x at time t (kg/m^3).
  - $q(x,t)$ is the mass flow rate across the x section at time t (kg/s).

The mass-weighted average velocity on section x is defined by

$$v\,(x,t) = \frac{q\,(x,t)}{A\rho\,(x,t)}.$$

- *Linear momentum equation*:

$$\begin{aligned}\frac{\partial(\rho v)}{\partial t}(x,t) + \frac{\partial(\rho v^2)}{\partial x}(x,t) + \frac{\partial p}{\partial x}(x,t)\\ +\frac{\lambda\rho(x,t)}{2D}|v(x,t)|v(x,t) - g\rho(x,t)h'(x) = 0.\end{aligned} \tag{2}$$

- *Energy equation*:

$$\begin{aligned}\frac{\partial(\rho E)}{\partial t}(x,t) + \frac{\partial((\rho E + p)v)}{\partial x}(x,t) =& \frac{4\beta}{D}(\theta_{ext}(x,t) - \theta(x,t))\\ &-g\rho(x,t)v(x,t)h'(x).\end{aligned} \tag{3}$$

  - ρ is the average mass density (kg/m^3),
  - p is the average thermodynamic pressure (N/m^2),
  - g is the gravity acceleration (m/s^2),
  - $h(x)$ is the height of the pipe at the x cross-section (m),
  - D is the diameter of the pipe (m),
  - λ is the friction factor between the gas and the pipe walls; it is a non-dimensional number depending on the diameter of the pipe, the rugosity of its wall and the Reynolds number of the flow,
  - E is the average specific total energy (J/kg),
  - β is a heat transfer coefficient (W/m^2K),
  - θ is the average temperature (K),

– θ_{ext} is the exterior temperature (K).

- State equations

$$\text{thermodynamic :} \qquad p = \hat{Z}(p,\theta)\rho R\theta, \tag{4}$$

$$E = e + \frac{1}{2}v^2, \tag{5}$$

$$\text{caloric :} \qquad e = \hat{e}(\theta) = \hat{e}(\theta_{ref}) + \int_{\theta_{ref}}^{\theta} \hat{c}_v(s)\, ds, \tag{6}$$

where

– $\hat{Z}(\theta, p)$ is the compressibility factor (nondimensional),
– R is the gas constant (J/(kg K)),
– e is the specific internal energy (J/kg),
– θ_{ref} is a reference temperature (K),
– $\hat{c}_v(\theta)$ is the specific heat at constant volume, at temperature θ (J/kg K).

The computation of λ will be done by using the *Colebrook's equation* (see [19]):

$$\frac{1}{\sqrt{\lambda}} = -2\log_{10}\left(\frac{2.51}{\mathrm{Re}\sqrt{\lambda}} + \frac{k}{3.7D}\right) = -2\log_{10}\left(\frac{2.51\pi D\eta}{4\,|q|\,\sqrt{\lambda}} + \frac{k}{3.7D}\right), \tag{7}$$

where k is the roughness coefficient of the pipe (m).

The last term in (2) arises from the gravity force. In fact, the correct expression of that term is $g\rho(x,t)\sin(\pi - \alpha(x))$ (see Fig. 2) but, if the slope of the pipeline is small, i.e., if

$$|h'(x)| \ll 1$$

then

$$\sin(\pi - \alpha(x)) \approx \tan(\pi - \alpha(x)) = -\tan\alpha(x) = -h'(x).$$

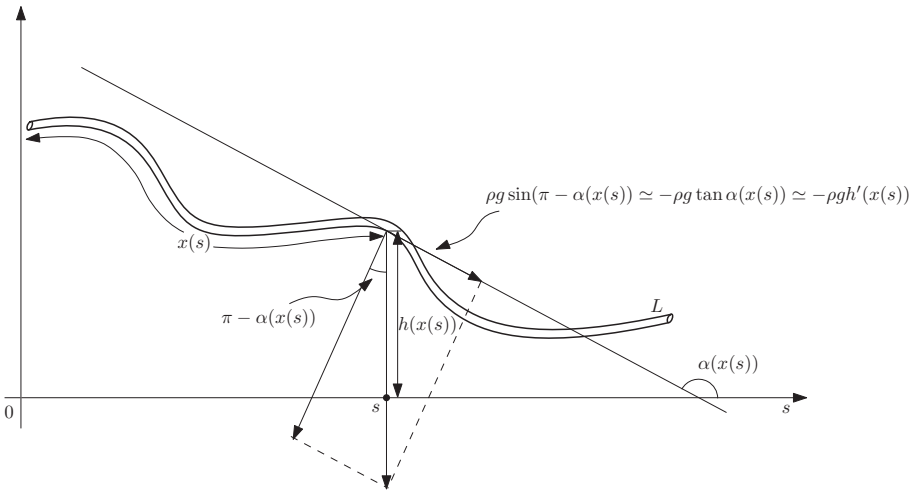

Figure 2: The gravity force term.

2.1 Steady state model

From this point forward, we will suppose that the flow is in steady-state and the temperature is given. Then, the partial derivatives with respect to time are null and the energy equation is not needed. Hence, the system of equations becomes

$$\frac{dq}{dx}(x) = 0, \tag{8}$$

$$A\frac{dp}{dx}(x) + \frac{\lambda(q(x))}{2DA}\frac{1}{\rho(x)}|q(x)|\,q(x) + Ag\rho(x)\frac{dh(x)}{dx} = 0, \tag{9}$$

$$\hat{Z}(p(x),\theta(x))\,\rho(x)\,R\theta(x) = p(x), \tag{10}$$

where θ is the absolute temperature, which is supposed to be known lengthwise the pipe. The last equation is the equation of state for real gases. Notations are as follows:

$$R = \frac{\mathcal{R}}{M},$$

where $\mathcal{R}$ is the universal gas constant (J/(k-mol K), and M is the molar mass (kg/k-mol). The compressibility factor, Z, depends on pressure and temperature. It can be determined using different equations, like the van der Waals equation, but in the gas transportation industry the AGA8 model is widely used. This model is an empirical equation proposed by the American Gas As-

sociation [20], namely,

$$Z = \hat{Z}\left(p, \theta\right) = 1 + p_r 0.257 - 0.533 \frac{p_r}{\theta_r}, \tag{11}$$

being $p_r := p/p_c$, $\theta_r := \theta/\theta_c$, and p_c and θ_c the *critical pressure* and the *critical temperature*, respectively. Let us recall that above the critical temperature it is impossible to liquefy a gas, while the critical pressure is the minimum pressure required to liquefy a gas at its critical temperature. For natural gas the critical temperature is around 170 K and the critical pressure around 5 MPa. Notice that the first equation implies that the mass flow is constant along the pipe, $q\left(x\right) = q \; \forall x \in (0, L)$.

2.2 Approximate model

For numerical simulation of gas transmission networks a simplified model is used which is deduced by integrating the equation (9) between the ends of the pipe, $x = 0$ and $x = L$ and making certain approximations.

Firstly, the mean density in the section is replaced with the following expression, deduced from the equation of state for real gases:

$$\rho\left(x\right) = \frac{p\left(x\right)}{Z\left(p\left(x\right), \theta\left(x\right)\right) \; R\, \theta\left(x\right)}.$$

Thus, we obtain

$$\begin{aligned} A p\left(x\right) \frac{dp}{dx}\left(x\right) + \frac{\lambda(q)}{2DA} Z\left(p\left(x\right), \theta\left(x\right)\right) \; R\, \theta\left(x\right) |q| \, q \\ + A g \frac{p^2\left(x\right)}{Z\left(p\left(x\right), \theta\left(x\right)\right) \; R\, \theta\left(x\right)} h'(x) = 0. \end{aligned} \tag{12}$$

Integrating this equation from $x = 0$ to $x = L$ and dividing by $A/2$ yields,

$$\begin{aligned} p^2\left(L\right) - p^2\left(0\right) = -\frac{\lambda\left(q\right)}{DA^2} R \, |q| \, q \int_0^L Z\left(p\left(x\right), \theta\left(x\right)\right) \theta\left(x\right) \; dx \\ - \frac{2g}{R} \int_0^L \frac{p^2\left(x\right)}{Z\left(p\left(x\right), \theta\left(x\right)\right) \theta\left(x\right)} h'(x) \, dx. \end{aligned} \tag{13}$$

At this point, we rewrite equation (13) by using the new variable $u\left(x\right) := p^2\left(x\right)$,

$$\begin{aligned} u\left(L\right) - u\left(0\right) = -\frac{\lambda\left(q\right)}{DA^2} R \, |q| \, q \int_0^L Z\left(p\left(x\right), \theta\left(x\right)\right) \theta\left(x\right) \; dx \\ - \frac{2g}{R} \int_0^L \frac{u\left(x\right)}{Z\left(p\left(x\right), \theta\left(x\right)\right) \theta\left(x\right)} \frac{dh\left(x\right)}{dx} \, dx. \end{aligned} \tag{14}$$

Now, the integrals on the right-hand side are approximated using average values of pressure and temperature in the pipe, denoted by p_m and θ_m, respectively, whose expression will be specified below:

$$\int_0^L Z\left(p\left(x\right),\theta\left(x\right)\right)\theta\left(x\right)\,dx \approx Z\left(p_m,\theta_m\right)\theta_m L,$$

$$\int_0^L \frac{u\left(x\right)}{Z\left(p\left(x\right),\theta\left(x\right)\right)\theta\left(x\right)}\frac{dh\left(x\right)}{dx}\,dx \approx \frac{u_m}{Z\left(p_m,\theta_m\right)\theta_m}(h\left(L\right)-h\left(0\right)).$$

Replacing in (14), we finally obtain,

$$u\left(0\right)-u\left(L\right)=\frac{\lambda\left(q\right)L}{DA^2}\,R\,\theta_m\left|q\right|qZ\left(p_m,\theta_m\right)+\frac{2g}{R\theta_m}\frac{u_m}{Z\left(p_m,\theta_m\right)}\left(h\left(L\right)-h\left(0\right)\right), \tag{15}$$

Assuming that the section of the pipe is circular ($A=\pi D^2/4$), we have,

$$u\left(0\right)-u\left(L\right)=G\left(p_m,\theta_m,q\right)+\frac{2g}{R\theta_m}\frac{u_m}{Z\left(p_m,\theta_m\right)}\left(h\left(L\right)-h\left(0\right)\right) \tag{16}$$

where

$$G\left(p_m,\theta_m,q\right):=\frac{16\lambda\left(q\right)L}{\pi^2D^5}\,R\,\theta_m\left|q\right|qZ\left(p_m,\theta_m\right), \tag{17}$$

or, introducing $\mu\left(q\right):=\lambda\left(q\right)\left|q\right|q$,

$$G\left(p_m,\theta_m,q\right)=\frac{16\mu\left(q\right)L}{\pi^2D^5}\,R\,\theta_m Z\left(p_m,\theta_m\right), \tag{18}$$

and the average u_m can be computed by the following alternatives:

$$u_m:=\frac{u\left(0\right)+u\left(L\right)}{2}, \tag{19}$$

$$u_m:=\frac{2}{3}\left(u\left(0\right)+u\left(L\right)-\frac{u\left(0\right)u\left(L\right)}{u\left(0\right)+u\left(L\right)}\right), \tag{20}$$

and similar expressions for θ_m. Let us recall that the absolute temperatures at points $x=0$ and $x=L$ are assumed to be known.

3 Modelling the network

The gas transport network is modeled as a directed graph $G=(N,E)$, where N represents the set of n nodes and E the set of e edges. Thus, each element of E is an ordered pair of elements in N.

- The nodes represent the gas supply points, the gas consumption points, the underground storages, the suction or discharge points in a compression station, the interconnection points among pipelines, and the points where the latter change diameter or some other property.

- The edges represent the pipelines, the compressors (each compressor links the suction node and the discharge node by the ratio of their increasing pressures), the flow control valves (FCV) (where the mass flow rate is imposed), the closed closing valves (where the mass flow is zero), the bypasses or open closing valves, the pressure control valves (PCV) (which link two nodes by the ratio of their decreasing pressures).

Concerning the flow, the magnitudes involved in the model are:

1. The pressure at the nodes: $\{p_i : i = 1, \cdots, n\}$. We denote by $\mathbf{p}$ the column vector of n components: $\mathbf{p} = (p_1, \cdots, p_n)^t$.

2. The mass flow rate exchanged with the outside of the network at the nodes: $\{c_i : i = 1, \cdots, n\}$. We denote by $\mathbf{c}$ the column vector of n components: $\mathbf{c} = (c_1, \cdots, c_n)^t$.

3. The mass flow rate along the edges: $\{q_j : j = 1, \cdots, e\}$. We denote by $\mathbf{q}$ the column vector of e components: $\mathbf{q} = (q_1, \cdots, q_e)^t$.

In order to analyze and solve the model, it is convenient to introduce the square pressure at the nodes: $\{u_i : i = 1, \cdots, n\}$. Vector $\mathbf{u}$ will denote the column vector of n components, $\mathbf{u} = (u_1, \cdots, u_n)^t = (p_1^2, \cdots, p_n^2)^t$.

The equations of the gas network model are going to be mathematical expressions of mass conservation at nodes and head loss along edges:

3.1 Mass conservation

It is also known as Kirchhoff's first law of the network because of its analogy with this law for electric circuits. It establishes that, at any node, the sum of the ingoing mass flow rates must be equal to the sum of outgoing mass flow rates. Thanks to the incidence matrix of the graph representing the network, $\mathcal{A}$, it can be written in a compact way as

$$\mathcal{A}\mathbf{q} = \mathbf{c}. \tag{21}$$

An important property of matrix $\mathcal{A}$ is the following. Let $\mathbf{e}$ be the vector of $\mathbb{R}^n$ whose components are all equal to 1. From the definition of $\mathcal{A}$ it is straightforward to check that $\mathcal{A}^t\mathbf{e} = \mathbf{0}$. Then, scalar multiplication of equation (21) by $\mathbf{e}$

leads to

$$\mathbf{c} \cdot \mathbf{e} = \sum_{i=1}^{n} c_i = \mathcal{A}\mathbf{q} \cdot \mathbf{e} = \mathbf{q} \cdot \mathcal{A}^t \mathbf{e} = 0, \tag{22}$$

which is an obvious necessary condition for the existence of a solution to the network model: since the network is in steady state, the algebraic sum of the mass flow rates exchanged with the outside of the network has to be null.

The above property implies that the maximum number of independent equations in the linear system (21) is $n-1$. Thus, even if all components of vector $\mathbf{c}$ are known, in general we need other equations to uniquely compute the flows in the network. These additional equations will be written in the next section and come from the linear momentum conservation principle. Meanwhile, let us analyze the set of solutions of the mass conservation equation (21) assuming that $\mathbf{c}$ is given satisfying (22). For this purpose, let us denote by $\mathbf{q}^*$ a particular solution orthogonal to $\ker(\mathcal{A})$. Then the set of solutions is the linear manifold $\mathbf{q}^* + \ker(\mathcal{A})$. Let us take any $\mathbf{w} \in \ker(\mathcal{A})$. This means that $\mathcal{A}\mathbf{w} = \mathbf{0}$. If the only physical constraint were mass conservation, the flow corresponding to vector $\mathbf{w}$ could be considered as superfluous because it does not help to transport gas from emission to consumption points. However, superfluous flows are often needed to meet the linear momentum conservation equations to be given below. In other words, it is unlikely that the vector of mass flow rates in a real network be orthogonal to the vector space $\ker(\mathcal{A})$.

The flow vectors belonging to the kernel of $\mathcal{A}$ are called *cycling flows*. The orthogonal projection of the actual vector of mass flow rates in a network onto the space of cycling flows will be called the *superfluous flows* vector. We want to emphasize once again that the latter are often needed in order to comply with the momentum conservation principle.

For some particular calculations it can be necessary to "eliminate" the superfluous flow vector. This can be done by making the projection of the mass flow rate vector onto the orthogonal space to $\ker(\mathcal{A})$. A basis of this kernel can be obtained from the so-called *cycle matrix* which, in its turn, can be obtained by means of "graph algorithms" like the *depth-first search* (DFS) or "algebraic methods" based on the *singular-value decomposition* (SVD) of matrix $\mathcal{A}$.

3.1.1 Notations

Firstly, let us define the dimension of the different kind of nodes and edges:

- n_p: number of nodes where the pressure is imposed,
- e_r: number of edges corresponding to compressors or pressure control valves,

- e_t: number of flow control valves,
- e_c: number of closed closing valves,
- $e_f = e - e_t - e_c - e_r$: number of edges which are neither flow control valves, nor closed closing valves, nor compressors, nor pressure control valves. We refer to these edges as *free edges* and, for the sake of exposition, they will be numbered first.

Then the *data* of the model are the following:

- $\boldsymbol{\alpha}^R$: vector of differences of square pressures between the two nodes of edges associated with compressors or pressure control valves (e_r components),
- $\mathbf{p}^U$: vector of imposed pressures (n_p components),
- $\mathbf{u}^U$: vector of imposed square pressures (n_p components),
- $\mathbf{c}^D$: vector of imposed mass flow rates exchanged with the outside of the network ($n - n_p$ components),
- $\mathbf{q}^V$: vector of imposed mass flow rates (e_v components, with $e_v = e_t + e_c$).

Consequently, the *unknowns* of the model are the following:

- $\mathbf{p}^D$: vector of pressures at nodes where pressure is not imposed ($n - n_p$ components),
- $\mathbf{u}^D$: vector of square pressures at nodes where square pressure is not imposed ($n - n_p$ components),
- $\mathbf{q}^R$: vector of mass flow rates along the edges associated with compressors or pressure control valves (e_r components),
- $\mathbf{q}^F$: vector of mass flow rates along the free edges (e_f components),
- $\mathbf{c}^U$: vector of mass flow rates exchanged with the outside of the network at nodes where pressure is imposed (n_p components),

According to the above notations, the mass conservation equation (21) can be rewritten in the form

$$\mathcal{A}_F\mathbf{q}^F + \mathcal{A}_R\mathbf{q}^R - \mathcal{U}^t\mathbf{c}^U = \mathcal{D}^t\mathbf{c}^D - \mathcal{A}_V\mathbf{q}^V. \tag{23}$$

Let us left-multiply this equality by matrix $\mathcal{D}$. We get (notice that $\mathcal{D}\mathcal{U}^t = 0$ and $\mathcal{D}\mathcal{D}^t = \mathcal{I}$),

$$\mathcal{D}\mathcal{A}_F\mathbf{q}^F + \mathcal{D}\mathcal{A}_R\mathbf{q}^R = \mathbf{g}, \tag{24}$$

with

$$\mathbf{g} := \mathbf{c}^D - \mathcal{D}\mathcal{A}_V\mathbf{q}^V. \tag{25}$$

3.2 Momentum conservation

It states that there is a pressure drop along pipelines due to the viscous stress arising from friction with their walls which can be computed with the function introduced in (18). This function can be rewritten as

$$G_j\left(p_{mj},\theta_{mj},q_j\right)=r_j\left(p_{mj},\theta_{mj}\right)\mu_j\left(q_j\right), \tag{26}$$

where

$$r_j\left(p_{mj},\theta_{mj}\right):=\frac{16L_j\,R}{\pi^2D_j^5}\theta_{mj}Z\left(p_{mj},\theta_{mj}\right). \tag{27}$$

Let us suppose that the free edges are numbered first. We define the "diagonal" mapping $\mathbf{G}_F:\mathbb{R}^{e_f}\to\mathbb{R}^{e_f}$ by

$$\mathbf{G}_F\left(\mathbf{p}_m,\boldsymbol{\theta}_m,\mathbf{q}^F\right)_j \;=\; G_j\left(p_{mj},\theta_{mj},q_j^F\right),\ j=1,\cdots,e_f$$

and the vector $\mathbf{b}^F\in\mathbb{R}^{e_f}$ by

$$b_j^F=\frac{2g}{R\theta_{mj}}\frac{u_{mj}}{Z\left(p_{mj},\theta_{mj}\right)}\left(H_{\mathcal{M}_{2,j}}-H_{\mathcal{M}_{1,j}}\right), \tag{28}$$

where H_i denotes the height of the i-th node, u_{mj} is the average value of u along the j-th edge given by

$$u_{mj}=\frac{u_{\mathcal{M}_{1,j}}+u_{\mathcal{M}_{2,j}}}{2},$$

and $\mathcal{M}_{1,j}$ and $\mathcal{M}_{2,j}$ are the two nodes of the j-th edge. We have,

$$\mathcal{A}_F^t\mathbf{u}-\mathbf{G}_F\left(\mathbf{p}_m,\boldsymbol{\theta}_m,\mathbf{q}^F\right)=\mathbf{b}^F(\mathbf{u}), \tag{29}$$

$$\mathcal{A}_R^t\mathbf{u}=\boldsymbol{\alpha}^R, \tag{30}$$

and, since $\mathbf{u}=\mathcal{U}^t\mathbf{u}^U+\mathcal{D}^t\mathbf{u}^D$, the first equation can also be written as

$$\mathcal{A}_F^t\mathcal{D}^t\mathbf{u}^D-\mathbf{G}_F\left(\mathbf{p}_m,\boldsymbol{\theta}_m,\mathbf{q}^F\right)=\mathbf{f}, \tag{31}$$

with

$$\mathbf{f}:=\mathbf{b}^F(\mathbf{u})-\mathcal{A}_F^t\mathcal{U}^t\mathbf{u}^U \tag{32}$$

and the second one as

$$\mathcal{A}_R^t\mathcal{D}^t\mathbf{u}^D=\mathbf{k}, \tag{33}$$

with

$$\mathbf{k}:=\boldsymbol{\alpha}^R-\mathcal{A}_R^t\mathcal{U}^t\mathbf{u}^U. \tag{34}$$

3.3 The full model

Let us summarize the model of the gas transportation network:
Given,

- $\mathbf{u}^U$*: the vector of imposed square pressures,*
- $\mathbf{q}^V$*: the vector of mass flow rates at the edges with flow control valves,*
- $\boldsymbol{\alpha}^R$*: the vector of differences of square pressures between the two nodes of edges associated with compressors or pressure control valves,*
- $\mathbf{c}^D$*: the vector of the mass flow rates exchanged with the outside of the network, at nodes where pressure is not imposed,*

find vectors $\mathbf{u}^D$, $\mathbf{q}^F$, $\mathbf{q}^R$ *and* $\mathbf{c}^U$ *such that*

$$\mathcal{D}\mathcal{A}_F\mathbf{q}^F + \mathcal{D}\mathcal{A}_R\mathbf{q}^R = \mathbf{g}, \tag{35}$$

$$\mathcal{A}_F^t\mathcal{D}^t\mathbf{u}^D - \mathbf{G}_F\left(\mathbf{q}^F\right) = \mathbf{f}, \tag{36}$$

$$\mathcal{A}_R^t\mathcal{D}^t\mathbf{u}^D = \mathbf{k}, \tag{37}$$

$$\mathcal{A}_F\mathbf{q}^F + \mathcal{A}_R\mathbf{q}^R - \mathcal{U}^t\mathbf{c}^U = \mathcal{D}^t\mathbf{c}^D - \mathcal{A}_V\mathbf{q}^V, \tag{38}$$

with $\mathbf{g}$, $\mathbf{f}$ *and* $\mathbf{k}$ *given by (25), (32) and (34), respectively.*

The unknowns of the model are $\mathbf{u}^D$ ($n - n_p$ numbers), $\mathbf{q}^F$ (e_f numbers), $\mathbf{q}^R$ (e_r numbers), and $\mathbf{c}^U$ (n_p numbers) so that the total number of unknowns is $n - n_p + e_f + e_r + n_p = n + e_f + e_r$, which is equal to the number of equations: $n - n_p + e_f + e_r + n_p = n + e_f + e_r$.

Let us notice that, if we can solve equations (35), (36) and (37) for $\mathbf{u}^D$, $\mathbf{q}^F$ and $\mathbf{q}^R$, then (38) allows us to compute $\mathbf{c}^U$ by

$$\mathbf{c}^U = \mathcal{U}\mathcal{A}_F\mathbf{q}^F + \mathcal{U}\mathcal{A}_R\mathbf{q}^R + \mathcal{U}\mathcal{A}_V\mathbf{q}^V,$$

in a second step. This is because $\mathcal{U}\mathcal{U}^t = \mathcal{I}$ and $\mathcal{U}\mathcal{D}^t = 0$.

We observe that unknown vector $\mathbf{u}^D$ appears in the expression of the right-hand side $\mathbf{f}$ of equation (36), namely, in vector $\mathbf{b}^F(\mathbf{u})$. Thus, it is important to rewrite this equation by putting this term on the left-hand side. For this purpose, let us introduce the following notation:

$$w_j = \frac{g}{R\theta_{mj}Z(p_m, \theta_{mj})}\left(H_{\mathcal{M}_{2j}} - H_{\mathcal{M}_{1j}}\right), \tag{39}$$

for $1 \leq j \leq e_f$, and $\mathcal{W}$ denotes the $e_f \times e_f$ diagonal matrix

$$\mathcal{W}_{lj} = w_j\delta_{lj}, \;\; 1 \leq l, j \leq e_f.$$

Let the $n \times e$ matrix Λ be defined, for $1 \leq i \leq n,\ 1 \leq j \leq e$, by

$$\Lambda_{ij} = \delta_{i\,\mathcal{M}_{1j}} + \delta_{i\,\mathcal{M}_{2j}}$$

where δ is the Kronecker's delta. Then vector $\mathbf{b}^F(\mathbf{u})$ can be written as

$$\mathbf{b}^F(\mathbf{u}) = \mathcal{W}\mathcal{F}\Lambda^t\mathbf{u} = \mathcal{W}\mathcal{F}\Lambda^t\big(\mathcal{D}^t\mathbf{u}^D + \mathcal{U}^t\mathbf{u}^U\big)$$

and (36) becomes

$$\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{G}_F\left(\mathbf{q}^F\right) = \mathbf{h}, \tag{40}$$

with

$$\mathbf{h} := \big(\mathcal{W}\mathcal{F}\Lambda^t - \mathcal{A}_F^t\big)\mathcal{U}^t\mathbf{u}^U.$$

Now, from (40) we can obtain $\mathbf{q}^F$ as

$$\mathbf{q}^F = \mathbf{G}_F^{-1}\Big(\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{h}\Big),$$

and replacing this expression in (35) it can be written in terms of $\mathbf{u}^D$ and $\mathbf{q}^R$, namely,

$$\mathcal{D}\mathcal{A}_F\mathbf{G}_F^{-1}\Big(\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{h}\Big) + \mathcal{D}\mathcal{A}_R\mathbf{q}^R = \mathbf{g}. \tag{41}$$

In order to prove the existence of a solution to (37) and (41) it is convenient to subtract the term

$$\mathcal{D}\Lambda\mathcal{F}^t\mathcal{W}\mathbf{G}_F^{-1}\Big(\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{h}\Big),$$

to both sides of (41). We get

$$\begin{aligned}\mathcal{D}\big(\mathcal{A}_F - \Lambda\mathcal{F}^t\mathcal{W}\big)\mathbf{G}_F^{-1}\Big(\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{h}\Big) + \mathcal{D}\mathcal{A}_R\mathbf{q}^R \\ = \mathbf{g} - \mathcal{D}\Lambda\mathcal{F}^t\mathcal{W}\mathbf{G}_F^{-1}\Big(\big(\mathcal{A}_F^t - \mathcal{W}\mathcal{F}\Lambda^t\big)\mathcal{D}^t\mathbf{u}^D - \mathbf{h}\Big).\end{aligned} \tag{42}$$

Finally, by introducing the $(n - n_p) \times e_f$ matrix

$$\mathcal{B} := \mathcal{D}\big(\mathcal{A}_F - \Lambda\mathcal{F}^t\mathcal{W}\big),$$

this equation can be rewritten as

$$\mathcal{B}\mathbf{G}_F^{-1}\Big(\mathcal{B}^t\mathbf{u}^D - \mathbf{h}\Big) + \mathcal{D}\mathcal{A}_R\mathbf{q}^R = \mathbf{g} - \mathcal{D}\Lambda\mathcal{F}^t\mathcal{W}\mathbf{G}_F^{-1}\Big(\mathcal{B}^t\mathbf{u}^D - \mathbf{h}\Big). \tag{43}$$

As mentioned before, matrix $\mathcal{W}$ depends on the solution through the compressibility factor Z because this parameter is a function of pressure which, in its turn, is the square root of u. The same is true for mapping $\mathbf{G}_F$.

3.4 Existence of solution. Numerical methods

Existence of solution to problem (43) has been shown in [11] under quite general assumptions. The proof consists of two step. In the first one, convex analysis tools are used and, in the second one, the Brouwer's fixed point theorem is applied. Moreover, as (43) is a nonlinear system of algebraic equations, it can be solved by using Newton's algorithm (see [18] for further details).

4 Optimization

In order to optimize the gas transport network, different optimization goals can be considered: minimize the self-consumption in the compressor stations, minimize the boil-off gas in the regasification plants, maximize the exportation from any area of the network to another area or reduce the bottlenecks. For the sake of simplicity, in this paper we will focus on minimizing the self-consumption in the compressor stations, that is, we want to minimize the function defined by

$$Q = \frac{1}{\varepsilon\xi\zeta LCV}\left\{\frac{\gamma}{\gamma-1}Z(p_1,\theta_1)R\theta_1\left((\frac{p_2}{p_1})^{\frac{\gamma-1}{\gamma}}-1\right)q\right\}, \quad \text{kg/s.}$$

This minimization is achieved by modifying the compression ratio at the compressor stations, the decompression ratio at PCVs, the flow at the FCVs, the flow at the regasification plants or at the international connections, and others variables. Let us point out that all these variables are also known, in the mathematical systems theory, as control variables. Once the optimization goal has been chosen, it is important to apply a set of constraints which reproduce the real conditions of the problem. These conditions can be put into three different groups:

- *Physical*: mass conservation equations and pressure loss equations; they coincide with the mathematical model of the network.
- *Security of supply*: imposed mass flow rate at exit points, minimum and maximum pressure allowed at each node of the network and capacity bounds at each pipe of the network.
- *Compressor stations*: every compressor must work accordingly to its operating diagram and its technical characteristics. Fig. 3 shows an example of operating diagram of a compressor. The functions defining this diagram lead to nonlinear constraints (see [16] or [18] for more details).

A two-stage procedure to tackle this problem has been developed. In the first stage the complexity of gas physics is reduced while taking all discrete

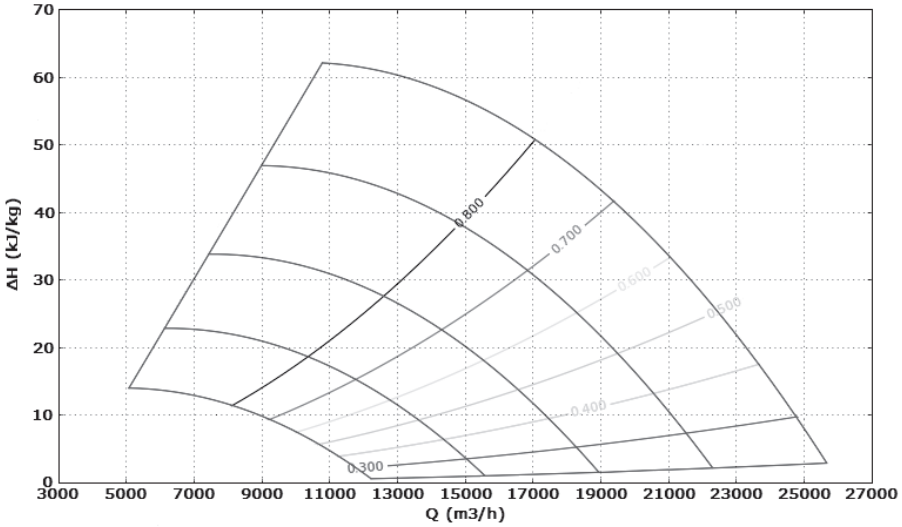

Figure 3: Compressor diagram.

decisions into account. Thus, the first stage provides all discrete decisions and gives an initial solution to the second stage. The second stage refines the solution obtained by the first stage, providing a result that uses a slightly more precise formulation of the physical constraints and that may be used for the study and management of the gas network.

4.1 First stage

The idea of this stage is to obtain an initial solution, which is used to configure the network (compressor stations, PCVs, ...), disregarding some second order physical effects. Notice that it involves solving a mixed integer nonlinear problem. Indeed, firstly there are a lot of nonlinear aspects, mainly due to the pressure loss in the pipes, the gas consumption and the operation range of the compressors. Secondly, there are binary decisions regarding whether or not a given valve or compressor is active. This approach does not use the simulator, which means that the group of conditions included in physics' (and then in the state equation) are imposed as a set of constraints of the problem. Regarding the optimization goal, the pressures and mass flow rates are independent variables. One of the algorithms that can be used to get a solution to this problem is the classical Sequential Linear Programming (SLP) algorithm. This algorithm is widely studied in the literature and it has a very good behavior in practice (see [21, Chap. 10]). It consists in solving iteratively linear

approximations of the nonlinear problem until the algorithm finds an optimal suitable solution. There are different ways to linearize the functions and the constraints, e.g. Taylor approximations. Its main characteristics are that it does local search based on bounded size steps at each iteration and it provides a sequence whose limit points are KKT (Karush-Kuhn-Tucker) points. For our purpose, the classical SLP has one limitation since it does not accommodate binary variables. In order to avoid this limitation, a modified version of the algorithm has been developed allowing us to introduce the binary variables. Besides, it also allows unbounded size steps, meaning that at every iteration a mixed integer linear. optimization problem is solved. On the downside, it is more common to observe convergence problems, such as cycling, in this modified version of classical SLP than in the standard version.

4.2 Second stage

The aim of this stage is to refine the solution given by the first stage to obtain a result which reproduces the physical behavior of the network and fulfills all the original constraints. This second stage is based on optimal control techniques. It employs the network model to implicitly express the state variables (pressures and mass flow rates) in terms of control variables. In this way, the independent variables for the optimization goal are only the control variables. Moreover, the final solution uses slightly more precise formulations of the network model. Given that the configuration provided by the first stage contains all the discrete decisions made, this approach deals with a continuous nonlinear problem. Again, the classical SLP can be used as an algorithm to solve the problem but, unlike the first stage, the optimization goal and the constraints are locally linearized by using the derivatives respect to the control variables. They are computed by using the so-called *adjoint state*.

5 Numerical results

In this section we show an application of GANESO code to the primary Spanish gas network. The conditions are the following:

- International connections and underground facilities are taken as fixed inputs.
- The optimizer has freedom to choose the distribution of the input mass flow rates from the regasification plants and the international connections.
- The optimizer has freedom to choose how to use compressor stations,

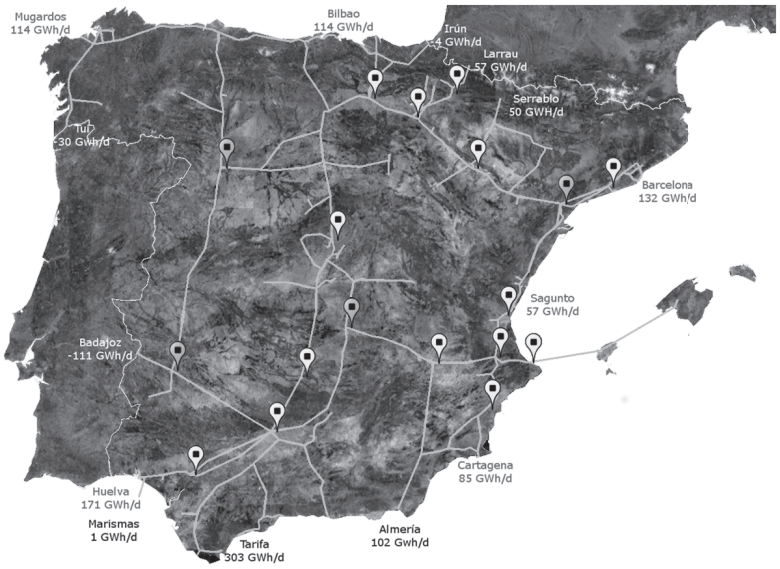

Figure 4: Usual management without optimization.

PCVs and FCVs.

- The cost function is based on the gas self-consumption in the compressor stations.
- Scenario: working day of January with low demand.

In Fig. 4 we show the real situation of the network, while Fig. 5 show the optimized management. Table 1 shows the optimized entry flows into the network and Table 2 the costs at the stations.

Before Vs After:

- From South = Cartagena + Huelva = -134.3099 GWh/d
- From North = Reganosa + Barcelona + Bilbao = +78.9250 GWh/d

5.1 Conclusions

- GANESO has optimized the distribution of flow among the regasification plants and the use of compressor stations.
- Based on this management, the cost is about one-sixth the usual one.
- The optimization took 5-10 minutes on a desktop computer.

Figure 5: Optimized management.

[GWh/day]	No opt.	With opt.
Barcelona	131.8407	241.6383
Bilbao	113.8560	90.6997
Cartagena	85.3920	38.2229
Huelva	170.7840	83.6432
Reganosa	114.1571	106.4408
Sagunto	56.9280	112.3129

Table 1: Optimized entry flows

[GWh/day]	No opt.	With opt.
Alcazar	0.2909	-
Algete	-	-
Almendralejo	0.2650	0.1587
Baneras	-	-
Chinchilla	-	-
Cordoba 1	-	-
Cordoba 2	-	-
Crevillente	-	-
Denia	-	-
Haro	-	-
Montesa	-	-
Navarra	-	-
Paterna	-	-
Puertollano	-	-
Sevilla	-	-
Tivisa	0.2229	-
V. Arnedo	-	-
Zamora	0.1516	-
Zaragoza	-	-
TOTAL	0.9304	0.1587

Table 2: Compression cost at the stations.

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