Comparing Finite Differences methods for gas network simulation

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Abstract— This is a study in gas modelling and simulation with a special focus on the simulation of a gas pipeline, the most important element of the network, which is represented by a quasi-hyperbolic PDE, linearised around operational levels. Different numerical schemata are presented for the solution of this problem, explicit and implicit, as well as cell centered discretisation methods. In order to have a well-posed initialboundary value problem (IBVP), we use two-port network transfer function models to calculate the initial value function. The numerical methods are implemented in Matlab, and we give special relevance to issues as consistency, stability and convergence. Furthermore, we apply each of the schemata to calculate the solution of a pipeline. The present work is part of a research study to evaluate comparatively different numerical methods for the solution of gas network models, in particular the hyperbolic model. We start with a isothermal, one-dimensional gas flow and considering horizontal pipelines.

Keywords: High pressure transmission pipelines, Finite difference methods, gas networks simulation.

I. INTRODUCTION.

The transient behaviour of gas in the pipelines is represented by partial differential equation (PDE), or a system of these equations, whose form varies with the considered assumptions and the particular operating conditions of the pipeline. Whenever the rate of change of the gas properties normal to the streamline direction may be considered negligible when compared to the rate of change of that streamline, the flow becomes unidimensional. This means that the gas properties are considered uniform over any cross-section, and give satisfactory solutions to problems where (i) the cross-section of the pipe has small variations along the streamline; (ii) the curvature radius of the pipeline is large when compared to its diameter; (iii) the velocity and temperature profiles are kept almost constant along the pipe. Therefore, gas flow, pressure, density, velocity, etc. can be considered functions of time and space along the axis of the pipe.

2-D transient models are always obtained from three physical laws: (i) Conservation of mass; (ii) Conservation of momentum; (iii) Conservation of energy. When simulating transient gas models, it is required on one hand that the result be accurate and on the other that the model is kept simple enough to be handled numerically. The simplified models are obtained by neglecting certain terms according to the particular pipeline in question, which means that the chosen transient model should fit the particular operating conditions of the pipeline.

The methods for solving PDEs can be classified into analytical or numerical; the analytical methods are very laborious and difficult to apply to models of this complexity. This work is devoted to the numerical solution of gas transient models, in particular to finite difference (FD) methods, where we discuss in particular a class of implicit/explicit methods.

A parabolic model is solved in [6] using the method of characteristics (MC) and the Crank-Nicolson method with different discretisation steps. In [11] is discussed comparatively finite difference (FD) and finite element (FE) methods to solve the same problem, where the criterion of comparison of results are the accuracy of the results and computation time. Helgaker *et al.* solve numerically the governing equations for one-dimension compressible flow using implicit FD methods.

As for a discontinuous change in inlet temperature the method is observed to introduce unphysical oscillations in the temperature profile along the pipeline, a solution strategy where the hydraulic and thermal models are solved separately using different discretisation techniques is suggested [5]. In [3], for the implicit method, the energy equation is solved one time step behind the continuity and momentum equation. Compared to solving all three equations simultaneously, this will decrease the computational time for each time step during the simulation.

In [4], since the one-dimension version is a result of averages over the pipe cross-section and the flow is normally turbulent, the order of averaging in space and time is an issue; in particular, for the dissipation term. In [2], one-dimension, nonisothermal gas flow model was solved to simulate the slow and fast fluid transients, such as those typically found in high-pressure gas transmission pipelines. The simulation results were used to understand the effect of different pipeline thermal models on the flow rate, pressure and temperature. For the same problem, in [13] the mathematical model constitutes a non-homogeneous system of non-linear hyperbolic conservation laws. At each time step, a non-homogeneous hyperbolic model is split into a homogeneous hyperbolic model and an ODE operator.

In [7], the equations for fast flow in short gas pipe are written in conservative form and solved by a predictorcorrector schema for the interior mesh points: an improved Lax-Friedricks schema as a predictor and a leapfrog schema as a corrector. MC and upwind method are used for the

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boundary conditions. For mass slow fluid in relatively long gas pipe, the equations are written in non-conservative form and resolved by a simple explicit FD schema. The boundary conditions are considered by using the characteristic form of the equations including an inertial multiplier (Yow model) and resolved by a Newton-Raphson method, which is claimed to gain more computational time and simplicity in comparison with other methods. In [8], the obtained equations are written in characteristic form and resolved by a predictor-corrector lambda schema for the interior mesh points. MC is used for the boundaries. Advantages of explicit form of these schemata and the flexibility of the MC are used for an isothermal fast transient gas flow in a short pipe. The results, obtained for a simple practical application, agree with those of other methods. Modisette discusses adaptive techniques for mesh points, where the benefit of dense meshes is discussed for different models, and an heuristic to estimate the needed mesh is suggested [9].

In Section II we linearise the quasi-hyperbolic PDE model around some operational levels. In Section III we present the class of FD implicit/explicit methods to be used and state convergence conditions. The numerical solution of problem (4)–(5) is calculated in Section IV within stability ranges stated in the previous section. We conclude by outlining the most important points of the work and stating some directions for future research in Section V.

II. LINEAR QUASI-HYPERBOLIC PDE

We consider a hyperbolic PDE to represent the gas dynamics in the pipes [10]. Hence:

$$\begin{pmatrix} \frac{\partial q(x,t)}{\partial t} = -S \frac{\partial p(x,t)}{\partial x} + \frac{\lambda c^2}{2dS} \frac{q^2(x,t)}{p(x,t)}, \\ \frac{\partial p(x,t)}{\partial t} = -\frac{c^2}{S} \frac{\partial q(x,t)}{\partial x},
\end{cases} (1)$$

where x is space, t is time, p is edge pressure-drop, q is massflow, S is the cross-sectional area, d is the pipe diameter, c is the isothermal speed of sound, and λ is the friction factor.

To linearise system (1), we consider p(x,t), q(x,t) as variations around some operational levels of pressure and massflow, (\bar{p}, \bar{q}) , that is, $p(x,t) = \bar{p} + \Delta p(x,t)$ and $q(x,t) = \bar{q} + \Delta q(x,t)$, with $\Delta p(x,t)$ and $\Delta q(x,t)$ as the deviations from the pressure-drop and mass-flow, respectively. Assuming $\frac{\Delta p(x,t)}{\bar{p}} \ll 1$, as well as $\frac{\Delta q(x,t)}{\bar{q}} \ll 1$, and neglecting terms of higher order and some simple calculations:

$$\frac{q^2(x,t)}{p(x,t)} \cong \frac{\bar{q}^2}{\bar{p}} + 2\frac{\bar{q}}{\bar{p}}\Delta q(x,t) - \frac{\bar{q}^2}{\bar{p}^2}\Delta p(x,t).$$
(2)

Substituting (2) into (1), yields:

$$\begin{cases} \frac{\partial q(x,t)}{\partial t} = -S \frac{\partial p(x,t)}{\partial x} - \alpha q(x,t), \\ \frac{\partial p(x,t)}{\partial t} = -\frac{c^2}{S} \frac{\partial q(x,t)}{\partial x}, \end{cases}$$
(3)

where $\alpha = \frac{\lambda c^2}{2dS} \frac{\bar{q}}{\bar{q}}$, (see [1] for more details). Hence, differentiating the first equation of (3) in order to time and the second in order to space, and eliminating p(x,t) in both, we obtain a quasi-hyperbolic PDE model of second order in terms of q(x,t):

$$\frac{\partial^2 q(x,t)}{\partial t^2} - c^2 \frac{\partial^2 q(x,t)}{\partial x^2} = -\alpha \frac{\partial q(x,t)}{\partial t}.$$
 (4)

An analogous model can be obtained in terms of p(x, t).

Concerning wave equation (4), we study the respective IBVP, where the problem is to find a continuous function $\tilde{q}(x,t)$ for $t \ge 0, 0 \le x \le L$, where L is the length of the pipeline, and satisfies (4) for t > 0 and 0 < x < L, and satisfies the initial and boundary conditions:

$$\begin{cases} \widetilde{q}(x,0) = f_1(x), & 0 \le x \le L, \\ \frac{\partial \widetilde{q}(x,0)}{\partial t} = f_2(x), & 0 < x < L, \\ \widetilde{q}(0,t) = g_1(t), & t \ge 0, \\ \widetilde{q}(L,t) = g_2(t), & t \ge 0, \end{cases}$$
(5)

where $f_1(x), f_2(x), g_1(t), g_2(t)$ are also continuous functions. The IBVP is defined on a semi-infinite strip.

III. NUMERICAL METHODS

According to Osiadacz [10], different classes of numerical methods to solve this problem exist. In this work we want to analyse the selection of implicit and explicit methods relating to the choice of the grid, with the evaluation of the functions at the grid points as well as inside the grid cell.

Consider $\Delta x = L/\ell$ and $\Delta t = T/N$, where T is a period of time considered in the gas behaviour. Partitioning the space interval, [0, L], in equal ℓ parts of width Δx , as well as the time interval, [0, T], in equal N parts of width Δt , we obtain a grid on the rectangle $R = \{(x, t) : 0 < x < L \land 0 < t < T\}$ by drawing vertical and horizontal lines through the points with coordinates (x_j, t_n) where $x_j = j\Delta x$, $j = 0, 1, \ldots, \ell$, and $t_n = n\Delta t$, $n = 0, 1, \ldots, N$, are the intersection of the grid lines x_j and t_n , and called the mesh points. We represent the value of mass-flow at every mesh point of the grid by q_j^n , that is, $q(x_j, t_n)$. Using this notation, we consider all the derivatives in (4) approximated by a centred schema. Thus:

$$q_{j}^{n+1} - 2q_{j}^{n} + q_{j}^{n-1} = \left(\frac{\Delta t}{\Delta x}c\right)^{2} \left(q_{j+1}^{n} - 2q_{j}^{n} + q_{j-1}^{n}\right) - \frac{\alpha}{2}\Delta t \left(q_{j}^{n+1} - q_{j}^{n-1}\right), \quad (6)$$

for every inner point $j = 1, \ldots, \ell - 1$. Defining $D_x^2 q_j^n := q_{j+1}^n - 2q_j^n + q_{j-1}^n$, and

$$r := \frac{\Delta t}{\Delta x}c, \quad a := \frac{\alpha}{2}\Delta t,$$
 (7)

and considering the convex linear combination

$$q_j^n = \theta q_j^{n+1} + (1 - 2\theta) q_j^n + \theta q_j^{n-1}, \qquad 0 \le \theta \le 1,$$
 (8)

we obtain a class of multi-level implicit FD schemata:

$$q_{j}^{n+1} - 2q_{j}^{n} + q_{j}^{n-1} = -a \left(q_{j}^{n+1} - q_{j}^{n-1} \right)$$
(9)
$$r^{2} \left(\theta D_{x}^{2} q_{j}^{n+1} + (1 - 2\theta) D_{x}^{2} q_{j}^{n} + \theta D_{x}^{2} q_{j}^{n-1} \right).$$

Whenever $\theta = 0$ in (9), we have an explicit centred method.

We analyse the consistency of (9) with (4), i.e., $|q(x,t) - q_j^n|$ as the mesh is refined, i.e., $\Delta x, \Delta t \to 0$.

Theorem 1 (Consistency of the FD implicit schemata): FD schemata (9) are consistent with the PDE of IBVP (4)–(5), in conditions of (8), when $\Delta x, \Delta t \rightarrow 0$. Therefore, the class of methods analysed is consistent. Moreover, the numerical approximation is of order $\mathcal{O}(\Delta x^2, \Delta t)$.

To guarantee convergence, we also study the behaviour of $|q(x,t) - q_j^n|$ as $n \to \infty$ for fixed $\Delta x, \Delta t$. Once, these two conditions are fulfilled, the solution of a numerical schema converges to the exact solution of (4) [12].

An explicit solution of (4) can be written as a Fourier series. Let M, ξ and m be constants, where m is an integer, and insert in FD (9) the trial solution $M\xi^n e^{i\Delta xmj}$ in place of q_j^n . Hence with (7) and $D = 4r^2 \sin^2\left(\frac{m\Delta x}{2}\right) > 0$:

$$\xi^2 \left(D\theta + 1 + a \right) + \xi \left(D(1 - 2\theta) - 2 \right) + \left(D\theta + 1 - a \right) = 0,$$

where

$$\xi = \frac{-(D(1-2\theta)-2) \pm \sqrt{D^2(1-4\theta)-4D+4a^2}}{2(D\theta+1+a)}$$

Consider $\chi = D^2(1 - 4\theta) - 4D + 4a^2$.

Theorem 2 (Stability of the FD implicit schemata): A FD schema (9) is stable,

I. for
$$\chi \leq 0$$
, and
(i) $\theta = \frac{1}{4}$, if $\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|} \in \left]0, \frac{4c}{\alpha}\right]$.
(ii) $\frac{1}{4} < \theta \leq 1$, if
 $\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|} \in \left]0, \frac{2c\Delta t\sqrt{4\theta-1}}{\sqrt{-2+\sqrt{4+(\alpha\Delta t)^2(4\theta-1)}}}\right[$.
(iii) $0 \leq \theta < \frac{1}{4}$, if $\Delta t \in \left[0, \frac{2}{\alpha\sqrt{1-4\theta}}\right]$
and $\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|}$ belongs to
 $\left]\frac{2c\Delta t\sqrt{1-4\theta}}{\sqrt{2+\sqrt{4-(\alpha\Delta t)^2(1-4\theta)}}}, \frac{2c\Delta t\sqrt{1-4\theta}}{\sqrt{2-\sqrt{4-(\alpha\Delta t)^2(1-4\theta)}}}\right[$

II. for $\chi > 0$, and

(i) for $\theta = \frac{1}{4}$, if $\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|} \in \left[\frac{4c}{\alpha}, +\infty\right[$. (ii) for $\frac{1}{4} < \theta \le 1$ if

$$\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|} \in \left] \frac{2c\Delta t\sqrt{4\theta-1}}{\sqrt{-2+\sqrt{4+(\alpha\Delta t)^2(4\theta-1)}}}, +\infty \right[.$$
(iii) for $0 \le \theta < \frac{1}{4}$ if $\Delta t \in \left] 0, \frac{2}{\alpha\sqrt{1-4\theta}} \right[$ and

$$\frac{\Delta x}{|\sin(\frac{m\Delta x}{2})|} \text{ belongs to}$$

$$\left] 2c\Delta t\sqrt{1-4\theta}, \frac{2c\Delta t\sqrt{1-4\theta}}{\sqrt{2+\sqrt{4-(\alpha\Delta t)^2(1-4\theta)}}} \right[$$

$$\cup \left] \frac{2c\Delta t\sqrt{1-4\theta}}{\sqrt{2-\sqrt{4-(\alpha\Delta t)^2(1-4\theta)}}}, +\infty \right[.$$

IV. SIMULATION AND ANALYSIS

Numerical methods (9) are applied to the well-posed problem (4)–(5). The boundary conditions are obtained from the interpolation of data supplied by a case study described next. The initial functions are calculated using the two-port transfer functions models developed in [1] from this data. Also, the numerical solutions are assessed using this case study, that is a mix of simulated and operational data supplied by REN-Gasodutos, the portuguese gas transmission and distribution company. The chosen numerical algorithms are applied to a single pipeline.

The pipeline is cylindrical with a diameter of d = 793 mm, a length of L = 35.58 Km, and a roughness factor of $\lambda = 0.005$ mm. The input, output and a middle point of the pipeline have the respective heights of 22.5 m, 43.2 m and 30.8 m. The simulation reproduces one normal working gas day (March, 2nd, 2009), in the closed interval [0h, 24h], with no leakages, and at the constant temperature of $18.5^{\circ}C$. The data was collected with a sampling rate of 2 minutes. Fig. 1 shows the source and offtake mass-flow for the referred period of time.



Fig. 1. Input and output mass-flow [Kg/s]: boundary conditions.

Fig. 2 shows $f_1(x)$ and the validation of mass-flow.

The procedure is validated by considering just one point in time and then verifying if the data generated by the just described procedure coincides with the outlet measured data.

As far as the simulations are done within the convergence region, we obtained similar results for any value of θ . In



(a) $f_1(x)$: mass-flow along the (b) Mass-flow. pipeline at t = 0.





(a) $\theta = 0.15$: mass-flow and the respective iteration error.

Fig. 3. Mass-flow along the pipeline: Implicit method.

particular, we made simulations for $\theta = 0, 0 < \theta < 1/4$, and $1/4 \le \theta \le 1$. Fig. 3 represents mass-flow for $0 < \theta < 1/4$. For the sake of comparison, the simulations were done with the same Δt and Δx .

V. CONCLUSIONS AND FUTURE WORK

We have investigated the numerical solution of IBVP (4)-(5). The initial value functions were calculated using a two-port network method, and the boundary from some operational data supplied by an industry case study. The resulting IBVP is numerically solved through a class of implicit schemata. The convergence of this class of methods is studied. The methods were implemented in Matlab to assess the theoretical stability conditions. For every method, defined by every θ , whenever the computations are done in the convergence region, the obtained results are very alike. Therefore, for a certain region, we can find the θ that best suits a required grid. The simulations have been done for mass-flow as well as pressure. We observed that when the transients are high, a finer space grid may be desirable. Therefore, in the future we would like to investigate the same problem considering irregular and adaptive grids. The results have been validated using the industry case study. We also want to study the nonlinear version of the same problem, as well as to consider the pipe elevation and the

temperature. Furthermore, we will study all these issues for a simple network. Our larger horizon of work also comprises a comparative study of other numerical methods for the same problem, that is, the simulation of models that represent the gas dynamics in the pipes. Having an efficient simulator is very useful to acquire a deeper knowledge of the system but also to test and develop possible future control strategies.

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