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A General Boundary Solution Method for 1D Gas Dynamic Models

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Abstract

This paper outlines a generalised boundary solution method for solving flow at boundaries of 1D duct models. It is adaptable to duct-duct connections and duct-volume connections with subsonic, choked and supersonic flows. It is fully non-homentropic (accounting for friction, and temperature and property variations). The generalised approach aids in reducing code complexity for the approximately 30 distinct flow types that can exist at the boundaries of 1D ducts.

Assumptions are described and numerical methods outlined. The solution requires solution of a number of non-linear simultaneous equations which is accomplished with the Newton-Raphson method. Sample results for a converging flow compared to experimental date are given.

Introduction

One dimensional gas dynamics modeling is an important tool in modern reciprocating internal combustion engine design. Despite a long history and the feeling by some that it is time to *close the book* on this field (see forward to [14]) high quality work continues to be reported in the literature eg [6, 12, 13]. Moreover, there remains an incredible variety of methods and codes in use in engine research laboratories around the world that reflect the particular historical needs and emphases of each research group, and the pedigree of its gas dynamics code, whether it be a Method of Characteristics (MOC) based formulation [1], other wave action method [4], or a finite difference based formulation [14]. Much of the current work reported in literature relates to improving boundary or junction models. Accuracy in modelling boundaries is critical in engine modelling, since there are numerous duct boundaries that trace the path from air inlet through the combustion cylinder to exhaust outlet. Also, new opportunities in detailed CFD present new challenges in interfacing. Boundary formulations are typically based on wave action concepts (even finite difference codes). Thus, work reported in this area has relevance for all 1D gas dynamics codes.

This paper and its companion [9] report the salient features of *another* 1D gas dynamics code which is based the method developed at Queens University, Belfast in the 1990's eg. [2, 3, 11]. It is an attempt to simplify gas dynamic calculations and maintain or improve accuracy. In the model, each computational cell is treated as an idealised constant-area, constant-property, frictionless duct, so that simple algebraic expression are sufficient to describe the passage of finite amplitude waves [9]. Area change, gas property change and friction are accounted for at the interfaces between cells. Connection at duct ends is treated in exactly the same way. Thus the model uses a uniform theoretical treatment of boundaries throughout.

The boundary solution algorithm summarised here was developed with careful consideration to the accuracy, numerical efficiency, and stability of the solution for a wide range of possible flow cases.

Pressure Wave Theory and Nomenclature

A pressure wave passing a gas particle induces a change in velocity in the particle which is given by Earnshaw [7] as

$$u - u_0 = \frac{2a_0}{(\gamma-1)}\left[\left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{2\gamma}} - 1\right] \tag{1}$$

Where u and u_0 are the final and initial velocities respectively, P and P_0 are the final and initial pressures, γ is the ratio of specific heats and a_0 is the speed of sound at the original pressure P_0. Equation (1) assumes a calorically perfect gas, and isentropic compression or expansion process, so the final speed of sound is found as:

$$a = a_0\left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{2\gamma}} \tag{2}$$

In equation (1) the positive direction of velocity is in the same direction as the motion of the pressure wave.

Earnshaw's equation can be extended to the general case of 1D duct flow where a both a rightward and leftward pressure wave superimpose. The pressure and velocity of the gas in the duct as a function of both waves is:

$$u = \frac{2a_0}{(\gamma-1)}\left(X_R - X_L\right) \tag{3}$$

$$X = X_R + X_L - 1 \tag{4}$$

Velocity u is positive in the rightward direction. The variable X is shorthand for

$$X = \left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{2\gamma}} \tag{5}$$

And the subscripts R and L signify the rightward and leftward travelling pressure waves respectively. Where X appears without a subscript, this signifies the superposition pressure – ie the static pressure. Note the reference pressure P_0 can be set to an arbitrary value, though it should be a similar pressure to that being modelled. It is conventional to set it to atmospheric pressure.

Figure 1 shows the mesh nodes of a 1D duct plotted in space and time. Right and left travelling waves propagate along the duct and intercept the nodes at cell boundaries. The values of the right and left travelling wave can be calculated if the pressure and velocity are known by re-arranging equations (3) and (4) as:

$$X_R = \left[X + u\frac{(\gamma-1)}{2a_0} + 1\right]/2 \tag{6}$$

$$X_L = \left[X - u\frac{(\gamma - 1)}{2a_0} + 1 \right] / 2 \qquad (7)$$

It is convenient to name the waves according to whether they are travelling toward the node (*incident*) or away (*reflected*). This is because the flow at a node is established only by the values of the *incident* waves (if the flow is sub-sonic).

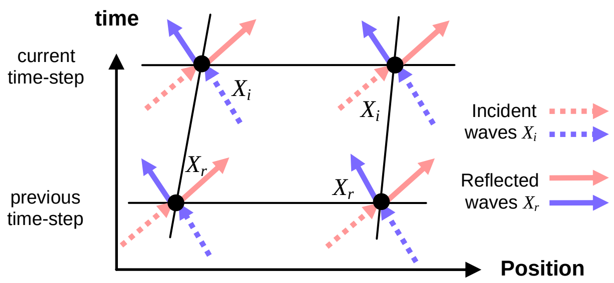

Figure 1 Duct cell boundary nodes in space and time

In general, to allow for varying gas composition and temperature within a duct, the gas properties on either side of a node will be different (in space *and* time). This is illustrated in Figure 2.

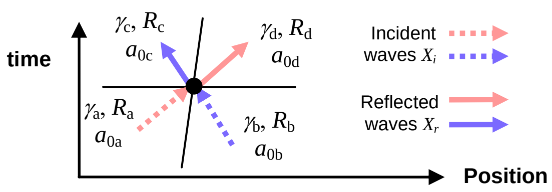

Figure 2 Variation of gas properties around a node in space and time.

The flow area may change from one cell to the next. This will occur between the end cells of two connected ducts of different cross section, and it will also occur between cells of a tapered duct (since the cell space is assumed to be constant area). More complex area changes are also discussed in the following section.

Flow Types

Considering all possible kinds of flow between duct sections and/or large volumes, there are about 31 distinct possibilities as shown pictorially in Figure 3. Constant area duct flow is a special case of type ~1 where the change in area is zero. Friction or reducing area may cause a choke point such as in type ~2. A sub-sonic diverging flow will typically experience increased pressure loss due to flow separation. (~3) If a diverging flow is sonic or super-sonic on the upstream side it will expand further unless it is decelerated and compressed by a standing shock. (~4-6). A super-sonic flow may pass entirely through a duct section (~7) unless it becomes choked, or a shock travelling upstream against the flow passes through the section. In both cases a travelling shock on the upstream side first slows the flow to a sub-sonic speed before it passes through section (~8-9). If the flow passes a restricted area between two ducts, the flow is in two stages. (~10-19). If a duct is connected to a volume which is supplying the flow, the kinetic energy and pressure of the gas in the volume is fixed. The inlet flow is assumed to be sub sonic, though the flow may choke. (~20-24) If the duct is supplying a flow to a volume, then the pressure on the downstream side is fixed to the volume pressure (~25, ~28) unless the flow has choked, in which case the sonic condition fixes the downstream pressure, and the flow will expand somewhat as it enters the volume (~26, ~27, ~29). If two volumes are connected directly by a short orifice, the flow may be sub-sonic or it may choke (~30-31).

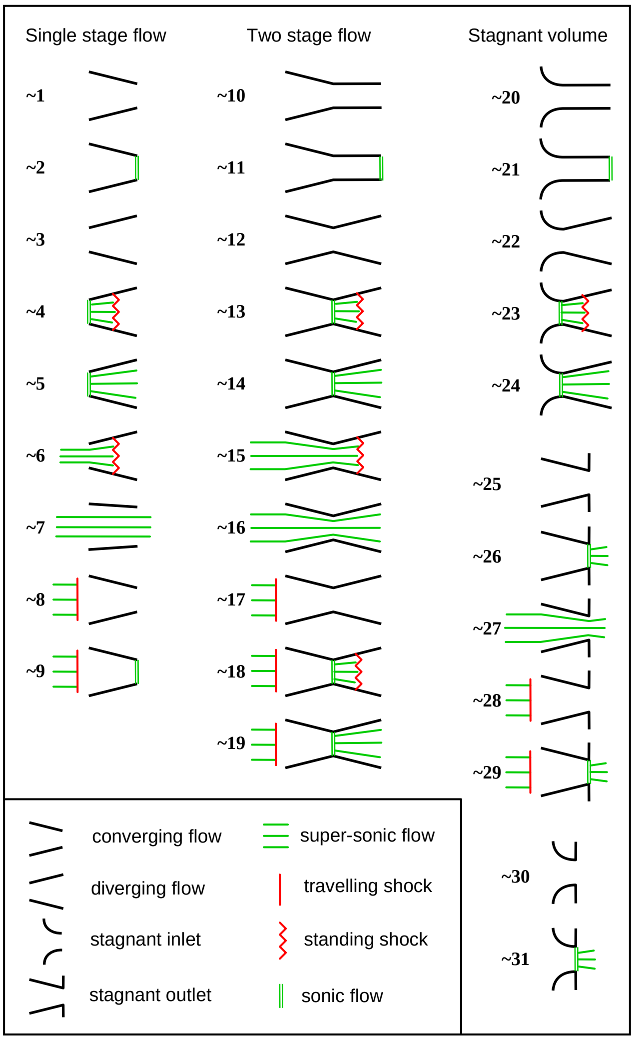

Figure 3 Catalogue of all flow types considered.
Flow is from left to right.

A correct solution for any one of the cases above is not especially difficult - the difficulty lies in managing the complexity in providing for so many possibilities. Increasing complexity runs the risk of inadvertent programming error or code maintenance problems. It is beneficial to arrange the different flow types according to families and use as much common code as possible.

Assumptions

Steady Flow

The flow at a node (be it a cell or duct boundary) conceptually passes through an infinitesimal control volume. This allows it to be solved as a steady state problem since there can be no accumulation of mass or energy within the (small) control volume. The flow is quasi-steady. It is unclear if there is any alternative to this approach. Chalet et al. [5] claim to avoid the assumption of steady flow, but are referring instead to the application of a tuning ‘governor coefficient’ which is a function of flow Mach number and not based on steady flow-bench data. The quasi steady assumption remains in place.

1D Flow

The flow is assumed to have uniform properties across any given cross section. The flow area may change, thus it is not truly 1D but quasi 1D. Clearly boundary layers, free jets and recirculation zones violate the 1D assumption, but experimental validation work such as [3, 13] show remarkably faithful simulation results notwithstanding. The influence of detached flow can be modelled by adding extra *friction* at these locations or by including an *area coefficient*. These methods are imperfect since they tend not to reproduce the experimental data at all operating conditions. [8] reports a model for separated flow which attempts to account for the recent flow history and its effect on flow separation.

Flow into a Volume

The pressure of a separated jet entering a large volume is assumed to be identical to the volume pressure. The exception is if the jet is sonic or supersonic at the exit, in which case upstream conditions determine the exit conditions.

Calorically Perfect Flow

Each quasi steady flow is assumed to have constant specific heats. Thus the gas is modelled as *locally* perfect, though specific heats are allowed to vary in both space and time. The calorically perfect flow assumption is not a serious impediment for engine modeling (since there are relatively low pressure ratios across flow restrictions), but may be problematic for high speed or high temperature (rapidly reacting) flows such as gas guns.

Solution Method

Figure 4 shows a typical single stage flow boundary (type ~1). The gas properties (γ, a_0) in the cell spaces are in general different to the gas properties of the boundary flow. Conceptually, contact surfaces exist immediately adjacent to the flow boundary. The pressure and velocity on either side of the flow boundary are usually different. Unless the flow is isentropic, the downstream reference pressure speed of sound a_0 also increases slightly.

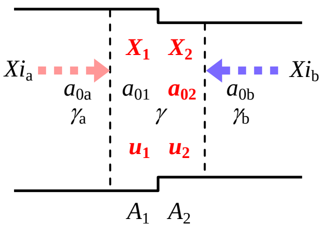

Figure 4 A typical flow boundary showing all flow properties. Unknown values in bold. Flow is from left to right.

Change of Reference Frame.

A flow boundary (node) is free to move relative to the duct's reference frame. If the node is moving, the value of the each wave must be modified to match the velocity of the nodal reference frame:

$$X_{\text{wave\_mod}} = X_{wave} - V_{node}\frac{(\gamma_{cell}-1)}{4a_{0cell}} \qquad (8)$$

Where X_{wave_mod} is the modified wave value and V_{node} is the velocity of the node relative to the wave's original reference frame with positive being in the same direction as the wave's direction of propagation. γ_{cell} and $a_{0\text{cell}}$ are the cell space gas properties in which the wave is travelling. Thus a wave's effective magnitude is increased by a node moving to meet it, and decreased if the node is moving with it.

Determining Flow Direction

It is useful to know the direction of the flow before performing detailed calculations, and this can be checked by calculating the stagnation pressure of the flow on both sides of the boundary. The inlet side will be the side with the highest stagnation pressure.

$$\frac{P_{stagnant}}{P_0} = (2X_i - 1)^{\frac{2\gamma_{cell}}{(\gamma_{cell}-1)}} \qquad (9)$$

Solving the Flow

The solution of the flow shown in Figure 4 is shown to illustrate the general procedure. This flow has five unknowns, namely upstream and downstream X and u, and downstream a_0. The flow must satisfy the conditions of conservation of energy – equation (10) and conservation of mass – equation (11). Equations (6) and (7) relate the incident pressure waves to X and u. After including the effect of the discontinuity in gas properties at the contact surface, they become equation (12 a,b). Finally, if a model for friction work is available, the change in a_0 from upstream to downstream can be written as equation (13)

Energy equation 1=>2

$$\frac{a_{01}{}^2 X_1{}^2}{(\gamma-1)} - \frac{a_{02}{}^2 X_2{}^2}{(\gamma-1)} + \frac{u_1{}^2}{2} - \frac{u_2{}^2}{2} = 0 \qquad (10)$$

Continuity Equation 1=>2

$$\frac{A_1 u_1 X_1^{\frac{2}{(\gamma-1)}}}{a_{01}{}^2} - \frac{A_2 u_2 X_2^{\frac{2}{(\gamma-1)}}}{a_{02}{}^2} = 0 \qquad (11)$$

Wave Equation a, b

$$X_{1,2}^{\frac{\gamma_{\text{a,b}}(\gamma-1)}{\gamma(\gamma_{\text{a,b}}-1)}} \pm u_{1,2}\frac{(\gamma_{\text{a,b}}-1)}{2a_{0\text{a,b}}} - 2Xi_{\text{a,b}} + 1 = 0 \qquad (12\text{ a,b})$$

a_0 Equation 1=>2

$$a_{01}{}^2 - a_{02}{}^2 + \frac{w_f}{X^2} = 0 \qquad (13)$$

These form a system of five non-linear algebraic equations in five unknowns which can be solved simultaneously using the Newton-Raphson method for simultaneous equations.

If the flow on the downstream side exceeds the local sonic velocity, the downstream wave equation (12b) must be replaced with the sonic equation:

$$a_{02} X_2 - u_2 = 0 \qquad (14)$$

Initial Guess

The Newton-Raphson method is generally robust, and fast-converging, but the process is greatly assisted if the initial guess supplied is near the solution. Moreover, problems occur if the flow solution lies outside of the parameters of the chosen flow equations (such as a supersonic flow developing at the throat of a sub-sonic problem). It is thus of great importance to do careful analysis of the flow before passing it to the final solver. There is a mass of detail in this process covering initial guesses for simple straight ducts, to highly restricted two stage flows with possible choking, to inflows from stagnant volumes and so on.

Shocks

The effect of a standing shock within a diverging section is automatically satisfied by the energy, continuity and downstream wave equation, but the possibility of a fully supersonic outlet must be checked, in which case the downstream wave equation must be replaced by the a_0 Equation (13).

On the other hand, if the upstream flow is supersonic, checks must be made to see if the flow will choke, or have a shock migrate upstream from the exit. If the upstream flow becomes shocked, a simple correction can be made to the upstream incident wave Xi_a on each iteration of the main Newton-Raphson solution. This works quite effectively, since the value of the incident wave changes only slightly when it traverses such a shock.

Sample Results

Results of experiments by Kirkparick [10] are used to test the model for flows with area change. The results shown in Figure 5 are for converging flow since flow separation effects are small. A single shot apparatus on the left side of a pipe system injects a pressure pulse into an 80mm pipe. The pulse propagates along the pipe toward the right and traverses an area change to a 25 mm pipe. The pressure is recorded at a location downstream of the area change. For better accuracy, the measured pressure on the upstream side was used to drive the simulation.

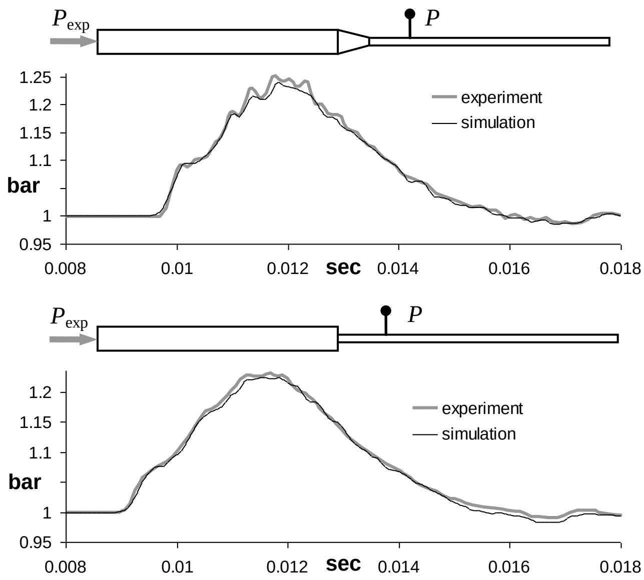

Figure 5 Single shot experimental pressure compared to simulation

Discussion and Conclusion

An overview of a boundary calculation method has been given, which rigorously considers flow losses (friction etc) and non-uniform gas properties. This method is applied both to duct ends and also to cell boundaries within ducts. Typically four or five equations are solved simultaneously for a single stage flow while two more equations are added for two stage flow. If the flow can be assumed isentropic (frictionless) then equation (13) can be eliminated. Further, uniform gas properties could remove another two equations. However, these special cases are not representative of most real flows, so it is considered better to solve the full set for general applicability.

The results of simulation compared to experiment are good for the cases tested here. Unfortunately the original experimental data is no longer available, so it was manually extracted from a photocopy of the original publication. Some error may be due to this process, since the resolution of the simulation results is higher than most of the printed experimental data.

This generalised approach to boundary flows aids in reducing simulation code complexity, while maintaining full rigour for ideal gas 1D flow models.

Nomenclature

A	area
a, a_0	speed of sound, isentropic reference pressure a
P, P_0	pressure, reference pressure
u	fluid velocity
w_f	friction work
γ	ratio of specific heats
$X = \left(\dfrac{P}{P_0}\right)^{\frac{\gamma-1}{2\gamma}}$	pressure amplitude ratio

References

[1] Benson, R.S., *The Thermodynamics and Gas Dynamics of Internal Combustion Engines Volume 1*, ed. J.H. Horlock and D.E. Winterbone. Vol. 1. 1982: Oxford University Press, Walton Street, Oxford.

[2] Blair, G.P., S.J. Kirkpatrick, and R. Fleck. *Experimental Validation of a 1d Modelling Code for a Pipe Containing Gas of Varying Properties*. 1995: SAE. Paper 950275

[3] Blair, G.P., et al. *Experimental Validation of 1-D Modelling Codes for a Pipe System Containing Area Discontinuities*. 1995: SAE. Paper 950276

[4] Blair, G.P., *Design and simulation of Four-Stroke Engines*. 1999: Society of Automotive Engineers, Warrendale PA U.S.A.

[5] Chalet, D., et al., *Inflow boundary condition for one-dimensional gas dynamics simulation code of internal combustion engine manifolds.* Proc. IMechE Part D: J. Automobile Engineering, 2009. **Vol. 223**

[6] Depcik, C., B. van Leer, and D. Assanis, *The Numerical Simulation of Variable-Property Reacting-Gas Dynamics: New Insights and Validation.* Numerical Heat Transfer, Part A: Applications, 2004. **47**(1): p. 27 - 56.

[7] Earnshaw, S., *On the Mathematical Theory of Sound.* Philosophical Transactions of the Royal Society of London, 1860. **150**: p. 133-148.

[8] Gibbes, G. and G. Hong. *A Model for Pressure Recovery of Flows in Expanding Ducts for 1D Gas Dynamic Simulations*. in *Asia Pacific Automotive Conference*. 2009. Hanoi, Vietnam: SAE.

[9] Gibbes, G. and G. Hong. *Improving the accuracy of a 1D Gas Dynamics Model*. in *17th Australasian Fluid Mechanics Conference*. 2010. Auckland, New Zealand.

[10] Kirkpatrick, S.J. *An Evaluation of One-Dimensional Simulation Techniques for Predicting Unsteady Gas Flow in Engine Ducting*. For degree of Doctor of Philosophy in *Department of Mechanical and Manufacturing Engineering*. 1994: The Queens University of Belfast.

[11] Kirkpatrick, S.J., et al. *Experimental Evaluation of 1-D Computer Codes for the Simulation of Unsteady Gas Flow Through Engines - a First Phase*. 1994: SAE. Paper 941685

[12] Pearson, R., et al. *Exhaust system gas dynamics in internal Combustion Engines*. in *ASME Internal Combustion Engine Division 2006 Spring Technical Conference*. 2006. Aachen, Germany. ICES2006-1444

[13] Thornhill, D., et al., *Particle image velocimetry investigation of a finite amplitude pressure wave.* Experiments in Fluids, 2006. **40**: p. 400-404.

[14] Winterbone, D.E. and R.J. Pearson, *Theory of Engine Manifold Design: Wave Action Methods for IC Engineers.* 1999: Professional Engineering Publishing Ltd, Suffolk, UK.